Green's Function Methods

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Part I
Fermi Liquid Theory

1 Weakly interacting fermions

(Taken from Giamarchi's notes "Interactions in Quantum Fluids" arXiv:1007.1030v1)

Consider independent electrons described by the Hamiltonian

$$H_{\rm kin} = \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{1.1}$$

where the sum over $\mathbf{k}$ runs in general over the first Brillouin zone. One usually incorporates the chemical potential in the energy $\xi(\mathbf{k}) = \varepsilon(\mathbf{k}) - E_{\rm F}$ to make sure that $\xi(\mathbf{k}) = 0$ at the Fermi level. The ground state of such system is the unpolarized Fermi sea

$$|{\rm F}\rangle = \prod_{\mathbf{k},\xi(\mathbf{k})\leq 0} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}\downarrow} |\varnothing\rangle \tag{1.2}$$

At finite temperature states are occupied with a probability given by the Fermi factor

$$n(\mathbf{k}) = \left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle = f_{\rm F}(\xi(\mathbf{k})) = \frac{1}{e^{\beta\xi(\mathbf{k})}+1} \tag{1.3}$$

A very important point, true for most solids, is that the order of magnitude of the Fermi energy is $E_{\rm F} \sim$ 1eV $\sim 12,000$ K. This means that the temperature, or most of the energies that are relevant for a solid (for example 30GHz $\sim 1K$) are extremely small compared to the Fermi energy. As a result the broadening of the Fermi distribution is extremely small. The important states are thus the ones in a tiny **shell** close to the Fermi level, as shown in (see Fig. 1.1 in reference). The other excitations are completely blocked by the Pauli principle. This hierarchy of energies is of course what confers to fermions in solids their unique properties and make them so different from a classical system. As a consequences some of the response of such a fermion gas are rather unique. The specific heat is linear with temperature (contrarily to the case of a classical gas for which it would be a constant)

$$C_V(T) = \frac{\pi^2}{3} k_{\rm B}^2 \mathcal{N}(E_{\rm F})\, T \tag{1.4}$$

where $\mathcal{N}(E_{\rm F})$ is the density of states per unit volume at the Fermi level. The compressibility of the fermion gas goes to a constant in the limit $T \to 0$, and the same goes for the spin susceptibility, namely the magnetization M of the electron gas in response to an applied magnetic field H.

$$\chi = \left(\frac{dM}{dH}\right)_T \tag{1.5}$$

Note that a system made of independent spins would have had a divergent spin susceptibility when $T \to 0$ instead of a constant one. The slope of the specific heat, the compressibility and the spin susceptibility of the free fermion gas are all controlled, by the same quantity namely the density of states at the Fermi level.

One could thus wonder what would be the effects of interactions on such a behavior. Because of the interactions, the energy of a particle can now fluctuate since the particle can give of take energy from the others. Thus one could naively imagine that the interactions produce an effect on the distribution function similar to the one of a thermal bath, with an effective "**temperature**" of the order of the **strength of the interaction**. In order to determine the consequences of such a broadening, one needs to estimate the strength of the interactions. In a solid the interaction is mostly the Coulomb interaction. However, in a metal this interaction is screened beyond a length λ that one can easily compute in the Thomas-Fermi approximation

$$\lambda^{-2} = \frac{e^2 \mathcal{N}(E_F)}{\epsilon_0} \tag{1.6}$$

where e is the charge of the particles and ϵ_0 the dielectric constant of the vacuum.

For 3d free fermions $\epsilon = \hbar^2 k^2/2m$, the density of states per unit volume is

$$\frac{2}{V}\frac{d^3k}{(2\pi/L)^3} = \frac{1}{\pi^2} k^2 dk = \mathcal{N}(\epsilon) d\epsilon \tag{1.7}$$

$$\mathcal{N}(\epsilon) = \frac{mk(\epsilon)}{\pi^2\hbar^2} = \frac{m}{\hbar^2\pi^2}\sqrt{\frac{2m\epsilon}{\hbar^2}} \tag{1.8}$$

At fermi level we have

$$\mathcal{N}(\epsilon_F) = \frac{mk_F}{\pi^2\hbar^2} \tag{1.9}$$

The number density of particles n is

$$n = \frac{2}{V}\frac{\frac{4\pi}{3}k_F^3}{(2\pi/L)^3} = \frac{k_F^3}{3\pi^2} \tag{1.10}$$

evidently, this also tells us that the Fermi wavelength is of the same order of magnitude as the lattice spacing a

$$a \sim (\frac{N}{V})^{-1/3} \sim 3k_F^{-1} \tag{1.11}$$

we can write

$$\mathcal{N}(\epsilon_F) = \frac{2}{3}\frac{n}{E_F} \tag{1.12}$$

To estimate λ we can use the fine structure constant

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} = \frac{1}{137} \tag{1.13}$$

to obtain

$$\lambda^{-2} = 4\pi\alpha\hbar c\mathcal{N}\left(E_{\mathrm{F}}\right) = 4\pi\alpha\hbar c\frac{3n}{2E_{\mathrm{F}}} \tag{1.14}$$

and $E_F = \hbar v_F k_F$ and $6\pi^2 n = k_F^3$ one gets

$$\lambda^{-2} = \frac{1}{\pi}\alpha\frac{c}{v_F}k_F^2 \tag{1.15}$$

Since $v_F/c \sim 10^{-2}$ in most systems (0.5×10^{-2} for copper), one finds that $k_{\mathrm{F}}\lambda \sim 1$. The screening length is of the order of the **inverse Fermi length**, i.e. essentially the **lattice spacing** in normal metals. This is a striking result: not only the Coulomb interaction is screened, but the screening is so efficient that the interaction is practically local. We will use extensively this fact in the definition of models below. Let us now estimate the order of magnitude of this screened interaction. The interaction between two particles can be written as

$$H_{\mathrm{int}} = \int d\mathbf{r}d\mathbf{r}'V\left(\mathbf{r}-\mathbf{r}'\right)\rho(\mathbf{r})\rho\left(\mathbf{r}'\right) \tag{1.16}$$

Since the interaction is screened it is convenient to replace it by a local interaction. Given our previous result let us simply replace the screening length by a the fermion-fermion distance. The effective potential seen at point $\mathbf{r}$ by one particle is

$$\int d\mathbf{r}'V\left(\mathbf{r}-\mathbf{r}'\right)\rho\left(\mathbf{r}'\right) \tag{1.17}$$

Due to screening we should only integrate within a radius a around the point $\mathbf{r}$. Assuming that the density is roughly constant one obtains

$$\int_{|\vec{r}-\vec{r}'|<a} d\mathbf{r}\frac{e^2}{4\pi\epsilon_0\left|\mathbf{r}-\mathbf{r}'\right|}\rho_0 \sim \frac{e^2\rho_0 S_d a^{d-1}}{4(d-1)\pi\epsilon_0} \tag{1.18}$$

where S_d is the surface of the sphere in d dimensions. Using $\rho_0 \sim 1/a^d$ and one gets

$$\frac{S_d}{(d-1)}\hbar\alpha c a^{-1} \tag{1.19}$$

This potential acting on a particle has to be compared with the kinetic energy of this particle at the Fermi level which is $E_{\mathrm{F}} = \hbar v_{\mathrm{F}} k_{\mathrm{F}}$. Since $k_{\mathrm{F}} \sim a^{-1}$ one has again to compare α and v_F/c. The two are about the same order of magnitude. The Coulomb energy, even if screened (i.e. even in a very good metal), is thus of the same order of magnitude than the kinetic energy. If such an interaction was acting as a temperature in smearing the Fermi function this would lead to an enormous smearing.

This would be in complete contradiction with data on most of solids. The specific heat in real materials is found to be linear, albeit with a slope different from the naive free electron picture at temperatures much smaller than the scale of the interactions. Similarly spin susceptibility and compressibility are still found, e.g. in 3-He to be essentially constant at low temperature, again implying that the Fermi distribution must remain quite sharp.

In addition, a remarkable experimental technique to look at the single particle excitations, and momenta distributions is provided by the photoemission technique (Damascelli, Hussain and Shen, 2003). Pending some hypothesis this technique is a direct measure of the spectral function $A(\mathbf{k},\omega)$ which is the probability of finding an excitation with the energy ω and a momentum $\mathbf{k}$. For free particles $A(\mathbf{k},\omega) = \delta(\omega - \xi(\mathbf{k}))$. Naively one would expect that, because an energy of the order of the interaction can be exchanged, these perfect peaks are broadened over an energy of the order of the interaction. This is not the case. Very sharp peaks exist, and become sharper and sharper as one gets closer to the Fermi energy. The momentum distribution seems to be **broadened uniquely by the temperature** when one is at the Fermi surface.

One is thus faced with a remarkable puzzle: the "free electron" picture seems, at least qualitatively, to work much better than it should, based on estimates of the interaction strength. This must hide a profound effect, and is thus a great theoretical challenge.

2 Landau Fermi Liquid Theory

The main idea behind Fermi liquids (Nozieres, 1961) is to look at the excitations that would exist above the ground state of the system. In the absence of interactions the ground state is the Fermi sea. Turning on the interaction will change the ground state into a very complicated object, that we will be unable to describe. What we need are the excitations that correspond to the addition or removal (creation of a hole) of a fermion in the ground state. In the absence of interactions one just add an electron in an empty $\mathbf{k}$ state and such an excitation does not care about the presence of all the other electrons in the ground state (otherwise than via the Pauli principle which prevents from creating it in an already occupied state). In the presence of interactions this will not be the case and the added particle interacts with the existing particles in the ground state. For example for repulsive interactions one can expect that this excitation repels other electrons in its vicinity. On the other hand if one is at low temperature (compared to the Fermi energy) there are very few of such excitations and one can thus neglect the interactions between them. This picture strongly suggests that **the main interaction is between the excitation and the ground state**. This defines a new composite object (fermion or hole surrounded by its own polarization cloud). This complex object essentially behaves as a particle, with the same quantum numbers (charge, spin) than the original fermion, albeit with **renormalized parameters**, for example its mass. This image thus strongly suggests that even in the presence of interactions good excitations looking like free particles, still exists. These particle resemble free fermions but with a renormalized energy $E(\mathbf{k})$ and thus a renormalized mass. Since the interaction has been incorporated in the definition of such objects, it will not act as a source of broadening for their momentum distribution and the momentum distribution for the quasiparticles will remain very sharp, with only the small temperature broadening.

Of course the above is just a qualitative idea. Let me now give a more formal treatment. For that we can consider the retarded single correlation function

$$G\left(\mathbf{k}, t_2 - t_1\right) = -i\theta\left(t_2 - t_1\right)\left\langle \left[c_{\mathbf{k},t_2}, c^{\dagger}_{\mathbf{k},t_1}\right]_+ \right\rangle \tag{2.1}$$

This correlation represents the creation of a particle in a well defined momentum state $\mathbf{k}$ at time t_1, let it propagate and then tries to destroy it in a well defined momentum state $\mathbf{k}$ at time t_2. The imaginary part of the Fourier transform of this correlation function is just the spectral function

$$A(\mathbf{k},\omega) = \frac{-1}{\pi}\Im G(\mathbf{k},\omega) \tag{2.2}$$

The spectral function measures the probability to find a single particle excitation with an energy ω and a momentum $\mathbf{k}$. It does obey the sum rule of probabilities $\int d\omega A(\mathbf{k},\omega) = 1$. The general form of the retarded correlation is

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \xi(\mathbf{k}) - \Sigma(\mathbf{k},\omega) + i\delta} \tag{2.3}$$

where $\Sigma(\mathbf{k},\omega)$, called the **self energy**, is a certain function of momenta and frequency. The relation also defines the function Σ. For noninteracting systems $\Sigma = 0$, and perturbative methods (Feynman diagrams) exist to

compute Σ in powers of the interaction. However we will not attempt here to compute the self energy Σ but simply to examine how it controls the spectral function. The spectral function is

$$A(\mathbf{k},\omega)=\frac{1}{\pi}\frac{-\Im\Sigma(\mathbf{k},\omega)}{(\omega-\xi(\mathbf{k})-\Re\Sigma(\mathbf{k},\omega))^2+(\Im\Sigma(\mathbf{k},\omega))^2} \tag{2.4}$$

We see that $\Im\Sigma$ and $\Re\Sigma$ play very different roles in the spectral function. Note that quite generally we need $\Im\Sigma(\mathbf{k},\omega)<0$ to get a positive spectral function. In the absence of interactions $\Sigma=0$ and one recovers

$$A(\mathbf{k},\omega)=\delta(\omega-\xi(\mathbf{k})) \tag{2.5}$$

Broadly speaking, for a given $\mathbf{k}$, $\Re\Sigma$ shifts the peak while $\Im\Sigma$ broadens the peak. However, this is only true when $\Im\Sigma$ is ω-independent. Assuming that $\Sigma(\omega)$ is now fast-varying enough to change the shape of the Lorentzian, we can make some characteristic statesments about the curve $A(\omega)$. As a Lorentzian function, it has a width of order $\Im\Sigma$ and a height or order $1/\Im\Sigma$, with peak located at ω_0 given by the solution of

$$\omega_0-\xi(\mathbf{k})-\Re\Sigma(\mathbf{k},\omega_0)=0 \tag{2.6}$$

The solution will be called $\omega_0\equiv E(\mathbf{k})$, serving as the new **dispersion relation**. Note that this is the definition of the dispersion for a quasiparticle, although strictly speaking this is not the exact peak of $A(\mathbf{k},\omega)$. If $\Re\Sigma$ is ω-independent, then the above equation simplifies to $E(\mathbf{k})=\xi(\mathbf{k})+\Re\Sigma(\mathbf{k})$.

For simplicity, if we assume Σ to be ω-independent, then

$$G(\mathbf{k},\omega)=\frac{1}{\omega-\xi(\mathbf{k})-\Sigma(\mathbf{k})+i\delta} \tag{2.7}$$

We already have

$$G(\mathbf{k},t)=-i\theta(t)e^{-i\xi(\mathbf{k})t}\to G(\mathbf{k},\omega)=\frac{1}{\omega-\xi(\mathbf{k})+i\delta} \tag{2.8}$$

now simply replace $\xi(\mathbf{k})$ by $\xi(\mathbf{k})+\Sigma(\mathbf{k})$ and we have

$$G(\mathbf{k},t)=-i\theta(t)e^{-i(\xi(\mathbf{k})+\Sigma(\mathbf{k}))t}\to G(\mathbf{k},\omega)=\frac{1}{\omega-\xi(\mathbf{k})-\Sigma(\mathbf{k})+i\delta} \tag{2.9}$$

$$\begin{aligned}G(\mathbf{k},t)&=-i\theta(t)e^{-i(\xi(\mathbf{k})+\Re\Sigma(\mathbf{k}))t}e^{-(-\Im\Sigma(\mathbf{k}))t}\\&\equiv-i\theta(t)e^{-iE(\mathbf{k})t}e^{-t/\tau(\mathbf{k})}\end{aligned} \tag{2.10}$$

where $1/\tau(\mathbf{k})\equiv-\Im\Sigma(\mathbf{k})$ is the life-time of the particle. In this language, we write

$$G(\mathbf{k},\omega)=\frac{1}{\omega-E(\mathbf{k})+i/\tau(\mathbf{k})} \tag{2.11}$$

$$A(\mathbf{k},\omega)=\frac{1}{\pi}\frac{1/\tau(\mathbf{k})}{(\omega-E(\mathbf{k}))^2+(1/\tau(\mathbf{k}))^2} \tag{2.12}$$

which is an exact Lorentzian.

2.1 Effective mass and quasiparticle weight

Consider the equation for the dispersion relation $E(\mathbf{k})$

$$E(\mathbf{k})-\xi(\mathbf{k})-\Re\Sigma(\mathbf{k},E(\mathbf{k}))=0 \tag{2.13}$$

For Fermi gas we can keep the lowest order Taylor expansion $\xi(\mathbf{k})=\frac{k_\mathrm{F}}{m}(k-k_F)$. For the shifted dispersion relation, if we assume it to be isotropic, then we may put it into a similar form $E(\mathbf{k})=\frac{k_\mathrm{F}}{m^*}(k-k_\mathrm{F})$ with a new effective mass m^* which is different from m. k_F stay the same due to Luttinger's theorem: **The volume enclosed by a material's Fermi surface is directly proportional to the particle density**. Since the density of particles is the same before and after we turn on the interaction, the volume in k-space is always $\frac{4\pi}{3}k_F^3$, so k_F must stay the same after we turn on the interaction. More strictly speaking, the Fermi surface is defined by $G(\omega=0,p)\to0$ or ∞.

Close to the Fermi level we only need to compute the effective mass m^* to fully determine (at least for a spherical Fermi surface) the effects of the interactions on the energy of single particle excitations. To relate the effective mass to the self energy we take d/dk of the dispersion relation

$$\frac{dE(k)}{dk} = \frac{d\xi(k)}{dk} + \left.\frac{\partial \Re\Sigma(k,\omega)}{\partial k}\right|_{\omega=E(k)} + \left.\frac{\partial \Re\Sigma(k,\omega)}{\partial \omega}\right|_{\omega=E(k)} \frac{dE(k)}{dk} \tag{2.14}$$

which gives the relation between m and m^*

$$\frac{m}{m^*} = \frac{1 + \left.\frac{m}{k_F}\frac{\partial \Re\Sigma(k,\omega)}{\partial k}\right|_{\omega=E(k)}}{1 - \left.\frac{\partial \Re\Sigma(k,\omega)}{\partial \omega}\right|_{\omega=E(k)}} \tag{2.15}$$

This renormalization of the mass by interaction is well consistent with the experimental findings showing that in the specific heat one had something that was resembling the behavior of free electrons but with a different mass m^*.

If we set the imaginary part to zero in the spectral function, we have

$$\begin{aligned} A(\mathbf{k},\omega) &= \delta(\omega - \xi(\mathbf{k}) - \Re\Sigma(\mathbf{k},\omega)) \\ &= Z_k \delta(\omega - E(\mathbf{k})) \end{aligned} \tag{2.16}$$

where we defined the **weight** at the peak

$$Z_k = \frac{1}{1 - \left.\frac{\partial \Re\Sigma(k,\omega)}{\partial \omega}\right|_{\omega=E(k)}} \tag{2.17}$$

using the identity

$$\delta(f(x)) = \sum_i \frac{\delta(x - a_i)}{|f'(a_i)|} \tag{2.18}$$

Because $\Re\Sigma(k,\omega)$ is frequency dependent, the total spectral weight in the peak is not one anymore, but the total **weight** is now $Z_k \leq 1$. It is as if only a faction Z_k of an electron is converted into a new particle with a diepersion relation $E(\mathbf{k})$. The integral of $A(\mathbf{k},\omega)$ in ω does not sum up to 1 anymore, breaking the conservation of probability. This is because we have set $\Im\Sigma \to 0$ but keep $\Re\Sigma$ finite, but this is not a valid procedure. $\Re\Sigma$ and $\Im\Sigma$ are in fact related by Kramers-Kronig relations, since Σ is retarded. However the reduction of the quasiparticle weight that we found is quite real.

To conclude, we see that the real part of the self energy controls the **dispersion relation** and the **total weight** of excitations which in the spectral function produce peaks exactly like free particles. The frequency and momentum dependence of the real part of the self energy lead to the two independent quantities m^* the effective mass of the excitations and Z_k the weight. In the particular case when the momentum dependence of the self energy is small one can see that

$$\frac{m}{m^*} = Z_{k_F} \tag{2.19}$$

2.2 Landau Quasiparticles

From the previous analysis of the spectral function and its connection with the self energy we have a schematic idea of the excitations as summarized in (ref Fig. 1.5). Quite generally we can thus distinguish two parts in the spectral function:

1. Lorentzian with dispersion $\omega = E(\mathbf{k})$ of width $-\Im\Sigma$, height $-1/\Im\Sigma$ and finite lifetime $\tau = -1/\Im\Sigma$.
2. Continuous background without any specific feature for which the probability to find a particle with an energy ω is practically independent of its momentum k.

Depending on the self energy, and thus the interactions, we can still have objects that we could identify with "free" particles, solving our problem of why the free electron picture works qualitatively so well with just a renormalization of the parameters.

This picture still need one more condition: the quasiparticles must be well-distinguished from each other, i.e. $A(\mathbf{k},\omega)$ must be sharp enough such that w can tell different Lorentzian apart. Therefore, one requires

$$E(k) \gg 1/\tau \tag{2.20}$$

As $k \to k_F$, we must have $E(k) \sim k - k_F \to 0$. So this requires $1/\tau$, or $\Im\Sigma$ to vanish faster than $E(k)$ with k. The lifetime τ is determined by all scattering processes which can change the quasiparticle into other momenta, with $1/\tau$ being the total scattering rate. It is not obvious that the scattering rate should vanish at the Fermi surface, not to mention vanish faster than $k - k_F$.

To estimate the lifetime τ, we start from the Fermi gas, and consider all the scattering which can take a particle at momentum k to another momentum. From Fermi golden rule, we have

$$1/\tau \sim \sum_f \Gamma_{if} = \frac{2\pi}{\hbar} \sum_f |\langle f\,|H'|\,i\rangle|^2\, \delta\left(E_f - E_i\right) \tag{2.21}$$

The lowest lying excitations in the Fermi gas are particle-hole excitations. As shown in (ref. Fig. 1.7) a particle coming in the system with an energy ω and a momentum k can excite a particle-hole excitation, taking a particle below the Fermi surface with an energy ω_1 and putting it above the Fermi level with an energy ω_2. The process is possible if the initial state is occupied and the final state is empty.

The specific values of $\langle f\,|H'|\,i\rangle$ do not affect the argument. The probability of transition then comes down to the sum over all possible initial states and final states that respect the constraints (energy conservation and initial state occupied, final state empty). Since the external particle has an energy ω it can give at most ω in the transition. Thus $\omega_2 - \omega_1 \leq \omega$. This implies also directly that the initial state cannot go deeper below the Fermi level than ω otherwise the final state would also be below the Fermi level and the transition would be forbidden. The probability of transition is thus

$$\tau^{-1} \propto P \propto \int_{-\omega}^{0} d\omega_1 \int_{0}^{\omega+\omega_1} d\omega_2 = \frac{1}{2}\omega^2 \tag{2.22}$$

this then vanishes faster than $E(k) \propto \omega$. The Landau quasiparticles become better and better defined as one gets closer to the Fermi level. This is a remarkable result guarantees that close to the Fermi surface, we can view the system as composed of well-defined quasiparticles.

However, the above argument works only when perturbation theory works, but this is questionable since the interaction is strong. One rescue may be Wilson's RG, where we perform the perturbative analysis step by step, in each step i we obtain an effective quasiparticle-i whose lifetime vanish close to the Fermi sea, until finally we obtain the final quasiparticle-n, which is the one with all interactions turned on.

Another way to understand this is by a "self-consistent" argument. Suppose the lifetime of a quasiparticle does vanish close the the Fermi sea, then we can do the above scattering phase volume argument for the quasiparticle directly, replacing all particles by quasiparticles in the argument. We would then reach the same conclusion that $\tau^{-1} \propto \omega^2$.

The phase volume argument is quite unusual. For a classical gas, the scattering rate is roughly proportional to the strength of the interaction, and the phase space volume does not play an essential role. In a Fermi liquid there are many electrons in the ground state, which are in principle strongly affected by the interactions. However there are very few excitations above this ground state at low energy. These excitations can interact strongly with the other electrons in the soup of the ground state, leading to a very strong change of the characteristics compared to free electron excitations. This can lead to very large effective masses or small quasiparticle weight. On the other hand the lifetime of the quasiparticles is controlled by a totally different mechanism since it is blocked by the Pauli principle, as shown in Fig. 1.3. Thus even if the interaction is strong the phase space available for such a scattering is going to zero close to the Fermi level, making the quasiparticle in practice infinitely long lived particles, and allowing to use them to describe the system.

The image of Fig. 1.7 also gives us a description of what a quasiparticle is: this is an electron that is surrounded by a cloud of particle-hole excitations, or in other words density fluctuations since $c^\dagger_{k+q}c_k$ is typically the type of terms entering the density operator. Such density fluctuations are of course neutral and do not change the spin. This composite object electron+density fluctuation cloud, thus represent a tightly bound object (just like an electron dressed with a cloud of photons in quantum electrodynamics), that is the Landau quasiparticle. Since the electron when moving must carry with it its polarization cloud, one can guess that its effective mass will indeed be affected.

The Fermi liquid theory is a direct explanation of the fact that "free" electrons theory works very well qualitatively (such as the specific heat linear in temperature) even when the change of parameters can be huge. We show in (ref. Fig. 1.8) the case of systems where the renormalization of the mass is about $m^* \sim 10^3$m indicating very strong interactions effects. Nevertheless we see that the specific heat varies linearly with temperature just like for

free electrons. The prediction for the quasiparticle peaks fits very well with the photoemission data, in which one clearly sees the peaks becoming sharper as one approaches the Fermi level. There is another direct consequence of the prediction for the lifetime. At finite temperature the typical fermions excited has energy $\omega \sim k_B T$, so the lifetime should vary as $\tau \sim 1/T^2$. If we put such a lifetime in the Drude formula for the conductivity we get

$$\sigma(T) = \frac{ne^2\tau}{m} \propto \frac{1}{T^2} \tag{2.23}$$

This result can be confirmed by a full calculation. This shows that the electron-electron interactions give an intrinsic contribution to the resistivity that varies as $\rho(T) \sim T^2$, and which also can be taken as one of the characteristic of Fermi liquid behavior. This is however difficult to test since this temperature dependence can easily be masked by other scattering phenomena (impurities, scattering by the phonons etc.) that must be added to the electron-electron scattering and that have quite different temperature dependence. Nevertheless there are some materials where the T^2 law can be well observed as shown in Fig. 1.8.

Another interesting consequence can be deduced by looking at the occupation factor $n(k)$ which can be expressed from the spectral function by

$$n(k) = \int d\omega' A\left(k, \omega'\right) f_{\mathrm{F}}\left(\omega'\right) \tag{2.24}$$

For free electrons $n(k)$ is a step function at $k = k_{\mathrm{F}}$. For a Fermi liquid, if we represent the spectral function as

$$A(k, \omega) = Z_k \delta(\omega - E(k)) + A_{\mathrm{inc}}(k, \omega) \tag{2.25}$$

where the incoherent part is a smooth flattish function without any salient feature, then $n(k)$ becomes

$$n(k) = Z_k f_{\mathrm{F}}(E(k)) + \text{ Cste} \tag{2.26}$$

Thus even in the presence of interaction there is still a discontinuity at the Fermi level, that is only rounded by the temperature. Contrarily to the case of free electron the amplitude of the singularity at $T = 0$ is not one anymore but is now $Z_{k_{\mathrm{F}}} < 1$. The existence of this discontinuity if quasiparticle exists tells us directly that the Fermi liquid theory is internally consistent since the very existence of the quasi particles (namely the large lifetime) was heavily resting on the existence of such a discontinuity at the Fermi level. One can thus in a way consider that the existence of a sharp discontinuity at the Fermi level is a good order parameters to characterize the existence of a Fermi liquid.

One important question is when the Fermi liquid theory does apply. This is of course a very delicate issue. One can see both from the arguments given above, and from direct perturbative calculations that when the interactions are weak the Fermi liquid theory will in general be valid. There are some notable exceptions that we will examine in the next section, and for which the phase space argument given above fails. However the main interest of the Fermi liquid theory is that it does not rest on the fact that the interactions are small and, as we have seen through examples, works also remarkably well for the case of strong interactions, **even when all perturbation theory fails to be controlled**. This is specially important for realistic systems since, as we showed, the interaction is routinely of the same order than the kinetic energy even in very good metals. The Fermi liquid theory has thus been the cornerstone of our description of most condensed matter systems in the last 50 years or so. Indeed it tells us that we can "forget" (or easily treat) the main perturbation, namely the interaction among fermions, by simply writing what is essentially a free fermion Hamiltonian with some parameters changed. It is not even important to compute microscopically these parameters since one can simply extract them from one experiment and then use them consistently in the others. This allows to go much further and treat effects caused by much smaller perturbations that one would otherwise have been totally unable to take into account. One of the most spectacular examples is the possibility to now look at the very tiny (compared to the electron-electron interactions) electron-phonon coupling, and to obtain from that the solution to the phenomenon of superconductivity, or other instabilities such as magnetic ordering.

3 Beyond Fermi Liquid

Of course not all materials follow the Fermi liquid theory. There are cases when this theory fails to apply. In that case the system is commonly referred to as **strongly correlated** or "**non Fermi liquid**" a term that hides our poor knowledge of their properties. For such systems, the question of the effects of interactions becomes again a formidable problem. As discussed in the introduction, most of the actual research in now devoted to such non fermi liquid systems. There are fortunately some situation where one can understand the physics and we will examine such cases in this section as well as define the main models that are at the heart of the study of these systems.

3.1 Instabilities of the FL

The Fermi liquid can become **unstable** for a variety of reasons. Some of them are well known. The simplest instability consists, at low temperature, for the system to go an **ordered state**. Many type of orders are possible, the most common are **spin order** such as **ferromagnetism**, **antiferromagnetism**, **charge order** such as a **charge density wave**, or **superconductivity**. In general analyzing such instabilities can be done by computing the corresponding **susceptibility** and looking for **divergences** as the temperature is lowered. When the normal system is well described by a Fermi liquid it is in general relatively easy to compute these susceptibilities by a mean field decoupling of the interaction. This is of course much more complex when one starts from a normal phase which is a non Fermi liquid.

Another important ingredient in the stability of the Fermi liquid phase is the **dimensionality** of the system. Intuitively we can expect that the lower the dimension the more important the effects of the interactions will be since the particles have a harder time to avoid each other. The ultimate case in that respect is the one dimensional situation where one particle moving will push the particle in front and so on, as anybody queuing in a line had already has chance to notice. This effect of dimensionality is confirmed by a direct perturbative calculation of the self energy (Mahan, 1981; Abrikosov, Gorkov and Dzyaloshinski, 1963)

$$\begin{aligned} \Sigma_{3D}(\omega) &\propto U^2\omega^2 \\ \Sigma_{2D}(\omega) &\propto U^2\omega^2\log(\omega) \\ \Sigma_{1D}(\omega) &\propto U^2\omega\log(\omega) \end{aligned} \tag{3.1}$$

where U is the strength of the interaction. In particular one immediately see that for the one dimensional case, the self energy becomes dominant compared to the mean energy ω. Using $Z_k = \left(1 - \frac{\partial \Re\Sigma(k,\omega)}{\partial\omega}\Big|_{\omega=E(k)}\right)^{-1}$ one sees that for one dimension the quasiparticle weight is zero at the Fermi level. This means the whole argument we used in the previous section to justify the existence of sharper and sharper peaks and thus the existence of Landau quasiparticles fails regardless of the strength of the interaction. In one dimension Fermi liquid always fails. This leads to a remarkable physics that we examine in more details in Section 1.4.

Part II
Linear Response Theory

In classical mechanics, for example, a damped Harmonic oscillator, we study the system with any given initial condition and predict how it evolves in time. The problem can be equivalently solved in frequency space by a Fourier Transform.

In many-body theory, it is hopeless that we start with **any initial** density matrix ϱ and predict how it would evolve in time, leading to some observable changes in the expectation of physical quantities, since the number of initial ϱ is practically infinite. The second law of thermodynamics come to help, making most of the condensed matter systems (metal, superconductor, superfluid...) we are able to do experiments on close to thermodynamic equilibrium. We almost always start with an equilibrium system, where we are sure $\varrho = Z^{-1}e^{-\beta H}$, and use some methods to couple the system to an external classical system that we can control. When we tune the nob of the external classical system (for example add an electric field), the many-body system is driven slightly out of thermodynamic equilibrium in a particular way (develop a current). It is difficult to describe the change of the system entirely, as it again involves describing the complex $\delta\varrho$. A simple and yet useful way to describe the change of the system is by studying the expectation value of some particular physical quantity $\delta\left\langle \hat{B}(t)\right\rangle$. Of course, $\delta\varrho$ will generate changes in the expectation value of all operators, but we shall focus on one at a time, as this is sufficient to explain experiments.

If the driving force is weak, and we are close to equilibrium, $\delta\varrho$ can be known almost exactly, although we will not calculate it explicitly. We will instead see that $\delta\left\langle B(t)\right\rangle$ becomes simple, since the perturbation at different times can be thought as independent of each other, this is the **linear response approximation**. As a concrete example, when we beat the drum once with a drumstick, the drum starts oscillating and then damps to a stop. The linear response approximation here says that when we keep beating the drum, the strike at time t and later $t+\delta t$ will combine to give a sound that is equal to the sum of sounds from the individual strikes. In frequency space this statement is even simpler: The force at each frequency induce response at the exact same frequency, which is directly proportional to the magnitude of the driving force. The Kubo formula describes exactly such a relation:

$$\delta\langle B(\mathbf{q},\omega)\rangle = \chi^R_{BA}(\mathbf{q},\omega)a(\mathbf{q},\omega) \tag{3.2}$$

The proportionality constant χ^R_{BA} is called the **generalized susceptibility** (or **response function**), which is an intrinsic property of the system independent of the magnitude of the driving force a. The pair a, B can also be thought of as a generalized force and a generalized displacement. As many-body system has so many degrees of freedom, there are countless many types of generalized forces that can be applied to the system and correspondingly infinite many ways the system ϱ can displace to $\varrho_{\approx eq}$ close-to-equilibrium.

All the information about the system close to equilibrium are thus captured by the generalized susceptibility $\chi^R_{BA}(\mathbf{q},\omega)$. We shall see this first in classical harmonic oscillators, where we will develop some intuition about it, and then see how to calculate it in a quantum system with Kubo formula. There are also many analytic properties of $\chi''_{AB}(\mathbf{q},\omega)$ in frequency space. As linear response works directly in frequency space, we should study all these quantities in frequency space. This of course contain the same information as the response in time, but give us much more theoretical conveniences.

The Green's function introduced in the Fermi-liquid theory chapter is also a special type of generalized susceptibility.

4 Relation to Experiments

The differential cross section due to inelastic electron scattering is given by

$$\frac{d\sigma}{d\epsilon_f d\Omega_f} = \left[\frac{m^2}{(2\pi)^3\hbar^5}\frac{k_f}{k_i}\left|V^c_{-\mathbf{q}}\right|^2\right] S_{\rho\rho}(\mathbf{q},\omega) \tag{4.1}$$

where $S_{\rho\rho}(\mathbf{q},\omega)$ represents the fluctuation of charge in space and time.

5 Classical linear response

5.1 Harmonic Oscillator

Consider a damped Harmonic oscillator

$$m\ddot{x}(t) + m\gamma\dot{x}(t) + kx(t) = F(t) \tag{5.1}$$

we can make γ retarded, which is more general

$$m\ddot{x}(t) + m\int_{-\infty}^{\infty} dt'\gamma(t-t')\dot{x}(t') + kx(t) = F(t) \tag{5.2}$$

here the dissipative force at time t depend in general on the velocity of the particle at all previous times t'. In Fourier Space this is

$$\left(-\omega^2 - i\omega\gamma(\omega) + \omega_0^2\right) x(\omega) = \frac{1}{m}F(\omega). \tag{5.3}$$

and

$$x(\omega) = \frac{1/m}{(-\omega^2 - i\omega\gamma(\omega) + \omega_0^2)}F(\omega) \tag{5.4}$$

Define

$$\begin{aligned} x(\omega) &= \chi^R(\omega)F(\omega) \\ \chi^R(\omega) &\equiv \frac{1/m}{-\omega^2 + \omega_0^2 - i\omega\gamma(\omega)} = \frac{1/m}{-\omega^2 + \omega_0^2 + \omega\gamma''(\omega) - i\omega\gamma'(\omega)} \end{aligned} \tag{5.5}$$

$$x(t) = \int_{-\infty}^{\infty} dt'\chi^R\left(t-t'\right)F\left(t'\right) \tag{5.6}$$

$$\chi^R(\omega) = \chi'(\omega) + i\chi''(\omega) \tag{5.7}$$

Since χ^R is causal, χ', χ'' must obey Kramer-Kronig relations.

5.1.1 Possitivity of $\omega\chi''(\omega)$

The work done by the external force in unit time

$$\begin{aligned} \dot{W} &= F(t)\dot{x} \\ &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}F(\omega)e^{-i\omega t}\dot{x} \\ &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Re\left[F(\omega)e^{-i\omega t}\right]\dot{x} \\ &\equiv \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\dot{W}_\omega \end{aligned} \tag{5.8}$$

can be calculated by summing over the work done by each Fourier component $\Re\left[F(\omega)e^{-i\omega t}\right]$. The average power done by the external force in a period $\mathcal{T}$(which can be taken to ∞) by the component $F(\omega)$ in an intever $\frac{d\omega}{2\pi}$ is given by

$$\begin{aligned} P(\omega) &\equiv \lim_{\mathcal{T}\to\infty}\frac{1}{\mathcal{T}}\int_{-\mathcal{T}/2}^{\mathcal{T}/2}dt\dot{W}_\omega \\ &= \Re\left[F(\omega)\lim_{\mathcal{T}\to\infty}\frac{1}{\mathcal{T}}\int_{-\mathcal{T}/2}^{\mathcal{T}/2}dte^{-i\omega t}\dot{x}(t)\right] \\ &= \Re\left[(i\omega)F(\omega)\lim_{\mathcal{T}\to\infty}\frac{1}{\mathcal{T}}\int_{-\mathcal{T}/2}^{\mathcal{T}/2}dte^{-i\omega t}x(t)\right] \\ &= \Re\left[i\omega F(\omega)x_\omega^*\right] \\ &= -\Im\left[\omega F(\omega)x_\omega^*\right] \\ &= -\left|F(\omega)\right|^2\Im\left[\omega\chi^{R*}(\omega)\right] \\ &= \left|F(\omega)\right|^2\omega\chi''(\omega) \end{aligned} \tag{5.9}$$

the work done is always positive in a period, so $P(\omega) \geq 0$ and

$$\omega\chi''(\omega) \geq 0 \tag{5.10}$$

we have

$$\chi''(\omega) = \frac{1}{m} \frac{\omega\gamma'(\omega)}{\left(-\omega^2 + \omega_0^2 + \omega\gamma''(\omega)\right)^2 + \left(\omega\gamma'(\omega)\right)^2} \tag{5.11}$$

so

$$\gamma'(\omega) \geq 0 \tag{5.12}$$

In addition, $\gamma(t)$ is real, so $\gamma(-\omega) = \gamma^*(\omega)$, so $\gamma'(\omega)$ is even and $\gamma''(\omega)$ is odd.

5.2 Coupled Harmonic Oscillator

(Andre's book I.Classical harmonic oscillator)

Looking at the problem of coupled harmonic oscillators, we will discover in this Chapter that in the limit where there is an infinite number of oscillators, irreversibility appears. Otherwise, the motion is periodic, or quasi-periodic. This is a very general result that demonstrates in a very simple context how irreversibility emerges in the limit of an infinite number of degrees of freedom. In practice, if we take the infinite-size limit before we take the $\eta \to 0$ limit, the response of the system will be irreversible.

Consider a harmonic oscillator attached to a one-dimensional chain of harmonic oscillators that plays the role of a bath or of a reservoir. (Fig.4-1 in ref) A mass M is attached on the left to a wall with a spring of constant k and on the right to a one-dimensional chain of oscillators. The deviation of the mass M with respect to equilibrium is denoted by x. Each of the masses m of the one-dimensional chain of oscillators is attached to its neighbor by a spring of constant k', except for the first link between M and m that I call k'' because it will play the role of a coupling constant between the bath and the mass M. The deviation from equilibrium of the mass at position i is u_i. A force F is also applied to the mass M. The potential energy is thus

$$V\left(x, \{u_i\}\right) = -Fx + \frac{1}{2}kx^2 + \frac{k''}{2}\left(x - u_1\right)^2 + \frac{k'}{2}\left(u_2 - u_1\right)^2 + \frac{k'}{2}\left(u_3 - u_2\right)^2 + \dots \tag{5.13}$$

the equations of motion are given by

$$\begin{aligned} M\ddot{x} &= -\frac{\partial V}{\partial x} = F - kx - k''(x - u_1) \\ m\ddot{u}_1 &= -\frac{\partial V}{\partial u_1} = -k''(u_1 - x) - k'(u_1 - u_2) \\ m\ddot{u}_2 &= -\frac{\partial V}{\partial u_2} = -k'(u_2 - u_1) - k'(u_2 - u_3) \\ &\dots \end{aligned} \tag{5.14}$$

The Fourier Transform gives

$$\begin{aligned} -M(\omega + i\eta)^2 x &= -\frac{\partial V}{\partial x} = F - kx - k''(x - u_1) \\ -m(\omega + i\eta)^2 u_1 &= -\frac{\partial V}{\partial u_1} = -k''(u_1 - x) - k'(u_1 - u_2) \\ -m(\omega + i\eta)^2 u_2 &= -\frac{\partial V}{\partial u_2} = -k'(u_2 - u_1) - k'(u_2 - u_3) \\ &\dots \end{aligned} \tag{5.15}$$

with $z = \omega + i\eta$, we write

$$\begin{bmatrix} -Mz^2 + k + k'' & -k'' & 0 & 0 & \cdots & 0 \\ -k'' & -mz^2 + k' + k'' & -k' & 0 & \cdots & 0 \\ 0 & -k' & -mz^2 + 2k' & -k' & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & & \\ \cdots & \cdots & \cdots & \cdots & & \\ 0 & 0 & 0 & \cdots & -k' & -mz^2 + 2k' \end{bmatrix} \begin{bmatrix} x \\ u_1 \\ u_2 \\ \cdots \\ \cdots \\ u_N \end{bmatrix} = \begin{bmatrix} F \\ 0 \\ 0 \\ \cdots \\ \cdots \\ 0 \end{bmatrix} \tag{5.16}$$

We rewrite the matrix equation as

$$\begin{bmatrix} \mathcal{D}_0^{-1}(z) & V^T \\ V & \mathcal{D}_b^{-1}(z) \end{bmatrix} \begin{bmatrix} x \\ u \end{bmatrix} = \begin{bmatrix} F \\ 0 \end{bmatrix} \tag{5.17}$$

where $\mathcal{D}_0^{-1}(z) = -Mz^2 + (k + k')$ is a scalar, V is a $N \times 1$ vector, V^T is its transpose, $\mathcal{D}_b^{-1}(z)$ is an $N \times N$ matrix for the bath, and u is a vector whose N components are u_i. The bottom block can easily be solved for u as follows in matrix notation, with Einstein summation implied

$$u^a = -\mathcal{D}_b^{ab}(z) V^b x \tag{5.18}$$

Substituting this in the first equation we find

$$x = \left(\mathcal{D}_0^{-1}(z) - V^T \mathcal{D}_b(z) V\right)^{-1} F \equiv \mathcal{D}(z) F \tag{5.19}$$

where $\mathcal{D}(z) \equiv \left(\mathcal{D}_0^{-1}(z) - V^T \mathcal{D}_b(z) V\right)$ is the overall propagator of x. In the case where there are no degrees of freedom in the bath, there is a single pair of eigenfrequencies at $\mathcal{D}_0^{-1}(z) = 0$, i.e. two poles infinitesimally close to the real axis at $\omega + i\eta = \pm\sqrt{(k + k'')/M}$. In the presence of the bath, there will be $N + 1$ pairs of poles. We can see that more explicitly as follows.

Define K as the real and symmetric matrix of spring constants

$$\mathcal{D}_b^{-1}(z) = \sqrt{m}\left(-z^2 + \frac{1}{\sqrt{m}} K \frac{1}{\sqrt{m}}\right)\sqrt{m} \tag{5.20}$$

$$\frac{1}{\sqrt{m}} K \frac{1}{\sqrt{m}} \equiv \frac{1}{m} \begin{bmatrix} (k' + k'') & -k' & 0 & \cdots & 0 \\ -k' & (2k') & -k' & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \\ \cdots & \cdots & \cdots & \cdots & -k' \\ 0 & 0 & \cdots & -k' & (2k') \end{bmatrix} \tag{5.21}$$

We now diagonalize $\frac{1}{\sqrt{m}} K \frac{1}{\sqrt{m}} = O^T D O$ with O orthogonal, and

$$\begin{aligned} \mathcal{D}_b^{-1}(z) &= \sqrt{m} O^T \left(-z^2 + D\right) O \sqrt{m} \\ \mathcal{D}_b(z) &= \frac{1}{\sqrt{m}} O^T \left(-z^2 + D\right)^{-1} O \frac{1}{\sqrt{m}} \end{aligned} \tag{5.22}$$

So

$$\begin{aligned} \mathcal{D}(z) &= \left(\mathcal{D}_0^{-1}(z) - V^T \frac{1}{\sqrt{m}} O^T \left(-z^2 + D\right)^{-1} O \frac{1}{\sqrt{m}} V\right)^{-1} \\ &= \left(\mathcal{D}_0^{-1}(z) - T^T \left(-z^2 + D\right)^{-1} T\right)^{-1} \end{aligned} \tag{5.23}$$

where we defined the $N \times 1$ vector $T = O \frac{1}{\sqrt{m}} V$. Since V has units of a spring constant and O is dimensionless, T has units of $\sqrt{k}\omega$. Labeling the eigenvalues in D by α, the propagator can be written as

$$\mathcal{D}^R(\omega) = \mathcal{D}(z = \omega + i\eta) = \lim_{\eta \to 0} \frac{1/M}{-(\omega + i\eta)^2 + \omega_0^2 - \frac{1}{M} \sum^N T_\alpha \frac{1}{-(\omega + i\eta)^2 + \omega_\alpha^2} T_\alpha^T} \tag{5.24}$$

where $\omega_0^2 \equiv \frac{(k + k'')}{M}$ is the 'bare' frequency of the oscillator. The poles in the presence of the bath are then given by the solution to

$$-(\omega + i\eta)^2 + \omega_0^2 - \frac{1}{M} \sum_{\alpha=1}^{N} \frac{T_\alpha^2}{-(\omega + i\eta)^2 + \omega_\alpha^2} = 0 \tag{5.25}$$

Rewriting with a common denominator, you see that we are looking for the zeros of a polynomial of order $N + 1$ in $(\omega + i\eta)^2$. The propagator will have $N + 1$ pairs of poles located symmetrically about the imaginary axis in the lower half plane, infinitesimally close to the real axis, as illustrated in (ref Fig.(4-2a)).

Any motion of the mass M can be written as a sum of oscillations at discrete frequencies. The motion may look complicated because the frequencies may not be commensurable, but it is in principle periodic. Physically, the mass M in the presence of the bath is a finite system and a disturbance will oscillate back and forth.

The effective equation that we obtained for the coordinate x takes into account the one-dimensional set of oscillators, that acts like a "bath" or reservoir. We have "**integrated out**" the bath, to obtain an equation of motion for the degree of liberty that we are interested in. The result contains $V\mathcal{D}_b(z)V^T$ that will be called a **hybridization function** in the context of the Anderson impurity problem that arises in dynamical mean-field theory. Also, $\mathcal{D}_b(z)$ is a propagator in the bath. It takes into account that a wave produced by a motion of x can go in the one-dimensional bath and come back in a retarded way later.

5.3 Infinite number of oscillators

What happens if the bath is infinite? Then, it looks as if the mass M was attached to some sort of infinite transmission line. A disturbance will propagate in the bath and **never come back**. This is how irreversibility arises. Mathematically, it is as if the motion was now represented by Fourier transforms instead of Fourier series.

If we take the number of degrees of freedom of the bath N to infinity, the summation in the denominator of the propagator can be promoted to an integral, to do this, we insert in delta functions

$$\begin{aligned}
&\frac{1}{M}\sum_{i=1}^{N}\frac{T_\alpha^2}{-(\omega+i\eta)^2+\omega_\alpha^2}\\
&=\int_0^\infty d\left(\Omega^2\right)\frac{1}{M}\sum_{i=1}^{N}\delta(\Omega^2-\omega_\alpha^2)T_\alpha^2\frac{1}{-(\omega+i\eta)^2+\Omega^2}\\
&\equiv\int_0^\infty d\left(\Omega^2\right)\frac{N(\Omega^2)}{-(\omega+i\eta)^2+\Omega^2}
\end{aligned}\tag{5.26}$$

where

$$N(\Omega^2)\equiv\frac{1}{M}\sum_{i=1}^{N}\delta(\Omega^2-\omega_\alpha^2)T_\alpha^2\tag{5.27}$$

In the limit where the number of eigenmodes goes to infinity, the coupling to the mass M represented by $T_\alpha T_a^T$ will scale as $1/N$, in other words, the more modes there are, the smaller the coupling to any given mode if we want a well defined continuum limit. Then $\frac{1}{N}\sum_{\alpha=1}^{N}$ can be transformed to an integral, and $N\left(\Omega^2\right)$ becomes a continuous function. Another way to look at this is to return to a finite η, in other words to the Lorentzian representation of the delta function. If within a width η there are many modes ω_α, then the function $N(\Omega^2)$ appears continuous. It is with a continuous $N(\Omega^2)$ that irreversibility appears as we shall see. In other words, if we take the limit of an infinite bath before the limit $\eta\to 0$, we introduce irreversibility.

Let us continue our derivation. We will see that any damping function $\gamma(\omega)$ can be represented by an appropriately constructed infinite bath. Since

$$\frac{1}{-(\omega+i\eta)^2+\Omega^2}=\frac{1}{2\Omega}\left(\frac{1}{\omega+i\eta+\Omega}-\frac{1}{\omega+i\eta-\Omega}\right)\tag{5.28}$$

The pole equation become

$$\begin{aligned}
&-\omega^2+\omega_0^2-\mathcal{P}\int_0^\infty\frac{N\left(\Omega^2\right)}{2\Omega}\left(\frac{1}{\omega+\Omega}-\frac{1}{\omega-\Omega}\right)2\Omega d\Omega\\
&+i\pi\int_0^\infty\frac{N\left(\Omega^2\right)}{2\Omega}(\delta(\omega+\Omega)-\delta(\omega-\Omega))2\Omega d\Omega=0.
\end{aligned}\tag{5.29}$$

$$\begin{aligned}
&-\omega^2+\omega_0^2-\mathcal{P}\int_0^\infty N\left(\Omega^2\right)\left(\frac{1}{\omega+\Omega}-\frac{1}{\omega-\Omega}\right)d\Omega\\
&-i\pi N(\omega^2)(\theta(\omega)-\theta(-\omega))=0
\end{aligned}\tag{5.30}$$

Now define

$$\begin{aligned}
\omega\gamma'(\omega)&\equiv\pi N(\omega^2)(\theta(\omega)-\theta(-\omega))\\
\omega\gamma''(\omega)&\equiv-\mathcal{P}\int_0^\infty N\left(\Omega^2\right)\left(\frac{1}{\omega+\Omega}-\frac{1}{\omega-\Omega}\right)d\Omega
\end{aligned}\tag{5.31}$$

where $\gamma'(\omega)$ is a real, positive, even function, $\gamma''(\omega)$ is real, odd, satisfying all the requirements that the real part of a dissipation function should have.

The propagator can be now written as

$$\chi^R(\omega) = \mathcal{D}^R(\omega) = \frac{1/M}{-\omega^2 + \omega_0^2 + \omega\gamma''(\omega) - i\omega\gamma'(\omega)} \tag{5.32}$$

with a finite imaginary part, which represent energy dissipation.

ref Fig. (4-3a) shows that in the infinite size limit, the poles of infinitesimal below the real axis collapse into a branch cut. The corresponding imaginary part of the susceptibility in Fig. (4-3b) is a continuous function. If we decide to approximate this continuous function by two Lorentzians, as in Fig. (4-3d) then the pole structure changes. There are now only two isolated poles far below the real axis as in Fig. (4-3c). The fact that the poles are no longer close to the real axis is often not a problem. We are just approximating continuous function representing the imaginary part of the susceptibility differently. However, the Lorentzian approximation has problems at high frequency so that sum rules can be violated.

6 Interaction Picture

Given Shrodinger equation

$$i\partial_t |\phi\rangle = H |\phi\rangle \tag{6.1}$$

Define the propagator

$$|\phi(t)\rangle = U(t,0) |\phi\rangle \tag{6.2}$$

where $|\psi\rangle \equiv |\psi(t=0)\rangle$. Shrodinger equation requires

$$i\partial_t U(t,0) = HU(t,0) \tag{6.3}$$

formally

$$U(t,0) = \mathcal{T} \exp\left\{-i\int_0^t H(t')dt'\right\} \tag{6.4}$$

If H is time-independent, we can write

$$U(t,0) = e^{-iHt} \tag{6.5}$$

Now consider a Hamiltonian which can be separated into a free Hamiltonian H_0 that we know how to solve and a time-dependent perturbation V:

$$H = H_0 + V(t) \tag{6.6}$$

where in general $[H_0, V] \neq 0$. In Shrodinger picture we have states and operators$|\phi_S(t)\rangle, \mathcal{O}_S$. For field operators we use the symbol ψ_S (Be sure to separate states and field operators). To define Heisenberg picture we rewrite the expectations

$$\langle\phi_S(t)| \mathcal{O}_S |\phi_S(t)\rangle = \langle\phi_S| U(0,t)\mathcal{O}_S U(t,0) |\phi_S\rangle = \langle\phi_H| \mathcal{O}_H(t) |\phi_H\rangle \tag{6.7}$$

where $|\phi_S\rangle \equiv |\phi_S(0)\rangle$. This gives

$$\begin{aligned} |\phi_H\rangle &= |\phi_S(t=0)\rangle = |\phi_S\rangle \\ \mathcal{O}_H(t) &= U(0,t)\mathcal{O}_S U(t,0) \end{aligned} \tag{6.8}$$

to define interaction picture,

$$\langle\phi_S(t)| \mathcal{O}_S |\phi_S(t)\rangle = \langle\phi_S(t)| e^{-iH_0t}e^{iH_0t}\mathcal{O}_S e^{-iH_0t}e^{iH_0t} |\phi_S(t)\rangle = \langle\phi_I(t)| \mathcal{O}_I(t) |\phi_I(t)\rangle \tag{6.9}$$

this gives

$$\begin{aligned} |\phi_I(t)\rangle &= e^{iH_0t} |\phi_S(t)\rangle = e^{iH_0t}U(t,0) |\phi_S\rangle \\ \mathcal{O}_I(t) &= e^{iH_0t}\mathcal{O}_S e^{-iH_0t} \end{aligned} \tag{6.10}$$

So we can define

$$\begin{aligned} |\phi_I(t)\rangle &\equiv U_I(t,0) |\phi_S\rangle \\ U_I(t,0) &= e^{iH_0t}U(t,0) \\ U_I(t,t_0) &= e^{iH_0t}U(t,t_0)e^{-iH_0t_0} \\ e^{-iH_0t}U_I(t,t_0)e^{iH_0t_0} &= U(t,t_0) \end{aligned} \tag{6.11}$$

we have also

$$\mathcal{O}_H(t) = U_I(0,t)\mathcal{O}_I(t)U_I(t,0) \tag{6.12}$$

Now differentiate $U_I(t,0)$ and get Shrodinger equation for the interaction propagator

$$\begin{aligned} i\partial_t U_I(t,0) &= -H_0 e^{iH_0 t}U(t,0) + e^{iH_0 t}i\partial_t U(t,0) \\ &= e^{iH_0 t}\left[H - H_0\right]U(t,0) \\ &= V_I(t)U_I(t,0) \end{aligned} \tag{6.13}$$

The formal solution will again be a time-ordered exponential

$$U_I\left(t,t_0\right) = \mathcal{T}\exp\left\{-i\int_{t_0}^{t} dt' V_I(t')\right\} \tag{6.14}$$

To see how time-ordering works, we can expand this

$$U_I\left(t,t_0\right) = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\mathcal{T}\left[\int_{t_0}^{t} dt' V_I(t')\right]^n \tag{6.15}$$

$$\begin{aligned} \mathcal{T}\left[\int_{t_0}^{t} dt' V_I(t')\right]^0 &= 1 \\ \mathcal{T}\left[\int_{t_0}^{t} dt' V_I(t')\right]^1 &= \int_{t_0}^{t} dt' V_I(t') \\ \mathcal{T}\left[\int_{t_0}^{t} dt' V_I(t')\right]^2 &= \int_{t_0}^{t} dt_1 V_I(t_1)\int_{t_0}^{t_1} dt_2 V_I(t_2) \\ \mathcal{T}\left[\int_{t_0}^{t} dt' V_I(t')\right]^3 &= \int_{t_0}^{t} dt_1 V_I(t_1)\int_{t_0}^{t_1} dt_2 V_I(t_2)\int_{t_0}^{t_2} dt_3 V_I(t_3) \\ ... &= ... \end{aligned} \tag{6.16}$$

to first order,

$$U_I\left(t,t_0\right) = 1 - i\int_{t_0}^{t} dt' V_I(t') + \mathcal{O}(V^2) \tag{6.17}$$

Notice that this formalism works only in zero-temperature, although it seems that in our derivation we have not assumed $\langle ... \rangle = \langle GS| ... |GS\rangle$. The reason is, when we consider finite temperature, the evolution of some expectation $\langle\mathcal{O}\rangle(t)$ is given by:

$$\langle\mathcal{O}\rangle(t) = \frac{1}{Z}\sum_n e^{-\beta E_n}\langle n(t)|\mathcal{O}|n(t)\rangle = \frac{\mathrm{Tr}\left(e^{-\beta H}\mathcal{O}_H\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)} \tag{6.18}$$

Notice that if $H(t) = H_0 + V(t)$ is explicitly time-dependent, the factor $e^{-\beta H} = e^{-\beta H(t)}$ or effectively $e^{-\beta E_n(t)}$ is explicitly time-dependent. This then is a "thermal force" coming out of $e^{-\beta H(t)}$, physically due to the thermal reservoir interacting with the system. In our formalism this thermal force is completely ignored. This could only be justified if we are at $T = 0$, where there is no thermal force. In general for $T =$ finite, the system is interacting with both the external perturbation and thermal reservoir, but the thermal interaction is assumed to be very fast, such that

$$\tau_{\text{thermal}} \ll \tau_{\text{perturbation}} \tag{6.19}$$

it is in this sense that we set $e^{-\beta H(t)}$, effectively making the thermal interaction "instantaneous" $\tau_{\text{thermal}} \to 0$. Later in imaginary time formalism we will make use of this assumption.

7 Kubo Formula

(From Andre's book on Quantum Materials, Chapter 9)

Let the Hamiltonian be written as the sum of a unperturbed Hamiltonian H_0 and a perturbation $\delta\mathcal{H}$

$$H(t) = H_0 + \delta\mathcal{H}(t) \tag{7.1}$$

the physical quantities can be written as linear combination of field operators, so we should consider a perturbation of the form:

$$\delta\mathcal{H}(t) = -\int d^3 r A_i(\mathbf{r}) a_i(\mathbf{r}, t) \tag{7.2}$$

with operators $A_i(\mathbf{r})$ and external classical fields $a_i(\mathbf{r}, t)$. In interacting picture

$$A_i(\mathbf{r}, t) = e^{iHt} A_i(\mathbf{r}) e^{-iHt} \tag{7.3}$$

so we have the corresponding perturbation in interaction picture

$$\delta\mathcal{H}_I(t) = -\int d^3 r A_i(\mathbf{r}, t) a_i(\mathbf{r}, t) \tag{7.4}$$

Starting in the equilibrium density matrix $\rho = \frac{1}{Z} e^{-\beta H_0}$ at time t_0, starting here, the system starts to evolve, in Heisenberg picture, ρ stay the same and we have

$$\mathcal{O}_H(t) = U^\dagger(t, t_0) \mathcal{O}_S U(t, t_0) \tag{7.5}$$

$$\begin{aligned} \langle B(\mathbf{r}, t)_{\text{n.e.}} \rangle &= \langle B_H(\mathbf{r}, t) \rangle \\ &= \left\langle U^\dagger(t, t_0) B(\mathbf{r}) U(t, t_0) \right\rangle \\ &= \frac{1}{Z} \operatorname{Tr}\left(e^{-\beta H_0} U^\dagger(t, t_0) B(\mathbf{r}) U(t, t_0) \right) \end{aligned} \tag{7.6}$$

where $\langle ... \rangle$ means a trace in basis $\{|i\rangle\}$: $\langle i| ... |i\rangle$ where $|i\rangle \equiv |i_S(t = t_0)\rangle$ is the Shrodinger picture state at t_0. In this expression, the subscript n.e. on the left reminds us that the time dependence includes that from the external perturbation. In interaction picture,

$$U_I(t, 0) = e^{iH_0 t} U(t, 0) \tag{7.7}$$

$$\begin{aligned} \langle B(\mathbf{r}, t)_{\text{n.e.}} \rangle &= \left\langle U^\dagger(t, t_0) B(\mathbf{r}) U(t, t_0) \right\rangle \\ &= \left\langle e^{-iH_0 t_0} U_I^\dagger(t, t_0) e^{iH_0 t} B(\mathbf{r}) e^{-iH_0 t} U_I(t, t_0) e^{iH_0 t_0} \right\rangle \\ &= \left\langle U_I^\dagger(t, t_0) B(\mathbf{r}, t) U_I(t, t_0) \right\rangle \end{aligned} \tag{7.8}$$

where the two factors $e^{\pm iH_0 t_0}$ cancel due to cyclic property of trace and that $[\rho, e^{\pm iH_0 t_0}] = 0$. Now we approximate U_I to first order

$$\begin{aligned} U_I(t, t_0) &\approx 1 - i \int_{t_0}^{t} dt' \delta\mathcal{H}_I(t') \\ &= 1 + i \int_{t_0}^{t} dt' \int d^3 r a_i(\mathbf{r}, t') A_i(\mathbf{r}, t') \end{aligned} \tag{7.9}$$

and evaluate the change due to the pertubation

$$\delta \langle B(\mathbf{r}, t) \rangle \equiv \langle B(\mathbf{r}, t)_{\text{n.e.}} \rangle - \langle B(\mathbf{r}, t) \rangle \tag{7.10}$$

$$\begin{aligned} \delta \langle B(\mathbf{r}, t) \rangle &= i \int_{t_0}^{t} dt' \int d^3 r' a_i(\mathbf{r}', t') \langle [B(\mathbf{r}, t), A_i(\mathbf{r}', t')] \rangle \\ &\to i \int_{-\infty}^{\infty} dt' \int d^3 r' a_i(\mathbf{r}', t') \theta(t - t') \langle [B(\mathbf{r}, t), A_i(\mathbf{r}', t')] \rangle \end{aligned} \tag{7.11}$$

where we have taken $t_0 \to -\infty$, which means the perturbation is turned on adiabatically. This is justified since linear response operates in the frequency domain, and Fourier Transform is not affected if we multiply the function by a slow-varying envelop function. For example,

$$\mathcal{F}\left\{ \left[e^{-t^2} t^2 \cos(t^2) \right] e^{-\frac{t^2}{100}} \right\}(\omega) \approx \mathcal{F}\left\{ \left[e^{-t^2} t^2 \cos(t^2) \right] \right\}(\omega) \tag{7.12}$$

the adiabatic switching does not affect the Fourier Transform of a function which vanish sufficiently fast.We have also moved the upper limit to $\theta(t-t_0)$. Now define the generalized susceptibility (or retarded response function)

$$\begin{aligned}\chi''_{BA_i}(\mathbf{r},t;\mathbf{r}',t') &\equiv \frac{1}{2}\langle[B(\mathbf{r},t),A_i(\mathbf{r}',t')]\rangle \\ \chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t') &\equiv 2i\chi''_{BA_i}(\mathbf{r},t;\mathbf{r}',t')\,\theta(t-t') \\ &= i\theta(t-t')\langle[B(\mathbf{r},t),A_i(\mathbf{r}',t')]\rangle\end{aligned} \tag{7.13}$$

We have the linear response equation in real time and coordinate space

$$\delta\langle B(\mathbf{r},t)\rangle = \int_{-\infty}^{\infty} dt' \int d^3r' \chi^R_{BA_i}(\mathbf{r},t;\mathbf{r}',t')\,a_i(\mathbf{r}',t') \tag{7.14}$$

since H_0 is time-independent, the commutator $\chi''_{BA_i}(\mathbf{r},t;\mathbf{r}',t') = \chi''_{BA_i}(\mathbf{r},\mathbf{r}',t-t')$. Performing a Fourier Transform $t-t'\to\omega$, we have, by convolution theorem,

$$\delta\langle B(\mathbf{r},\omega)\rangle = \int d^3r' \chi^R_{BA_i}(\mathbf{r},\mathbf{r}',\omega)\,a_i(\mathbf{r}',\omega) \tag{7.15}$$

if the system has translation symmetry, $\chi''_{BA_i}(\mathbf{r},t;\mathbf{r}',t') = \chi''_{BA_i}(\mathbf{r}-\mathbf{r}',t-t')$. Now perform the Fourier Transform $\mathbf{r}-\mathbf{r}'\to\mathbf{q}$, we have the Kubo formula in momentum-frequency space

$$\delta\langle B(\mathbf{q},\omega)\rangle = \chi^R_{BA_i}(\mathbf{q},\omega)\,a_i(\mathbf{q},\omega) \tag{7.16}$$

8 Analytic Properties of generalized susceptibilities

(Andre Marie Tremblay: Quantum Material Theory, from perturbation theory to dynamical-mean field)

In this section we use the following Fourier Transforms

$$\begin{aligned} f_{\mathbf{q}} &= \int d^3r f(\mathbf{r})\mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}} \\ f(\mathbf{r}) &= \int \frac{d^3k}{(2\pi)^3} f_{\mathbf{q}}\mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}} \\ g_\omega &= \int dt g(t) e^{i\omega t} \\ g(t) &= \int \frac{d\omega}{2\pi} g_\omega e^{-i\omega t} \end{aligned} \tag{8.1}$$

Recall our general expression for the response function

$$\chi^R_{BA}(\mathbf{r},t;\mathbf{r}',t') \equiv i\theta(t-t')\langle[B(t),A(t')]\rangle \tag{8.2}$$

where operators A, B are in interaction picture. Define

$$\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t') = \frac{1}{2\hbar}\langle[B(\mathbf{r},t),A(\mathbf{r}',t')]\rangle \tag{8.3}$$

which contain all the physics except the causality. The factor of two will allow χ'' to satisfy the Kramers-Kronig relations in their standard form. the function. These two functions are related by

$$\chi^R_{BA}(\mathbf{r},t;\mathbf{r}',t') = 2i\chi''_{BA}(\mathbf{r},t;\mathbf{r}',t')\,\theta(t-t') \tag{8.4}$$

We will use a short-hand notation

$$\chi^R_{A_iA_j}(t-t') = \frac{i}{\hbar}\langle[A_i(t),A_j(t')]\rangle\,\theta(t-t') \tag{8.5}$$

where we include in the indices i and j the positions as well as any other label of the operator such as vector or spin component. In this notation, we have not assumed translational invariance. We did however assume time-translation invariance. Since we are working with equilibrium averages above, this is always true. In this notation, we have

$$\begin{aligned}\chi''_{A_iA_j}(t-t') &\equiv \frac{1}{2}\langle[A_i(t),A_j(t')]\rangle \\ \chi^R_{A_iA_j}(t-t') &= 2i\chi''_{A_iA_j}(t-t')\,\theta(t-t')\end{aligned} \tag{8.6}$$

If A_i, A_j are Hermitian, then their commutator will be anti-Hermitian, whose average is imaginary. So $\chi''_{A_iA_j}$ would be purely imaginary, thus the two primes. We have omitted a $\hbar$ also, and $\chi''_{A_iA_j}(t-t') \equiv \frac{1}{2\hbar}\langle[A_i(t), A_j(t')]\rangle$ in full dimensional form.

8.1 The $i\eta$ prescription

In this section we shall be studying retarded functions

$$g^R(t) = g''(t)\theta(t) \tag{8.7}$$

and its Fourier Transform

$$g^R_\omega = \int_{-\infty}^{\infty} dt g^R(t) e^{i\omega t} = \int_0^{\infty} dt g''(t) e^{i\omega t} \tag{8.8}$$

However, the usual Fourier Transform has a problem of convergence, the solution of which is to introduce distributions which has meaning only when multiplied with other functions, for example

$$\mathcal{F}(x^2)(k) = -\sqrt{2\pi}\delta''(k) \tag{8.9}$$

$$\int dk \delta''(k) f(k) = f''(0) \tag{8.10}$$

We do not want "distributions" in g^R_ω since it would result in unphysical situations where the response keeps amplifying to infinity. So we insist that any perturbation be adiabatically turned on and off, so the response function has to vanish at $t \to \infty$, this adiabatic process is represented by the factor $e^{-\eta t}$:

$$g^R(t) = g''(t)\theta(t)e^{-\eta t} \tag{8.11}$$

This will ensure that its Fourier Transform converges, if the remaining part of $g^R(t)$ is at least not increasing exponentially (which should never happen physically). Equivalently, this could be considered as a modified Fourier Transform of $g''(t)$ with lower bound set to zero and $\omega \to \omega + i\eta$:

$$g^R_\omega = \int_0^{\infty} dt g''(t) e^{i(\omega+i\eta)t} \tag{8.12}$$

As we shall see in the Kramer Kronig relation section, we will arrive at the Fourier Transform of such a class of functions

$$\begin{aligned} \chi^R(t) &= 2i\chi''(t)\theta(t)e^{-\eta t} \\ \chi^R(\omega) &= \int \frac{d\omega'}{\pi} \frac{\chi''(\omega')}{\omega' - (\omega + i\eta)} \end{aligned} \tag{8.13}$$

8.2 Symmetry properties of H and symmetry of the response functions

The quantity $\chi''_{A_iA_j}(t-t')$ contains all the non-trivial information on the response. Indeed, the causal response is simply obtained by multiplying by a trivial $\theta(t-t')$ function. Certain symmetries of this response function depend on the particular symmetry of the Hamiltonian, others are quite general. We begin with properties that depend on the symmetry of H.

Let S be a symmetry of H, then

$$[H, S] = 0 \tag{8.14}$$

in the context of statistical mechanics, we say a system has symmetry S when it commute with the density matrix

$$[\varrho, S] = 0 \tag{8.15}$$

S is in general unitary or antiunitary. To extract non-trivial consequences of the existence of a symmetry, note that the cyclic property of the trace allows us to act on the operators instead of on the basis functions. In other words, we have

$$\langle\mathcal{O}\rangle = \mathrm{Tr}[\rho\mathcal{O}] = \mathrm{Tr}\left[S\varrho S^{-1}\mathcal{O}\right] = \mathrm{Tr}\left[\varrho S^{-1}\mathcal{O}S\right] \tag{8.16}$$

so we have

$$\left\langle S^{-1}\mathcal{O}S\right\rangle = \langle\mathcal{O}\rangle \tag{8.17}$$

It is because S and $\mathcal{O}$ in general do not commute that the above equation leads to non-trivial consequences. When two different operators are involved in the expectation value, as will be the case below for χ'', note that

$$\left\langle S^{-1}\mathcal{O}_1\mathcal{O}_2 S\right\rangle = \left\langle \left(S^{-1}\mathcal{O}_1 S\right)\left(S^{-1}\mathcal{O}_2 S\right)\right\rangle \tag{8.18}$$

which is valid even if $\mathcal{O}_1$ and $\mathcal{O}_2$ are not at the same time since by hypothesis S commutes with H and hence with the time-evolution operator.

Let us look in turn at the consequences of translational invariance and of invariance under a parity transformation $\mathbf{r}_\alpha \to -\mathbf{r}_\alpha$.

8.2.1 Translational invariance

When there is translational invariance, it means that if all operators are translated by $\mathbf{R}$, the thermal averages are unchanged. In other words,

$$\chi''_{BA}\left(\mathbf{r},t;\mathbf{r}',t'\right) = \chi''_{BA}\left(\mathbf{r}+\mathbf{R},t;\mathbf{r}'+\mathbf{R},t'\right) \tag{8.19}$$

so that χ''_{BA} is a function of $\mathbf{r}-\mathbf{r}'$ only. Since we already know that χ''_{BA} is a function only of $t-t'$, in such cases we write

$$\chi''_{BA}\left(\mathbf{r},t;\mathbf{r}',t'\right) = \chi''_{BA}\left(\mathbf{r}-\mathbf{r}';t-t'\right) \tag{8.20}$$

8.2.2 Parity

Under a parity transformation, operators transform as follows

$$P^{-1}\mathcal{O}(\mathbf{r})P = \varepsilon^P \mathcal{O}(-\mathbf{r}) \tag{8.21}$$

where $\varepsilon^P = \pm 1$. This number is known as the "signature" under parity transformation. That $\varepsilon^P = \pm 1$ is the only possibility for simple operators like density and momentum follows from the fact that applying the parity operation twice is the same as doing nothing. In other words, $P^2 = 1$. To be more specific, $\varepsilon^P_\rho = 1$ for density since under $\mathbf{r}_\alpha \to -\mathbf{r}_\alpha$ for every particle coordinate in the first quantization form

$$\rho(\mathbf{r}) = \sum_{\alpha=1}^{N} e_\alpha \delta\left(\mathbf{r}-\mathbf{r}_\alpha\right) \tag{8.22}$$

results in

$$P^{-1}\rho(\mathbf{r})P = \sum_{\alpha=1}^{N} e_\alpha \delta\left(\mathbf{r}+\mathbf{r}_\alpha\right) = \sum_{\alpha=1}^{N} e_\alpha \delta\left(-\mathbf{r}-\mathbf{r}_\alpha\right) = \rho(-\mathbf{r}) \tag{8.23}$$

For the momentum operator, $\varepsilon^P_p = -1$, since in first quantization form

$$\sum_{\alpha=1}^{N} \frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\delta\left(\mathbf{r}-\mathbf{r}_\alpha\right) \tag{8.24}$$

$$P^{-1}\mathbf{p}(\mathbf{r})P = \sum_{\alpha=1}^{N} -\frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\delta\left(\mathbf{r}+\mathbf{r}_\alpha\right) = \sum_{\alpha=1}^{N} \frac{\hbar}{i}\nabla_{\mathbf{r}_\alpha}\delta\left(-\mathbf{r}-\mathbf{r}_\alpha\right) = -\mathbf{p}(-\mathbf{r}) \tag{8.25}$$

In general then, this implies that

$$\chi''_{BA}\left(\mathbf{r},t;\mathbf{r}',t'\right) = \varepsilon^P_B\varepsilon^P_A\chi''_{BA}\left(-\mathbf{r},t;-\mathbf{r}',t'\right) \tag{8.26}$$

When we also have translational invariance, the last result means that $\chi''_{BA}(\mathbf{r}-\mathbf{r}';t-t')$ is even or odd in $\mathbf{r}-\mathbf{r}'$ depending on whether the operators have the same or opposite signatures under parity. Correspondingly, the Fourier transform in the translationally invariant case is odd or even, as can easily be proven by a change of integration variables in the Fourier transform

$$\chi''_{BA}\left(\mathbf{q};t-t'\right) = \varepsilon^P_B\varepsilon^P_A\chi''_{BA}\left(-\mathbf{q};t-t'\right) \tag{8.27}$$

8.2.3 Time-reversal symmetry

Time-reversal symmetry in the absence of spin is represented by complex conjugation for the wave function and by the transpose for operators. We can easily guess the time reversal transformation to an operator by knowing the classical limit. To take simple cases, position does not change but velocity and momentum change sign. To achieve the latter result with the momentum density operator

$$\mathbf{p}(\mathbf{r}) = \sum_{\alpha=1}^{N} \frac{\hbar}{i} \nabla_{\mathbf{r}_\alpha} \delta\left(\mathbf{r} - \mathbf{r}_\alpha\right) \tag{8.28}$$

it appears that complex conjugation suffices. It works because $\mathbf{p}(\mathbf{r})$ is hermitian. Does this mean that for the wave function, the operation of time reversal is simply complex conjugation? The answer is yes, except that in the most general case, there can be an additional unitary operation. Inverting time twice would mean taking the complex conjugate again and hence returning to the original state. If we accept that time reversing an operator is taking its complex conjugate, then H^* should correspond to time reversal of H.

A system in equilibrium obeys time-inversion symmetry, unless an external magnetic field is applied. This means that equilibrium averages evaluated with time-reversed states are equal to equilibrium averages evaluated with the original bases. Let us call T_t the operator that time-reverse a state. This is the operation of complex conjugation that we will call K. Since time-reversal is anti-unitary, we must use Dirac notation with care. Standard operators have associative law

$$\langle\alpha|X|\beta\rangle = \langle\alpha| \quad (X|\beta\rangle) = (\langle\alpha|X) \quad |\beta\rangle \tag{8.29}$$

this is not true of X is complex conjugation operator. Hence, we must absolutely specify if it acts on the right or on the left. Hence, we will write $\underrightarrow{K}$ when we want to take the complex conjugate of a ket, and $\underleftarrow{K}$ to take complex conjugate to a bra.

Time reversal is an antiunitary operation. The key property that differentiates an anti-unitary operator from a unitary one is its action on a linear combination

$$T_t\left(a_1\left|\psi_1\right\rangle + a_2\left|\psi_2\right\rangle\right) = a_1^* T_t\left|\psi_1\right\rangle + a_2^* T_t\left|\psi_2\right\rangle \tag{8.30}$$

Notice also that $T_t^\dagger T_t = \underleftarrow{K}\underrightarrow{K}$ is not equal to 1.

Returning to the action of the time reversal operation on a Shrodinger operator, we see that the expectation value of an arbitrary operator between time reversed states is

$$\langle i|\underleftarrow{K}\mathcal{O}\underrightarrow{K}|j\rangle = (\langle i|\underleftarrow{K})\left(\underrightarrow{K}\mathcal{O}^*|j\rangle\right) = \langle i|\underleftarrow{K}\underrightarrow{K}\left(\mathcal{O}^*|j\rangle\right) = \langle i|\mathcal{O}^*|j\rangle^* = \langle j|\,\mathcal{O}^{*\dagger}\,|i\rangle \tag{8.31}$$

for equilibrium averages

$$\left\langle \underleftarrow{K}\mathcal{O}\underrightarrow{K}\right\rangle = \left\langle \mathcal{O}^{*\dagger}\right\rangle = \varepsilon^t\left\langle \mathcal{O}^\dagger\right\rangle \tag{8.32}$$

The last equality defines the signature of the time-reversal operation for operators. One easily finds that $\epsilon^t = +1$ for position while $\epsilon^t = -1$ for velocity or momentum, etc... Note that $\mathcal{O}^{\dagger *}$ is the transpose of the operator. The signature under complex conjugation can only be ± 1, since applying complex conjugation twice is equivalent to the identity.

We can use this last result to find the effect of the time-reversal invariance on general correlation functions. The action of time reversal gives, when A and B are self-adjoint operators, and in addition the Hamiltonian is real ($\underrightarrow{K}H = H\underrightarrow{K}$)

$$\begin{aligned}
\langle\underleftarrow{K}A(t)B\underrightarrow{K}\rangle &= \langle\underleftarrow{K}e^{iHt}Ae^{-iHt}B\underrightarrow{K}\rangle \\
&= \langle\underleftarrow{K}\underrightarrow{K}e^{-iHt}A^*e^{iHt}B^*\rangle \\
&= \langle e^{-iHt}A^*e^{iHt}B^*\rangle^* \\
&= \left\langle B^*e^{-iHt/\hbar}A^*e^{iHt/\hbar}\right\rangle \\
&= \epsilon_A^t\epsilon_B^t\langle BA(-t)\rangle
\end{aligned} \tag{8.33}$$

In addition to the signature, the order of operators is changed as well as the sign of time. For $\chi''_{A_iA_j}(t-t')$ this immediately leads to

$$\chi''_{A_iA_j}(t-t') = \epsilon^t_{A_i}\epsilon^t_{A_j}\chi''_{A_jA_i}(-t'-(-t)) \tag{8.34}$$

and for the corresponding Fourier transform in frequency,

$$\chi''_{A_iA_j}(\omega) = \epsilon^t_{A_i}\epsilon^t_{A_j}\chi''_{A_jA_i}(\omega) \tag{8.35}$$

Seeing $\chi''_{A_iA_j}(\omega)$ as a matrix in A_iA_j, helps to remember this result a stating that time reversal transposes this matrix and multiplies it by the signature of each of its operators.

8.3 Properties that follow from the definiton

In this section, several exact results are shown, but the one I will use most often is $\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = -\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(-\omega)$. Let us thus write down the general symmetry properties of $\chi''_{A_iA_j}(t-t')$ that simply follow from its definition. These properties are independent of the specific form of the Hamiltonian. It only needs to be Hermitian.

- Commutator: Since it is a commutator

$$\chi''_{A_iA_j}(t-t') = -\chi''_{A_jA_i}(t'-t) \tag{8.36}$$

$$\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega) \tag{8.37}$$

- Hermiticity: Taking the observables as Hermitian, as is the case most of the time (superconductivity leads to an exception), one can use the cyclic property of the trace and the Hermiticity of the density matrix to show that

$$\chi''_{A_iA_j}(t-t') = \left[\chi''_{A_jA_i}(t'-t)\right]^* \tag{8.38}$$

$$\chi''_{A_iA_j}(\omega) = \left[\chi''_{A_jA_i}(\omega)\right]^* \tag{8.39}$$

  In other words, seen as a matrix in the indices A_i, A_j, the matrix $\chi''_{A_iA_j}(\omega)$ is hermitian at all frequencies.

As an example of the use of the last equation, consider $\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega)$ for density response. We obtain the equality $\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) = \left[\chi''_{\rho_{\mathbf{r}'}\rho_{\mathbf{r}}}(\omega)\right]^*$. Taking Fourier transforms in space, this implies that this response function, measurable through energy-loss electron spectroscopy, is real:

$$\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega) = \left[\chi''_{\rho_{\mathbf{q}}\rho_{-\mathbf{q}}}(\omega)\right]^* \tag{8.40}$$

this could be seen from

$$\begin{aligned}
\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}(\omega) &= \int \frac{d\mathbf{p}d\mathbf{p}'}{(2\pi)^6} e^{i(\mathbf{p}\cdot\mathbf{r}+\mathbf{p}'\cdot\mathbf{r}')}\chi''_{\rho_{\mathbf{p}}\rho_{\mathbf{p}'}}(\omega) \\
&= \int \frac{d\mathbf{p}d\mathbf{p}'}{(2\pi)^6} e^{i(\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')+(\mathbf{p}+\mathbf{p}')\cdot\mathbf{r}')}\chi''_{\rho_{\mathbf{p}}\rho_{\mathbf{p}'}}(\omega) \\
&= \int \frac{d\mathbf{p}d\mathbf{p}'}{(2\pi)^6} e^{i(\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')+(\mathbf{p}+\mathbf{p}')\cdot\mathbf{r}')}\chi''_{\rho_{\mathbf{p}}\rho_{\mathbf{p}'}}(\omega)(2\pi)^3\delta(\mathbf{p}+\mathbf{p}') \\
&= \int \frac{d\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')}\chi''_{\rho_{\mathbf{p}}\rho_{-\mathbf{p}}}(\omega)
\end{aligned} \tag{8.41}$$

In the second to the third step, we treat the variables of Fourier Transform as $(\mathbf{r}-\mathbf{r}', \mathbf{r}') \to (\mathbf{p}, \mathbf{p}+\mathbf{p}')$. Since $\chi''_{\rho_{\mathbf{r}}\rho_{\mathbf{r}'}}$ depends on $\mathbf{r}-\mathbf{r}'$ only instead of $\mathbf{r}'$, $\chi''_{\rho_{\mathbf{p}}\rho_{\mathbf{p}'}}$ must be a delta function of $\mathbf{p}+\mathbf{p}'$. To see the exact argument, take $f(x_1, x_2) = \tilde{f}(x_1)$ which only depends on x_1, and perform two Fourier Transforms

$$\begin{aligned}
f(k_1, k_2) &= \int dx_1 e^{-ik_1x_1} \int dx_2 e^{-ik_2x_2} f(x_1, x_2) \\
&= \int dx_1 e^{-ik_1x_1} \tilde{f}(x_1) \int dx_2 e^{-ik_2x_2} \\
&= f(k_1) \times (2\pi)\delta(k_2)
\end{aligned} \tag{8.42}$$

we see that in this case $f(k_1, k_2) = f(k_1) \times (2\pi)\delta(k_2)$.

Quite generally, using the commutator property and time-reversal symmetry to interchange the two operators, we see that for operators that have the same signature under time reversal

$$\chi''_{A_iA_j}(\omega) = -\chi''_{A_iA_j}(-\omega) \tag{8.43}$$

8.4 Kramer Kronig Relations

Kramer Kronig relations are general to all the response functions which satisfy causality. Here we take a simple example: a damped Harmonic Oscillator

$$m\frac{d^2x}{dt^2} + m\int_{-\infty}^{\infty} dt'\gamma\left(t-t'\right)\frac{dx}{dt'} + kx = F(t) \tag{8.44}$$

$$\left(-\omega^2 - i\omega\gamma(\omega) + \omega_0^2\right)x(\omega) = \frac{1}{m}F(\omega) \tag{8.45}$$

Here, $\gamma(t-t')$ is the retarded response and $\gamma(\omega)$ is its Fourier Transform. If $\gamma(\omega)$ has a real and an imaginary part, the imaginary part will renormalize ω_0 and the real part will give dissipation. The resonance frequency will be modified by both the real and the imaginary parts of $\gamma(\omega)$.

It should be understood that before the analytic continuity, the two functions

$$\gamma_t : \mathbb{R} \to \mathbb{R}, \quad \gamma_\omega : \mathbb{R} \to \mathbb{C} \tag{8.46}$$

after analytic continuity

$$\gamma_t : \mathbb{R} \to \mathbb{R}, \quad \gamma_\omega : \mathbb{C}^{\text{upper-half}} \to \mathbb{C} \tag{8.47}$$

this extension is possible since $\gamma(t) \propto \theta(t)$ so

$$\gamma(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}\gamma(t)dt = \int_{0}^{\infty} e^{i\omega t}\gamma(t)dt \tag{8.48}$$

converge even when ω has a positive imaginary part. Actually, $\gamma(\omega)$ is analytic in the upper complex ω half-plane. We need to prove this in two directions. Consider $\gamma(\omega)$ that is analytic in the upper complex ω half-plane, the integral

$$\gamma(t) = \int_{-\infty}^{\infty} e^{-i\omega t}\gamma(\omega)\frac{d\omega}{2\pi} \tag{8.49}$$

for $t < 0$ can be converted to an integral in the upper half plane, which gives 0 since there are no poles.

Suppose we start from the assumption that $\gamma(t) \propto \theta(t-t')$, then

$$\gamma(\omega) = \int_{0}^{\infty} e^{i\omega t}\gamma(t)dt \tag{8.50}$$

for any ω in the upper half plane, this integral always converge. For this to be true on the real axis, all we need is that the Fourier Transform of $\gamma(t)$ exist. We can assume $\gamma(t) \propto e^{-\eta t}$ where $\eta \to 0^+$. This ensures that there are no poles on the upper half plane.

A function that is analytic in the upper half-pane is called **retarded**, as suggested by the fact that the effect comes after the cause. A function that is analytic in the lower-half plane is called **advanced** because the effect occurs before the cause. Not very physical in the latter case, but mathematically well defined, and even useful as we shall see.

Using analyticity in the upper half-plane, we can derive the Kramers-Kronig relations:

$$\oint \frac{d\omega'}{2\pi}\frac{\gamma(\omega')}{\omega'-\omega} = 0 \tag{8.51}$$

where we assume $\gamma(\omega = \infty) = 0$ (if not, replace $\gamma(\omega')$ by $\gamma(\omega') - \gamma(\infty)$). The integral vanish on the contour illustrated in (Andre Fig. (2-2)). Indeed, the contour has two parts, and assuming that $\gamma(\omega')$ vanishes at least like a small power of ω' in the upper half-plane, the two parts add up to zero since we can complete the contour in the upper half-plane and there is no singularity there.

The contour on the infinitesimal half-circle is $-\frac{i}{2}\gamma(\omega)$, and we have thus

$$\mathcal{P}\int_{-\infty}^{\infty}\frac{\gamma(\omega')}{\omega'-\omega}\frac{d\omega'}{2\pi} - \frac{i}{2}\gamma(\omega) = 0 \tag{8.52}$$

now write $\gamma(\omega) = \gamma'(\omega) + i\gamma''(\omega)$ (Notice that we use $\prime, \prime\prime$ for the real and imaginary part of $\gamma(\omega)$, and that "imaginary part" and Fourier Transform do not commute). We have the Kramer-Kronig relations

$$\begin{aligned} \mathcal{P}\int_{-\infty}^{\infty} \frac{\gamma''(\omega')}{\omega' - \omega}\frac{d\omega'}{\pi} &= \gamma'(\omega) \\ -\mathcal{P}\int_{-\infty}^{\infty} \frac{\gamma'(\omega')}{\omega' - \omega}\frac{d\omega'}{\pi} &= \gamma''(\omega) \end{aligned} \tag{8.53}$$

This is a very important result that applies to all causal response functions, such as optical conductivity, impedance of an electrical circuit. It means that if I know for all frequencies either the real or the imaginary part of a response functions, I can find the missing one with the Kramers-Kronig relations.

In practice, if we know $\gamma''(\omega)$, we don't want to evaluate $\mathcal{P}$ integrals. A smart way to do this is by defining the **spectral representation**

$$\gamma(z) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi}\frac{\gamma''(\omega')}{\omega' - z} \tag{8.54}$$

where z is complex. (is the domain $\gamma_z : \mathbb{C} - \mathbb{R} \to \mathbb{C}$?) If we can calculate $\gamma(z)$, we can then directly recover $\gamma^R(\omega)$

$$\gamma^R(\omega) = \lim_{\eta\to 0}\gamma(\omega + i\eta) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi}\frac{\gamma''(\omega')}{\omega' - (\omega + i\eta)} \tag{8.55}$$

to see this, use the Sokhatsky-Weierstrass formula

$$\lim_{\eta\to 0^+}\frac{1}{\omega \pm i\eta} = \mathcal{P}\left(\frac{1}{\omega}\right) \mp i\pi\delta(\omega) \tag{8.56}$$

$$\begin{aligned} \lim_{\eta\to 0^+}\gamma(z = \omega + i\eta) &= \lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\gamma''(\omega')}{\omega' - \omega - i\eta} \\ &= \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\gamma''(\omega')\left[\mathcal{P}\frac{1}{\omega' - \omega} + i\pi\delta(\omega' - \omega)\right] \\ &= \mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\gamma''(\omega')}{\omega' - \omega} + i\gamma''(\omega) \\ &= \gamma'(\omega) + i\gamma''(\omega) \\ &= \gamma(\omega) \end{aligned} \tag{8.57}$$

correspondingly, the advanced function is

$$\gamma^A(\omega) = \lim_{\eta\to 0^+}\gamma(\omega - i\eta) \tag{8.58}$$

It has poles only in the upper half of the complex plane because $\gamma''(\omega)$ in the spectral representation is real. This function is acausal, in other words, the effect always happen before the cause.

Given the retarded response function in spectral representation

$$\gamma^R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi}\frac{\gamma''(\omega')}{\omega' - (\omega + i\eta)} \tag{8.59}$$

we can performa Fourier Transform to recover the real-time correlation function

$$\begin{aligned} \gamma(t) &= \int \frac{d\omega}{(2\pi)}e^{-i\omega t}\gamma^R(\omega) \\ &= -\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\gamma''(\omega')\int_{-\infty}^{\infty}\frac{d\omega}{(2\pi)}\frac{e^{-i\omega t}}{\omega - (\omega' - i\eta)} \\ &= i\theta(t)\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\gamma''(\omega')\mathrm{Res}\left[\frac{e^{-i\omega t}}{\omega - (\omega' - i\eta)}, \omega = \omega' - i\eta\right] \\ &= i\theta(t)\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\gamma''(\omega')e^{-i(\omega' - i\eta)t} \\ &= 2i\theta(t)e^{-\eta t}\gamma''(t) \end{aligned} \tag{8.60}$$

if $t < 0$, we can close a contour in the upper half plane, which doesn't have a pole, so $\gamma(t < 0) = 0$. For $t > 0$, we close the contour in the lower half plane, which has a residue at $\omega' - i\eta$. We see that the the spectral representation include all the nice properties that a response function should have.

8.4.1 General Response functions

The fact that there is a Heaviside $\theta(t-t')$ function implies that the Fourier transform of $\chi^R_{A_iA_j}(t-t')$ cannot have any pole in the complex upper half-plane of frequency because of the exponential. Conversely, analyticity of $\chi^R_{A_iA_j}(\omega)$ implies that in time there is a $\theta(t-t')$ function. Analyticity of the response $\chi^R_{A_iA_j}(\omega)$ in the upper half-plane and the contour shown in (Andre's notes Fig. (22)) that avoids the singularity on the real axis implies that if we define $\chi^R_{A_iA_j}(\omega) = \Re\chi^R_{A_iA_j}(\omega) + i\Im\chi^R_{A_iA_j}(\omega)$ then the Kramers-Kronig relation follow:

$$\begin{aligned}\Re\chi^R_{A_iA_j}(\omega) &= \mathcal{P}\int\frac{d\omega'}{\pi}\frac{\Im\chi^R_{A_iA_j}(\omega)}{\omega'-\omega}\\ \Im\chi^R_{A_iA_j}(\omega) &= -\mathcal{P}\int\frac{d\omega'}{\pi}\frac{\Re\chi^R_{A_iA_j}(\omega)}{\omega'-\omega}\end{aligned} \tag{8.61}$$

8.4.2 Summary

We can identify The Fourier Transform pairs for a generalized retarded susceptibility

$$\begin{aligned}\chi^R(t) &= 2i\chi''(t)\theta(t)e^{-\eta t}\\ \chi^R(\omega) &= \int\frac{d\omega'}{\pi}\frac{\chi''(\omega')}{\omega'-(\omega+i\eta)}\end{aligned} \tag{8.62}$$

We know that $\chi''(\omega)$ has no poles in the upper half plane. From our knowledge of the infinite coupled-harmonic oscillator, we know that there could be many poles in the lower half plane, so many that they merge into branch cuts. Depending on how far these poles are from the real axis (which depends on the universal small damping coefficient η) and depending how strong (coupling strength) they are, they will affect $\chi''(\omega)$ in the real axis. $\chi''(\omega')$ in the real axis then affect $\chi^R(\omega)$ in the way expressed above. We see that the value of $\chi^R(\omega)$ is determined mainly by $\chi''(\omega')$ around ω, and we can treat $\chi^R(\omega)$ in a sense as a "**smoothing**" of $\chi''(\omega)$ in the real axis.

From another angle, we can claim that we've found an inverse of the $\Im$ operator

$$\begin{aligned}[\Im]\left[\int\frac{d\omega'}{-\pi}\frac{\cdot(\omega')}{\omega'-\omega+i\eta}\right] &= 1_{\mathbb{R}}\\ \left[\int\frac{d\omega'}{-\pi}\frac{\cdot(\omega')}{\omega'-\omega+i\eta}\right][\Im] &= 1_{\mathbb{C},\mathrm{R}}\end{aligned} \tag{8.63}$$

both identities work in frequency space. $1_{\mathbb{R}}$ represent identity operator on real functions, such as $A(\omega)$, $1_{\mathbb{C},R}$ represent identity operator on complex retarded functions in frequency space, such as $G^R(\omega)$.

More concretely, this is

$$\begin{aligned}\int\frac{d\omega'}{-\pi}\left(\Im\frac{1}{\omega'-\omega+i\eta}\right)A(\omega') &= A(\omega)\\ \int\frac{d\omega'}{-\pi}\frac{\Im G^R(\omega')}{\omega'-\omega+i\eta} &= A(\omega)\end{aligned} \tag{8.64}$$

the first equation need only Sokhatsky-Weierstrass formula to prove, while the second need both SW formula and Kramer Kronig relation.

8.5 Spectral representation

It is instructive to perform a derivation of Kramers-Kronig relations that starts from our explicit expression for the susceptibility in terms of χ''. By definition, we can write

$$\chi^R_{A_iA_j}(t-t')\,e^{-\eta(t-t')} = 2i\chi''_{A_iA_j}(t-t')\,\theta(t-t')\,e^{-\eta(t-t')} \tag{8.65}$$

where the factor $e^{-\eta(t-t')}$ ensures that the effect of a perturbation at time t' will eventually vanish after long enough time $t-t'$. (we will take $\eta\to 0^+$ at the end). Here, however $\Im\chi^R_{A_iA_j}(\omega) \neq \chi''_{A_iA_j}(\omega)$ in general.

$$\chi^R_{A_iA_j}(\omega) = \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-(\omega+i\eta)} \tag{8.66}$$

The Fourier Transform of this function gives back the first equation. This is true no matter $\chi''_{A_iA_j}(\omega')$ is real or imaginary. The spectral function is

$$\chi_{A_iA_j}(z) = \int \frac{d\omega'}{\pi} \frac{\chi''_{A_iA_j}(\omega')}{\omega' - z} \tag{8.67}$$

The retarded and advanced responses are then

$$\chi^R_{A_iA_j}(\omega) = \lim_{\eta\to 0} \chi_{A_iA_j}(z)\Big|_{z=\omega+i\eta} \tag{8.68}$$

$$\chi^A_{A_iA_j}(\omega) = \lim_{\eta\to 0} \chi_{A_iA_j}(z)\Big|_{z=\omega-i\eta} \tag{8.69}$$

$\chi_{A_iA_j}(z)$ is a function which is equal to $\chi^R_{A_iA_j}(\omega)$ for z infinitesimally above the real axis, and to $\chi^A_{A_iA_j}(\omega)$ for z infinitesimally below the real axis. On the real axis of the complex z plane $\chi_{A_iA_j}(z)$ has a cut whenever $\chi''_{A_iA_j}(\omega) \neq 0$ since, using the Sokhatsky Weirstrass formula

$$\begin{aligned} \left[\chi_{A_iA_j}(\omega + i\eta) - \chi_{A_iA_j}(\omega - i\eta)\right] &= 2i\chi''_{A_iA_j}(\omega) \\ \chi^R_{A_iA_j}(\omega) - \chi^A_{A_iA_j}(\omega) &= 2i\chi''_{A_iA_j}(\omega) \end{aligned} \tag{8.70}$$

8.6 Positivity of $\omega\chi''(\omega)$ and dissipation

The proof of this section essentially follows the steps used for the simple harmonic oscillator. We want to show that the key function of the previous discussion, namely $\chi''_{A_iA_j}(\omega)$, contains all the information on the **dissipation**. Since stability of a thermodynamic system implies that an external applied field of any frequency must do work, the dissipation must be positive, which in turns means, as we now demonstrate, that $\omega\chi''_{A_iA_j}(\omega)$ is a positive-definite matrix.

Since the change in the energy of the system due to the external perturbation is given by the perturbation Hamiltonian $\delta\mathcal{H}$

$$\delta\mathcal{H}(t) \equiv -\int d^3r A_i(\mathbf{r}) a_i(\mathbf{r}, t) \tag{8.71}$$

the power dissipated by the external force is

$$\frac{dW}{dt} = \frac{d\delta\mathcal{H}(t)}{dt} = -\int d^3r A_i(\mathbf{r}) \frac{da_i(\mathbf{r}, t)}{dt} = -A_i \frac{da_i(t)}{dt} \tag{8.72}$$

In the last equality, we have used our short-hand notation and included position in the index i. The integral over $\mathbf{r}$ then becomes a sum over i which is not written explicitly since we take the convention that repeated indices are summed over. Taking the expectation value in the presence of the external perturbation, we find

$$\frac{dW}{dt} = -\left[\langle A_i\rangle + \langle \delta A_i\rangle\right] \frac{da_i(t)}{dt} \tag{8.73}$$

where $\langle A_i\rangle$ is the equilibrium expectation value, and $\langle \delta A_i\rangle$ the linear response. In a time period

$$\bar{W} = -\int_{-T/2}^{T/2} dt \left\langle \delta A_i(t)\right\rangle \frac{da_i(t)}{dt} \tag{8.74}$$

where the equilibrium part is dropped since $\langle A_i\rangle$ is t-independent. Taking $T \to \infty$ and using Parseval's theorem, we have

$$\begin{aligned} \bar{W} &= -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left\langle \delta A_i(\omega)\right\rangle (i\omega) a_i(-\omega) \\ &= -i\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega\chi^R_{A_iA_j}(\omega) a_i(-\omega) a_j(\omega) \end{aligned} \tag{8.75}$$

Changing dummy indices as follows, $\omega \to -\omega, i \to j, j \to i$ and adding the new expression to the old one, we obtain the requirement,

$$\bar{W} = -i\frac{1}{2}\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega \left[\chi^R_{A_iA_j}(\omega) - \chi^R_{A_jA_i}(-\omega)\right] a_j(\omega) a_i(-\omega) \tag{8.76}$$

spectral representation gives

$$\begin{aligned}
\chi^R_{A_iA_j}(\omega) - \chi^R_{A_jA_i}(-\omega) &= \int \frac{d\omega'}{\pi}\left[\frac{\chi''_{A_iA_j}(\omega')}{\omega' - (\omega + i\eta)} - \frac{\chi''_{A_jA_i}(\omega')}{\omega' - (-\omega + i\eta)}\right] \\
&= \int \frac{d\omega'}{\pi}\left[\frac{\chi''_{A_iA_j}(\omega')}{\omega' - (\omega + i\eta)} - \frac{-\chi''_{A_iA_j}(-\omega')}{\omega' - (-\omega + i\eta)}\right] \\
&= \int \frac{d\omega'}{\pi}\left[\frac{\chi''_{A_iA_j}(\omega')}{\omega' - (\omega + i\eta)} - \frac{\chi''_{A_iA_j}(\omega')}{\omega' - (\omega - i\eta)}\right] \\
&= \chi^R_{A_iA_j}(\omega) - \chi^A_{A_iA_j}(\omega) \\
&= 2i\chi''_{A_iA_j}(\omega)
\end{aligned} \tag{8.77}$$

so we have,

$$\bar{W} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} a_i^*(\omega)\left(\omega\chi''_{A_iA_j}(\omega)\right) a_j(\omega) \tag{8.78}$$

where $a_i(-\omega) = a_i^*(\omega)$ since $a_i(t)$ is real.

We require that any perturbation must dissipate energy for a thermal equilibrium, so $\bar{W} > 0$ for any list of functions a_i at any frequency, this means that each frequency mode must be positive

$$a_i^*(\omega)\left(\omega\chi''_{A_iA_j}(\omega)\right) a_j(\omega) > 0 \tag{8.79}$$

for all frequencies. If A_i, A_j are Hermitian, then $\chi''_{A_iA_j} = \left[\chi''_{A_jA_i}(\omega)\right]^*$ is a Hermitian matrix in index i, j, so its eigenvalues are real. Going to the basis where $\chi''_{A_iA_j}$ is diagonal, we see that the previous equation implies that all the eigenvalues must be positive. So $\omega\chi''_{A_iA_j}$ must be a positive definite matrix in i, j.

In particular, when there is only one kind of external perturbation applied,

$$\chi''_{A_iA_i}(\omega)\omega > 0 \tag{8.80}$$

so any "self-susceptibility" satisfies the same positivity condition as harmonic oscillators.

8.7 Summary of the analytic properties

We summarize the results of the last few sections that concern χ''. In the first row, we explicitly write the $\mathbf{r}, \mathbf{r}'$ dependence, in the second rwo we take the space fourier transform and in the rest the spatial indices are hidden in the indicies i and j appearing with A_i. $\epsilon^t_{A_i}$ is the signature under time reversal of the operator A_i, while $\epsilon^P_{A_i}$ is the signature under parity of the operator A_i.

Table 8.1: Summary of the analytic properties of the spectral function

Basic Property	Implies for χ''
H is invariant under translation	$\chi''_{BA}(\mathbf{r}, t; \mathbf{r}', t') = \chi''_{BA}(\mathbf{r} - \mathbf{r}'; t - t')$
H is invariant under parity	$\chi''_{BA}(\mathbf{q}; \omega) = \varepsilon^P_B \varepsilon^P_A \chi''_{BA}(-\mathbf{q}; \omega)$
H is invariant under time reversal	$\chi''_{A_iA_j}(\omega) = \epsilon^t_{A_i}\epsilon^t_{A_j}\chi''_{A_jA_i}(\omega)$
χ'' is a commutator	$\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega)$
χ'' contains hermitian operators only	$\chi''_{A_iA_j}(\omega) = \left[\chi''_{A_jA_i}(\omega)\right]^*$
positivity of dissipation	$\chi''_{A_iA_j}(\omega)$ is a positive definite matrix

8.8 Fluctuation Dissipation Theorem

Fluctuation dissipation theory is a very useful theorem relating linear response to equilibrium fluctuation measured in scattering experiments. Here I give the derivation in the general quantum case. It takes the form,

$$S_{A_iA_j}(\omega) = \frac{2\hbar}{1 - e^{-\beta\hbar\omega}}\chi''_{A_iA_j}(\omega) = 2\hbar\left(1 + n_B(\omega)\right)\chi''_{A_iA_j}(\omega) \tag{8.81}$$

where $n_B(\omega) = 1/\left(e^{\beta\hbar\omega} - 1\right)$ is the Bose factor. The "structure factor" or correlation function $S_{A_iA_j}(\omega)$ is defined by,

$$S_{A_iA_j}(t) \equiv \langle A_i(t)A_j\rangle - \langle A_i\rangle\langle A_j\rangle = \langle (A_i(t) - \langle A_i\rangle)(A_j(0) - \langle A_j\rangle)\rangle \equiv \langle \delta A_i(t)\delta A_j\rangle \tag{8.82}$$

Note that the fluctuations are with respect to an equilibrium system, and we are not adding any external potential, so H is time-independent, thus $\langle A_i(t)\rangle = \langle A_i(0)\rangle = \langle A_i\rangle$. This is a key theorem of statistical physics.

To prove the theorem, it suffice to trivially relate the definitions

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\langle [A_i(t), A_j]\rangle = \frac{1}{2\hbar}\langle [\delta A_i(t), \delta A_j]\rangle = \frac{1}{2\hbar}\left(S_{A_iA_j}(t) - S_{A_jA_i}(-t)\right) \tag{8.83}$$

then to use the key following identity that we set to prove,

$$S_{A_jA_i}(-t) = S_{A_iA_j}(t - i\hbar\beta) \tag{8.84}$$

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\left(S_{A_iA_j}(t) - S_{A_iA_j}(t - i\hbar\beta)\right) \tag{8.85}$$

$$\begin{aligned}\chi''_{A_iA_j}(\omega) &= \frac{1}{2\hbar}\left(S_{A_iA_j}(\omega) - \int dt e^{i\omega(t+i\hbar\beta)} S_{A_iA_j}(t)\right) \\ &= \frac{1}{2\hbar} S_{A_iA_j}(\omega)\left(1 - e^{-\beta\hbar\omega}\right)\end{aligned} \tag{8.86}$$

and finally, inverting the equation,

$$S_{A_iA_j}(\omega) = 2\hbar\chi''_{A_iA_j}(\omega)\left(1 + n_B(\omega)\right) \tag{8.87}$$

In the integration of $S_{A_iA_j}(t - i\hbar\beta)$, we have moved the integration from $-\infty, +\infty$ to $-\infty - i\hbar\beta, +\infty - i\hbar\beta$. This is valid only when $S_{A_iA_j}(t)$ has no poles inside $-\hbar\beta < \Im t < 0$. This is proved in the next section with Lehmann representation.

We now prove the periodicity condition $S_{A_jA_i}(-t) = S_{A_iA_j}(t - i\hbar\beta)$:

$$\begin{aligned}S_{A_jA_i}(-t) &= Z^{-1}\,\mathrm{Tr}\left[e^{-\beta H}\delta A_j\delta A_i(t)\right] \\ &= Z^{-1}\,\mathrm{Tr}\left[\delta A_i(t)e^{-\beta H}\delta A_j\right] \\ &= Z^{-1}\,\mathrm{Tr}\left[e^{-\beta H}e^{\beta H}\delta A_i(t)e^{-\beta H}\delta A_j\right] \\ &= Z^{-1}\,\mathrm{Tr}\left[e^{-\beta H}\delta A_i(t - i\beta\hbar)\delta A_j\right] \\ &= S_{A_iA_j}(t - i\beta\hbar)\end{aligned} \tag{8.88}$$

8.9 Lehmann representation

(Andre II. correlation functions, general properties, Lehmann representation)

Definition: The function that contain all the information: $\chi''_{A_iA_j}(\omega')$ is called the spectral function. The reason for this name is that $\chi''_{A_iA_j}(\omega')$ contains information on dissipation or, alternatively, on the spectrum of excitations. Hence, in that kind of equations, the response is expressed in terms of the spectrum of excitations. We will also have spectral representations for Green's functions.

In this section, I introduce the **Lehmann representation**. It is extremely useful to prove exact properties of the spectral function and to obtain relations between different kinds of correlation function. For example, here I will show again the fluctuation-dissipation theorem. Later, the relation between retarded functions and their expression in Matsubara frequencies will also be easy to see from the Lehmann representation. That representation also allows us to see the connection with the spectrum of excitations and develop physical intuition, since it express $\chi''_{A_iA_j}(\omega')$ in terms of matrix elements and excitation energies.

I begin with the definition and use the Heisenberg equations of motion and insert a complete set of energy eigenstates so that we find

$$\begin{aligned}\chi''_{A_iA_j}(t) &= \frac{1}{2\hbar}\,\mathrm{Tr}\left[\varrho\left(A_i(t)A_j(0) - A_j(0)A_i(t)\right)\right] \\ &= \frac{1}{2\hbar}\sum_{n,m}\frac{e^{-\beta E_n}}{Z}\left[\left\langle n\left|e^{iE_nt/\hbar}A_ie^{-iE_mt/\hbar}\right|m\right\rangle\langle m\,|A_j|\,n\rangle - \langle n\,|A_j|\,m\rangle\left\langle m\left|e^{iE_mt/\hbar}A_ie^{-iE_nt/\hbar}\right|n\right\rangle\right]\end{aligned} \tag{8.89}$$

Changing dummy indices m and n in the last term, we have

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\sum_{n,m}\frac{e^{-\beta E_n}-e^{-\beta E_m}}{Z}\langle n|A_i|m\rangle\langle m|A_j|n\rangle e^{i(E_n-E_m)t/\hbar} \tag{8.90}$$

The Fourier Transform is

$$\begin{aligned}\chi''_{A_iA_j}(\omega) &= \frac{1}{2\hbar}\sum_{n,m}\frac{e^{-\beta E_n}-e^{-\beta E_m}}{Z}\langle n|A_i|m\rangle\langle m|A_j|n\rangle\int_{-\infty}^{\infty}dt e^{i\frac{t}{\hbar}(\hbar\omega-(E_m-E_n))}\\ &= \sum_{n,m}\frac{e^{-\beta E_n}-e^{-\beta E_m}}{Z}\langle n|A_i|m\rangle\langle m|A_j|n\rangle\pi\delta(\hbar\omega-(E_m-E_n))\\ &= \sum_{n,m}\frac{e^{-\beta E_n}}{Z}\langle n|A_i|m\rangle\langle m|A_j|n\rangle\pi\delta(\hbar\omega-(E_m-E_n))\left(1-e^{-\beta\hbar\omega}\right)\end{aligned} \tag{8.91}$$

Substituting this into the spectral representation we have

$$\chi^R_{A_iA_j}(\omega) = \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-(\omega+i\eta)} \tag{8.92}$$

$$\begin{aligned}\chi_{A_iA_j}(z) &= \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-z}\\ &= \sum_{n,m}\frac{e^{-\beta E_n}-e^{-\beta E_m}}{Z}\frac{\langle n|A_i|m\rangle\langle m|A_j|n\rangle}{E_m-E_n-\hbar z}\end{aligned} \tag{8.93}$$

and the retarded Green's function

$$\begin{aligned}\chi^R_{A_iA_j}(\omega) &= \int\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega'-z}\\ &= \sum_{n,m}\frac{e^{-\beta E_n}-e^{-\beta E_m}}{Z}\frac{\langle n|A_i|m\rangle\langle m|A_j|n\rangle}{E_m-E_n-\hbar(\omega+i\eta)}\end{aligned} \tag{8.94}$$

The poles are indeed simple poles in the lower-half frequency plane, as we wanted to prove. They are just below the real axis, a distance along the imaginary direction. The position of the poles carries information on the excitation energies of the system. The residue at a given pole will depend on the value of $\chi''_{A_iA_j}$ at the corresponding value of the A_i, A_j real coordinate of the pole. The residues tell us how strongly the external probe and system connect the two states. The Lehmann representation reminds us of low order perturbation theory in the external probe.

Note that for $\chi''(\omega)$, $\omega\to-\omega$ is equivalent to exchanging m and n, so we clearly have

$$\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega) \tag{8.95}$$

which we discussed as a consequence of the commutator property.

Bohr's correspondence principle: Consider the diagonal case, $A_i = A_j$. We have seen in Sec.(10.6) that $\chi''_{A_iA_i}(\omega)$ is related to **absorption**. The absorption will occur at energies $\hbar\omega$ that correspond to the difference in energy between eigenstates, $E_m - E_n$, in accord with Bohr's correspondence principle.

Since $\langle n|A|m\rangle\langle m|A|n\rangle$ is equal to $|\langle m|A|n\rangle|^2$ for a Hermitian operator A, it is clear that the spectral weight $\chi''_{A_iA_j}(\omega)$ is positive when $A_i = A_j$. This will be the case when we compute conductivity for example, but this is not the case for thermopower, for example, where the measured quantity A_i is electrical current and the perturbation is a temperature gradient that couples to the energy density A_j.

We can write the correlation function in Lehnmann representation also

$$\begin{aligned}S_{A_iA_i}(t) &= \langle\delta A_i(t)\delta A_j\rangle\\ &= \mathrm{Tr}\left[\varrho\delta A_i(t)\delta A_j\right]\\ &= \sum_n\frac{1}{Z}\langle n|e^{-\beta H}e^{iHt}\delta A_i|m\rangle\langle m|e^{-iHt}\delta A_j|n\rangle\\ &= \sum_n\frac{e^{-\beta E_n}}{Z}e^{i(E_n-E_m)t}\langle n|\delta A_i|m\rangle\langle m|\delta A_j|n\rangle\end{aligned} \tag{8.96}$$

$$S_{A_iA_j}(\omega) = \sum_n \frac{e^{-\beta E_n}}{Z} \langle n| \delta A_i |m\rangle \langle m| \delta A_j |n\rangle 2\pi\delta(\omega - (E_m - E_n)) \tag{8.97}$$

compare this with

$$\chi''_{A_iA_j}(\omega) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} \langle n |A_i| m\rangle \langle m |A_j| n\rangle \pi\delta(\hbar\omega - (E_m - E_n)) \left(1 - e^{-\beta\hbar\omega}\right) \tag{8.98}$$

and notice that we can replace $[A_i, A_j] \to [\delta A_i, \delta A_j]$ so $\chi''_{A_iA_j}(\omega) = \chi''_{\delta A_i \delta A_j}(\omega)$. We have the Fluctuation dissipation theorem directly

$$S_{A_iA_j}(\omega) = 2\hbar(1 + n_B(\omega))\chi''_{A_iA_j}(\omega) \tag{8.99}$$

going back to the fluctuation dissipation section, $S_{A_iA_i}(t)$ is analytic whenever the summation converges. We know that the summation goes over E_n, E_m from the ground state energy to infinity. The convergence can be guarenteed by the exponential factor

$$e^{-\beta E_n} e^{-(E_n - E_m)\Im t} = e^{-(\beta + \Im t)E_n} e^{+E_m \Im t} \tag{8.100}$$

for $\Im t \in (-\beta, 0)$, when both factors are decaying, so there are no poles in $\Im t \in (-\beta, 0)$.

8.10 Sum rules

(Andre II. correlation functions, general properties, Sum rules)

All the many-body Physics of the response or scattering experiments is in the calculation of unequal-time commutators. These commutators in general involve the time evolution of the systems and thus they are non-trivial to evaluate. However, equal-time commutators are easy to evaluate in general using the usual commu- tation relations. Equal-time corresponds to integral over frequency as seen from Fourier space. Hence the name sum rules. We will not in general be able to satisfy all possible sum-rules since this would mean basically an exact solution to the problem, or computing infinite order high-frequency expansion. In brief, sum-rules are useful to

- Relate different experiments to each other
- Establish high frequency limits of correlation functions
- Provide constraints on phenomenological parameters or on approximate theories.

In this section, I show that our formalism is consistent with well known facts in elementary quantum statistical mechanics. Recall that in the grand canonical ensemble, the average number of particles is given by,

$$\langle N\rangle = \mathrm{Tr}\left[e^{-\beta(H-\mu N)}N\right]/Z = Z^{-1}\frac{\partial}{\beta\partial\mu}Z \tag{8.101}$$

$$\begin{aligned}
\left\langle N^2\right\rangle &= Z^{-1}\left(\frac{\partial}{\beta\partial\mu}\right)^2 Z \\
&= Z^{-1}\frac{\partial}{\beta\partial\mu}\left[ZZ^{-1}\frac{\partial}{\beta\partial\mu}Z\right] \\
&= Z^{-1}\frac{\partial}{\beta\partial\mu}\left[Z\langle N\rangle\right] \\
&= Z^{-1}\frac{\partial}{\beta\partial\mu}Z\langle N\rangle + \frac{\partial}{\beta\partial\mu}\langle N\rangle \\
&= \langle N\rangle^2 + \frac{\partial}{\beta\partial\mu}\langle N\rangle
\end{aligned} \tag{8.102}$$

we have

$$\Delta N^2 = \langle N^2\rangle - \langle N\rangle^2 = \frac{1}{\beta}\left(\frac{\partial N}{\partial\mu}\right)_{T,V} \tag{8.103}$$

In a way, this is a relation between fluctuation on the left-hand side, and response on the right-hand side. Let us see if this can be derived from the fluctuation-dissipation theorem.

By definition

$$S_{nn}(\mathbf{r},t) = \langle \delta n(\mathbf{r},t)\delta n(\mathbf{r}=0,t=0)\rangle \tag{8.104}$$

Notice we are doing Fourier Transform in the continuum, where N/V is fixed but $V, N \to \infty$, so here N has the unit of $[N/V]$ and represent the number of particles per unit volume, we effectively set $V = 1$.

$$\begin{aligned}
\Delta N^2 &= \lim_{t\to 0} \langle \delta N(t)\delta N\rangle \\
&= \lim_{t\to 0} \int d^3r d^3r' \, \langle \delta n(\mathbf{r},t)\delta n(\mathbf{r}',t=0)\rangle \\
&= \lim_{t\to 0} \int d^3r d^3r' \, \langle \delta n(\mathbf{r}-\mathbf{r}',t)\delta n\rangle \\
&= \lim_{t\to 0} \int d^3r S_{nn}(\mathbf{r},t) \\
&= \lim_{\mathbf{q}\to 0} \lim_{t\to 0} S_{nn}(\mathbf{q},t) \\
&= \lim_{\mathbf{q}\to 0} \int \frac{d\omega}{2\pi} S_{nn}(\mathbf{q},\omega)
\end{aligned} \tag{8.105}$$

From Lehmann representation,

$$S_{nn}(\mathbf{q},\omega) = \sum_n \frac{e^{-\beta E_n}}{Z} \langle n|\, \delta n \,|m\rangle \langle m|\, \delta n \,|n\rangle \, 2\pi\delta(\omega - (E_m - E_n)) \tag{8.106}$$

as $\mathbf{q} \to 0$, all the weights $\langle n|\, \delta n \,|m\rangle$ will approach zero except those with very small small ω. Using the Fluctuation Dissipation theorem, we can thus Taylor expand $e^{-\beta\hbar\omega}$

$$\lim_{\mathbf{q}\to 0} S_{nn}(\omega) = \lim_{\mathbf{q}\to 0} \frac{2\hbar}{1-e^{-\beta\hbar\omega}} \chi''_{nn}(\omega) = \lim_{\mathbf{q}\to 0} \frac{2\hbar}{\beta\hbar\omega} \chi''_{nn}(\omega) \tag{8.107}$$

We have

$$\langle NN\rangle - \langle N\rangle^2 = \lim_{\mathbf{q}\to 0} \int \frac{d\omega}{2\pi} S_{nn}(\mathbf{q},\omega) = \lim_{\mathbf{q}\to \mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\beta\omega} = \frac{1}{\beta} \left(\frac{\partial N}{\partial \mu}\right)_{T,V} = \frac{1}{\beta}\chi_{nn} \tag{8.108}$$

where χ_{nn} is another susceptibility. Another way to write it is

$$k_B T \chi_{nn} = S_{nn} \tag{8.109}$$

In this form, the density fluctuations are related to the response $(\partial N/\partial\mu)_{T,V}$ (itself related to the compressibility) and we have what is known as the **thermodynamic sum rule**

$$\lim_{\mathbf{q}\to \mathbf{0}} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} = \left(\frac{\partial N}{\partial \mu}\right)_{T,V} = \chi_{nn} \tag{8.110}$$

which in this case is known as the **compressibility sum rule**.

Thermodynamic sum rules can be seen from another point of view. Suppose we compute the linear response to a time-independent perturbation. In addition to the previous example where we looked at the response of the the density to a chem- ical potential shift, another example would be the response of the magnetization to a time-independent magnetic field. This should be the **magnetic susceptibility**. To remain general, I look at the response of operator A_i to the external field a_j coupled to A_j. However, I have to assume that A_i and A_j are **conserved quantities** so that the above assumptions about the limit $\mathbf{q} \to \mathbf{0}$ apply.

Linear response theory gives, at $\omega = 0$

$$\delta \langle A_i(\mathbf{q},\omega=0)\rangle = \chi^R_{A_iA_j}(\mathbf{q},\omega=0) a_j(\mathbf{q},\omega=0) \tag{8.111}$$

Recalling that the thermodynamic derivatives are in general for uniform ($\mathbf{q} = 0$) applied probes, the above formula becomes,

$$\lim_{\mathbf{q}\to\mathbf{0}} \chi^R_{A_iA_j}(\mathbf{q},\omega=0) = \frac{\partial A_i}{\partial a_j} \equiv \chi_{A_iA_j} \tag{8.112}$$

where $\chi_{A_iA_j}$ is the thermodynamic susceptibility. The spectral representation gives

$$\begin{aligned}\chi^R_{A_iA_j}(\mathbf{q},\omega=0) &= \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\mathbf{q},\omega')}{\omega'-i\eta} \\ &= \mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\mathbf{q},\omega')}{\omega'} + i\chi''_{A_iA_j}(\mathbf{q},0)\end{aligned} \tag{8.113}$$

Assuming that A_i, A_j have the same time reversal signature, we have $\chi''_{A_iA_j}(\omega) = \chi''_{A_jA_i}(\omega)$, in addition the commutator property gives $\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega)$, so we have $\chi''_{A_iA_j}(\omega) = -\chi''_{A_iA_j}(-\omega)$ is an odd function. We thus have $\chi''_{A_iA_j}(\omega=0)=0$ and the imaginary part in the above equation vanishes. Physically, this means that there is no zero-frequency dissipation in a stable system. The limit $\lim_{\mathbf{q}\to\mathbf{0}}$ again includes only small frequency transitions. From Lehmann representation, at small ω

$$\begin{aligned}\chi''_{A_iA_j}(\omega) &= \sum_{n,m}\frac{e^{-\beta E_n}}{Z}\langle n|A_i|m\rangle\langle m|A_j|n\rangle\,\pi\delta(\hbar\omega-(E_m-E_n))\left(1-e^{-\beta\hbar\omega}\right) \\ &\to \sum_{n,m}\frac{e^{-\beta E_n}}{Z}\langle n|A_i|m\rangle\langle m|A_j|n\rangle\,\pi\delta(\hbar\omega-(E_m-E_n))\,(\beta\hbar\omega) \\ &\propto \omega\end{aligned} \tag{8.114}$$

so there is no divergence for $\frac{\chi''_{A_iA_j}(\mathbf{q},\omega')}{\omega'}$ as $\omega'\to 0$, and the principle value operator $\mathcal{P}$ is superfluous. So we have the general expression relating the thermodynamic susceptibility $\chi_{A_iA_j}$ to the spectral function $\chi''_{A_iA_j}(\mathbf{q},\omega)$:

$$\chi_{A_iA_j} = \lim_{\mathbf{q}\to\mathbf{0}}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{A_iA_j}(\mathbf{q},\omega)}{\omega} \tag{8.115}$$

$$\chi_{A_iA_j} = \lim_{\mathbf{q}\to\mathbf{0}}\lim_{\omega\to 0}\chi^R_{A_iA_j}(\mathbf{q},\omega). \tag{8.116}$$

For thermodynamic quantities, the $\omega\to 0$ limit is always taken before the $\mathbf{q}\to\mathbf{0}$ limit. It will be the other way around for transport coefficients.

8.10.1 The order of limit for frequency and wavevector

It is extremely important to note that for thermodynamic sum rules, the $\omega\to 0$ limit is taken first, before the $\mathbf{q}\to 0$ limit. The other limit describes transport properties as we shall see. Take as an example of a $\mathbf{q}=\mathbf{0}$ quantity: the total number of particles. Then

$$\chi''_{NN}(t) = \frac{1}{2\hbar}\langle[N(t),N]\rangle = 0 \tag{8.117}$$

This quantity vanishes for all times because N is a conserved quantity independent of time, and it commutes with itself. Taking Fourier transforms, $\chi''_{NN}(\omega)$ vanishes for all frequencies. This implies that for conserved quantities

$$\chi^R_{A_iA_j}(\mathbf{q}=\mathbf{0},\omega) = 0 \tag{8.118}$$

Hence, we must take the $\mathbf{q}\to\mathbf{0}$ limit after the $\omega\to 0$ limit to obtain thermodynamic sum rules.

8.10.2 Moments, sum rules, and their relation to high-frequency expansions

The nth moment of a probability distribution is defined as the average of the random variable to the power n. By analogy, we define the nth moment of the spectral function by $\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^n\chi''_{A_iA_j}(\omega)$. For operators with the same signature under time reversal, even moments vanish while odd moments of $\chi_{A_iA_j}$ are related to equal-time

commutators that are easy to compute, at least formally:

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^n\chi''_{A_iA_j}(\omega) &= \left[\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\left(i\frac{\partial}{\partial t}\right)^n e^{-i\omega t}2\chi''_{A_iA_j}(\omega)\right]_{t=0}\\ &= \left[\left(i\frac{\partial}{\partial t}\right)^n 2\chi''_{A_iA_j}(t)\right]_{t=0}\\ &= \frac{1}{\hbar}\left\langle\left[\left(i\frac{\partial}{\partial t}\right)^n A_i(t),A_j(0)\right]\right\rangle_{t=0}\\ &= \frac{1}{\hbar}\left\langle\left[\left[\left[A_i(t),\frac{H}{\hbar}\right],\frac{H}{\hbar}\right]\ldots,A_j(0)\right]\right\rangle_{t=0}\end{aligned} \tag{8.119}$$

This may all easily be computed through n equal-time commutations with the Hamiltonian.

These moments determine the high frequency behavior of response functions. One does expect that high frequencies are related to short times, and if time is short enough it is natural that commutators be involved. Let us see this. Suppose the spectrum of excitations is bounded, as usually happens when the input momentum $\mathbf{q}$ is finite. Then, $\chi''_{A_iA_j}(\omega')=0$ for $\omega'>\Lambda$ where Λ is some large frequency. Then, for $\omega>\Lambda$, we can expand the denominator since the condition $\omega'/\omega\ll 1$ will always be satisfied within the integration range. This gives us a high-frequency expansion,

$$\begin{aligned}\chi^R_{A_iA_j}(\mathbf{q},\omega) &= \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\mathbf{q},\omega')}{\omega'-\omega-i\eta}\\ &\approx \sum_{n=1}^{\infty}\frac{-1}{\omega^{2n}}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}(\omega')^{2n-1}\chi''_{A_iA_j}(\mathbf{q},\omega')\end{aligned} \tag{8.120}$$

where we have assumed that we are in a situation where $\chi''_{A_iA_j}$ is odd, which implies that only odd moments of $\chi''_{A_iA_j}$ do not vanish. Clearly, in the $\omega\to\infty$ limit, the susceptibilities in general scale as $1/\omega^2$, a property we will use later in the context of analytic continuations.

The f-sum rule is one of the most widely used moment of a correlation function, particularly in the context of optical conductivity experiments. It is quite remarkable that this sum rule does not depend on interactions, so it should be valid independently of many details of the system. If we now focus on the first term of the high-frequency expansion, we have

$$\chi^R_{nn}(\mathbf{q},\omega)\approx\frac{-1}{\omega^2}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\omega'\chi''_{nn}(\mathbf{q},\omega')+\ldots=-\frac{n\mathbf{q}^2}{m\omega^2}+\ldots \tag{8.121}$$

This is equivalent to saying that at very high frequency the system reacts as if it was composed of free particles. It is the inertia that determines the response, like for a harmonic oscilator well above the resonance frequency. Let us derive that sum rule, which is basically a consequence of particle conservation. When the potential-energy part of the Hamiltonian commutes with the density operator, while the kinetic-energy part is that of free electrons (not true for tight-binding electrons) we find that

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega)=\frac{n\mathbf{q}^2}{m} \tag{8.122}$$

this is the f-sum rule, valid for any value of the momentum $\mathbf{q}$.

Using translation invariance we can write

$$\int d(\mathbf{r}-\mathbf{r}')e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}f(\mathbf{r}-\mathbf{r}')=\frac{1}{\mathcal{V}}\int d\mathbf{r}e^{-i\mathbf{q}\cdot r}\int d\mathbf{r}'e^{+i\mathbf{q}\cdot r'}f(\mathbf{r}-\mathbf{r}') \tag{8.123}$$

from the commutator expansion we have

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega) &= -\frac{1}{\hbar^2\mathcal{V}}\langle[[H,n_{\mathbf{q}}(t)],n_{-\mathbf{q}}(t)]\rangle\\ &= -\frac{1}{\hbar^2\mathcal{V}}\langle[[H,n_{\mathbf{q}}],n_{-\mathbf{q}}]\rangle\end{aligned} \tag{8.124}$$

We now calculate this commutator:

$$\begin{aligned} n_{\mathbf{q}} &= \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} n(\mathbf{r}) \\ &= \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \psi^\dagger_\sigma(\mathbf{r})\psi_\sigma(\mathbf{r}) \\ &= \frac{1}{V}\sum_{\mathbf{q}_1,\mathbf{q}_2} a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_2\sigma} \int d\mathbf{r} e^{i(\mathbf{q}_1-\mathbf{q}_2-\mathbf{q})\cdot\mathbf{r}} \\ &= \sum_{\mathbf{k}} a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}\sigma} \end{aligned} \tag{8.125}$$

where we used

$$\begin{aligned} a^\dagger_{\mathbf{p}} &= \int d^3r \frac{e^{-i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}} \psi^\dagger(\mathbf{r}) \\ f_{\mathbf{q}} &= \int d^3r f(\mathbf{r}) \mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}} \\ f(\mathbf{r}) &= \frac{1}{V}\sum_{\mathbf{q}} \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}} f_{\mathbf{q}} \end{aligned} \tag{8.126}$$

Now, The Hamiltonian is

$$H = \sum_{\mathbf{p}} (\frac{\mathbf{p}^2}{2m} - \mu) a^\dagger_{\mathbf{p}\alpha} a_{\mathbf{p}\alpha} \tag{8.127}$$

so the commutator

$$\begin{aligned} [H, n_{\mathbf{q}}] &= \sum_{\mathbf{p},\mathbf{k}} (\frac{\mathbf{p}^2}{2m} - \mu) \left[a^\dagger_{\mathbf{p}\alpha} a_{\mathbf{p}\alpha}, a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}\sigma} \right] \\ &= \sum_{\mathbf{p},\mathbf{k}} (\frac{\mathbf{p}^2}{2m} - \mu) \left(a^\dagger_{\mathbf{p}\alpha} a_{\mathbf{k}\alpha} \delta_{\mathbf{p},\mathbf{k}+\mathbf{q}} - a^\dagger_{\mathbf{k}+\mathbf{q}\alpha} a_{\mathbf{p}\alpha} \delta_{\mathbf{p},\mathbf{k}} \right) \\ &= \sum_{\mathbf{p}} (\frac{\mathbf{p}^2}{2m} - \mu) \left(a^\dagger_{\mathbf{p}\alpha} a_{\mathbf{p}-\mathbf{q}\alpha} - a^\dagger_{\mathbf{p}+\mathbf{q}\alpha} a_{\mathbf{p}\alpha} \right) \end{aligned} \tag{8.128}$$

$$\left[a^\dagger_{\mathbf{p}\alpha} a_{\mathbf{p}\alpha}, a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}\sigma} \right] = a^\dagger_{\mathbf{p}\alpha} a_{\mathbf{k}\alpha} \delta_{\mathbf{p},\mathbf{k}+\mathbf{q}} - a^\dagger_{\mathbf{k}+\mathbf{q}\alpha} a_{\mathbf{p}\alpha} \delta_{\mathbf{p},\mathbf{k}} \tag{8.129}$$

Now

$$\begin{aligned} [[H, n_{\mathbf{q}}], n_{-\mathbf{q}}] &= \sum_{\mathbf{p},\mathbf{k}} (\frac{\mathbf{p}^2}{2m} - \mu) \left[a^\dagger_{\mathbf{p}\alpha} a_{\mathbf{p}-\mathbf{q}\alpha} - a^\dagger_{\mathbf{p}+\mathbf{q}\alpha} a_{\mathbf{p}\alpha}, a^\dagger_{\mathbf{k}-\mathbf{q}\sigma} a_{\mathbf{k}\sigma} \right] \\ &= \sum_{\mathbf{p},\mathbf{k}} (\frac{\mathbf{p}^2}{2m} - \mu) \left(\delta_{k-q,p-q} a^\dagger_p a_k - \delta_{k,p} a^\dagger_{k-q} a_{p-q} + \delta_{k,p+q} a^\dagger_{k-q} a_p - \delta_{p,k-q} a^\dagger_{p+q} a_k \right) \\ &= \sum_{\mathbf{p}} (\frac{\mathbf{p}^2}{2m} - \mu) \left(2a^\dagger_p a_p - a^\dagger_{p-q} a_{p-q} - a^\dagger_{p+q} a_{p+q} \right) \\ &= \sum_{\mathbf{p}} \left[2\frac{\mathbf{p}^2}{2m} - \frac{(\mathbf{p}+\mathbf{q})^2}{2m} - \frac{(\mathbf{p}-\mathbf{q})^2}{2m} \right] \left(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} \right) \\ &= -\frac{\mathbf{q}^2}{m} \sum_{\mathbf{p}} a^\dagger_{\mathbf{p}} a_{\mathbf{p}} \\ &= \frac{-\mathbf{q}^2 \hat{N}}{m} \end{aligned} \tag{8.130}$$

so we have

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{nn}(\mathbf{q},\omega) = \frac{n\mathbf{q}^2}{m} \tag{8.131}$$

where $n = N/\mathcal{V}$.

9 Screening

(Ashcroft Mermin Chapter 17 Independent electron approximation, section: screening)

The effect of screening is one of the simplest and most important manifestation of electron-electron interactions. We consider here only screening of a free electron gas. Suppose a positively charged particle is placed at a given position in the electron gas and rigidly held there. It will then attract electrons, creating a surplus of negative charge in its neighborhood, which reduces or "screens" its field. In treating this screening it is convenient to introduce two electrostatic potentials. The first ϕ^{ext}, arises solely from the positively charged particle itself, and therefore satisfies Poisson's equation in the form (and its Fourier component form)

$$\begin{aligned} -\nabla^2\phi^{ext}(\mathbf{r}) &= 4\pi\rho^{ext}(\mathbf{r}) \\ q^2\phi^{ext}(\mathbf{q}) &= 4\pi\rho^{ext}(\mathbf{q}) \end{aligned} \tag{9.1}$$

where $\rho(\mathbf{r})$ is the particle's charge density. The second ϕ, is the full physical potential, produced by both the positively charged particle and the cloud of screening electrons it induces. It therefore satisfies

$$\begin{aligned} -\nabla^2\phi(\mathbf{r}) &= 4\pi\rho(\mathbf{r}) \\ q^2\phi(\mathbf{q}) &= 4\pi\rho(\mathbf{q}) \end{aligned} \tag{9.2}$$

where

$$\rho = \rho^{ext} + \rho^{ind} \tag{9.3}$$

We assume ϕ^{ext} and ϕ to be linearly related (linear response)

$$\phi^{ext}(\mathbf{r}) = \int d\mathbf{r}'\epsilon(\mathbf{r},\mathbf{r}')\phi(\mathbf{r}') \tag{9.4}$$

for homogeneous electron gas $\epsilon(\mathbf{r},\mathbf{r}') = \epsilon(\mathbf{r}-\mathbf{r}')$ and we have

$$\phi^{ext}(\mathbf{r}) = \int d\mathbf{r}'\epsilon(\mathbf{r}-\mathbf{r}')\phi(\mathbf{r}') \tag{9.5}$$

performing a Fourier Transform, using convolution theorem

$$\phi^{ext}(\mathbf{q}) = \epsilon(\mathbf{q})\phi(\mathbf{q}) \tag{9.6}$$

$$\begin{aligned} \epsilon(\mathbf{q}) &= \int d\mathbf{r}e^{-i\mathbf{q}\cdot\mathbf{r}}\epsilon(\mathbf{r}) \\ \epsilon(\mathbf{r}) &= \int \frac{d\mathbf{q}}{(2\pi)^3}e^{i\mathbf{q}\cdot\mathbf{r}}\epsilon(\mathbf{q}) \end{aligned} \tag{9.7}$$

the constant $\epsilon(\mathbf{q})$ is called the **dielectric constant** of the metal. When written in the form

$$\phi(\mathbf{q}) = \frac{1}{\epsilon(\mathbf{q})}\phi^{ext}(\mathbf{q}) \tag{9.8}$$

it asserts that the $\mathbf{q}$th Fourier component of the total potential present in the electron gas is just the $\mathbf{q}$th Fourier Component of the external potential, reduced by the factor $1/\epsilon(\mathbf{q})$. The quantity that turns out to be the most natural to calculate directly is the charge density induced by the total potential $\phi(\mathbf{r})$. Due to the linear response that relates the Fourier components directly, we can represent this susceptibility as

$$\rho^{ind}(\mathbf{q}) = \chi(\mathbf{q})\phi(\mathbf{q}) \tag{9.9}$$

we can show that this gives

$$\phi(\mathbf{q}) = \frac{1}{1-\frac{4\pi}{q^2}\chi(\mathbf{q})}\phi^{ext}(\mathbf{q}) \tag{9.10}$$

and $\chi(\mathbf{q})$ is related to $\epsilon(\mathbf{q})$ by

$$\epsilon(\mathbf{q}) = 1 - \frac{4\pi}{q^2}\chi(\mathbf{q}) \tag{9.11}$$

The problem of screening reduces to the calculation of the charge susceptibility $\chi(\mathbf{q})$. So far, the only approximation we have made is that the external charge is weak enough to produce only a linear response in the electron gas. Two methods to calculate $\chi(\mathbf{q})$ exist : Thomas-Fermi method and Lindhard method (or RPA). Thomas-Fermi method is based on the classical limit of Hartree theory, while Lindhard method is based on an exact Hartree calculation of the charge density in the presence of the self-consistent field of the external charge plus electron gas, except we only require ρ^{ind} to linear order in ϕ.

9.1 Thomas Fermi Screening

In principle, to find the charge density in the presence of the total potential $\phi = \phi^{ext} + \phi^{ind}$ we must solve the one-electron Shrodinger equation

$$-\frac{\hbar^2}{2m}\nabla\psi_i(\mathbf{r}) - e\phi(\mathbf{r})\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r}) \tag{9.12}$$

and then construct the electron density from the one-electron wave functions using

$$\rho(\mathbf{r}) = -e\sum_i |\psi_i(\mathbf{r})|^2 \tag{9.13}$$

TF approximation is based on a simplification in this procedure that can be made when the total potential $\phi(\mathbf{r})$ is a very slowly varying function of $\mathbf{r}$, then electrons feel a "**local dispersion**":

$$\varepsilon_{\mathbf{r}}(\mathbf{k}) = \frac{\hbar^2k^2}{2m} - e\phi(\mathbf{r}) \tag{9.14}$$

this make sense only in terms of wavepackets, which have a typical spread in position at least of the order $1/k_F$. We must therefore require that $\phi(\mathbf{r})$ vary slowly in the scale of the Fermi-wavelength or that the Fourier components $\chi(\mathbf{q})$ is reliable for $q \ll k_F$ only. We then have the electronic number density at position $\mathbf{r}$

$$\begin{aligned} n(\mathbf{r}) &= 2\int \frac{d\mathbf{k}}{(2\pi)^3} f_F(\varepsilon_{\mathbf{r}}(\mathbf{k})) \\ &= 2\int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\exp\left[\beta(\frac{\hbar^2k^2}{2m} - e\phi(\mathbf{r}) - \mu)\right] + 1} \end{aligned} \tag{9.15}$$

The induced charge density $\rho^{ind}(\mathbf{r}) = -en(\mathbf{r}) + en_0$ where en_0 is the charge density of the uniform positive background. Without external perturbation and thus without $\phi(\mathbf{r})$, n_0 should be the number density of electrons, in order that the metal stay neutral. So we have

$$n_0(\mu) = 2\int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\exp\left[\beta(\frac{\hbar^2k^2}{2m} - \mu)\right] + 1} \tag{9.16}$$

it can now be seen that these two functions are related

$$n(\mathbf{r}) = n_0(\mu + e\phi(\mathbf{r})) \tag{9.17}$$

and we can write

$$\begin{aligned} \rho^{ind}(\mathbf{r}) &= -e\left[n_0(\mu + e\phi(\mathbf{r})) - n_0(\mu)\right] \\ &\approx -e^2\frac{\partial n_0}{\partial\mu}\phi(\mathbf{r}) \end{aligned} \tag{9.18}$$

After a Fourier Transform, this gives a $\mathbf{q}$-independent charge susceptibility

$$\chi(\mathbf{q}) = -e^2\frac{\partial n_0}{\partial\mu} \tag{9.19}$$

and

$$\epsilon(\mathbf{q}) = 1 + \frac{4\pi e^2}{q^2}\frac{\partial n_0}{\partial\mu} \tag{9.20}$$

We can define a Thomas-Fermi wavevector

$$k_0 \equiv 4\pi e^2\frac{\partial n_0}{\partial\mu} \tag{9.21}$$

so that

$$\epsilon(\mathbf{q}) = 1 + \frac{k_0^2}{q^2} \tag{9.22}$$

$$\phi(\mathbf{q}) = \frac{q^2}{q^2 + k_0^2}\phi^{ext}(\mathbf{q}) \tag{9.23}$$

Suppose the external potential is a point charge

$$\phi^{ext}(\mathbf{r}) = \frac{Q}{r}, \quad \phi^{ext}(\mathbf{q}) = \frac{4\pi Q}{q^2} \tag{9.24}$$

the **screened Coulomb potential** is then

$$\phi(\mathbf{r}) = \frac{Q}{r}e^{-k_0 r}, \quad \phi(\mathbf{q}) = \frac{4\pi Q}{q^2 + k_0^2} \tag{9.25}$$

which is also called a **Yukawa potential**.
We now go back to the function $\frac{\partial n_0}{\partial \mu}$, at low T, we perform a Sommerfeld expansion of n_0:

$$\begin{aligned} n_0(\mu) &= 2\int \frac{d\mathbf{k}}{(2\pi)^3} f(\varepsilon_{\mathbf{k}}) \\ &= \int_0^\infty d\varepsilon \mathcal{N}(\varepsilon) f(\varepsilon) \\ &\approx \int_0^\mu d\varepsilon \mathcal{N}(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 \frac{d\mathcal{N}}{d\varepsilon}|_{\varepsilon=\mu} \\ &= \frac{m}{\hbar^2\pi^2}\sqrt{\frac{2m}{\hbar^2}}\left[\frac{2}{3}\mu^{3/2} + \frac{\pi^2}{12}(k_B T)^2 \mu^{-1/2}\right] \end{aligned} \tag{9.26}$$

$$\frac{\partial n_0}{\partial \mu} = \frac{m}{\hbar^2\pi^2}\sqrt{\frac{2m}{\hbar^2}}\left[\mu^{1/2} - \frac{\pi^2}{24}(k_B T)^2 \mu^{-3/2}\right] = \mathcal{N}(\mu) - ... \tag{9.27}$$

where $\mathcal{N}$ is the density of states function. For 3d free fermions $\epsilon = \hbar^2 k^2/2m$, the density of states per unit volume is

$$\frac{2}{V}\frac{d^3k}{(2\pi/L)^3} = \frac{1}{\pi^2}k^2 dk = \mathcal{N}(\epsilon)d\epsilon \tag{9.28}$$

$$\mathcal{N}(\varepsilon) = \frac{mk(\varepsilon)}{\pi^2\hbar^2} = \frac{m}{\hbar^2\pi^2}\sqrt{\frac{2m\varepsilon}{\hbar^2}} \tag{9.29}$$

We then have, to lowest order approximation and assuming $\mu \approx E_F$

$$k_0^2 \equiv 4\pi e^2 \mathcal{N}(\mu) \approx 4\pi e^2 \mathcal{N}(E_F) \tag{9.30}$$

We can also define a wavelength $\lambda = k_0^{-1}$ called the Thomas Fermi wavelength. After some simplification we can write

$$\lambda^{-2} = 4\pi e^2 \mathcal{N}(E_F) \rightarrow_{SI} \frac{e^2 \mathcal{N}(E_F)}{\epsilon_0} \tag{9.31}$$

where in the last step we used SI unit.

9.2 Lindhard Scrrening (RPA Approximation)

Consider linear response theory with the perturbation operator

$$H' = \int d\mathbf{r}\rho^{ind}(\mathbf{r})\phi(\mathbf{r}, t) \tag{9.32}$$

We wish to know the response of $\rho_e(\mathbf{r})$ with respect to this perturbation. Kubo formula gives

$$\bar{\rho}^{ind}(\mathbf{q}, \omega) = \alpha_{yx}(\mathbf{q}, \omega)\chi(\mathbf{q}, \omega) \tag{9.33}$$

since we are interested in $\rho^{ind}(\mathbf{q}) = \chi(\mathbf{q})\phi(\mathbf{q})$, we can set $\omega = 0$ and

$$\begin{aligned}
\chi(\mathbf{q}) &= ie^2 \lim_{\omega\to 0+i\eta} \int_0^\infty \mathrm{d}t e^{i\omega t} \int d^3r e^{-i\mathbf{q}\cdot\mathbf{r}} \langle[\rho_I(\mathbf{r},t), \rho_I(0,0)]\rangle \\
&= ie^2 \lim_{\omega\to 0+i\eta} \int_0^\infty \mathrm{d}t e^{i\omega t} \int d^3r \int \frac{d\mathbf{q}_1 d\mathbf{q}_2 d\mathbf{q}_3 d\mathbf{q}_4}{(2\pi)^{12}} e^{-i(\mathbf{q}+\mathbf{q}_1-\mathbf{q}_2)\cdot\mathbf{r}} e^{-i\xi_{\mathbf{q}_1}t} e^{i\xi_{\mathbf{q}_2}t} \left\langle[a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_2\sigma}, a^\dagger_{\mathbf{q}_3\alpha} a_{\mathbf{q}_4\alpha}]\right\rangle \\
&= i2e^2 \lim_{\omega\to 0+i\eta} \int_0^\infty \mathrm{d}t e^{i\omega t} \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^6} \int d^3r e^{-i(\mathbf{q}+\mathbf{q}_1-\mathbf{q}_2)\cdot\mathbf{r}} e^{-i\xi_{\mathbf{q}_1}t} e^{i\xi_{\mathbf{q}_2}t} \left(f_{\mathbf{q}_1} - f_{\mathbf{q}_2}\right) \\
&= i2e^2 \int \frac{d\mathbf{q}_1}{(2\pi)^3} \left(f_{\mathbf{q}_1} - f_{\mathbf{q}_1+\mathbf{q}}\right) \int_0^\infty \mathrm{d}t e^{i(\xi_{\mathbf{q}_1+\mathbf{q}} - \xi_{\mathbf{q}_1} + i\eta)t} \\
&= -2e^2 \int \frac{d\mathbf{q}_1}{(2\pi)^3} \frac{f_{\mathbf{q}_1} - f_{\mathbf{q}_1+\mathbf{q}}}{\xi_{\mathbf{q}_1+\mathbf{q}} - \xi_{\mathbf{q}_1} + i\eta} \\
&= -2e^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{f_{\mathbf{k}-\mathbf{q}/2} - f_{\mathbf{k}+\mathbf{q}/2}}{\xi_{\mathbf{k}+\mathbf{q}/2} - \xi_{\mathbf{k}-\mathbf{q}/2} + i\eta}
\end{aligned} \tag{9.34}$$

where $\mathbf{k} \equiv \mathbf{q}_1 + \mathbf{q}/2$. We used the number operator

$$\rho_I(\mathbf{r},t) = \Psi^\dagger_{0\sigma}(\mathbf{r},t)\Psi_{0\sigma}(\mathbf{r},t). \tag{9.35}$$

$$\begin{aligned}
a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_2\sigma} a^\dagger_{\mathbf{q}_3\alpha} a_{\mathbf{q}_4\alpha} &= a^\dagger_{\mathbf{q}_1\sigma} \left((2\pi)^3\delta(\mathbf{q}_3 - \mathbf{q}_2)\delta_{\alpha\sigma} - a^\dagger_{\mathbf{q}_3\alpha} a_{\mathbf{q}_2\sigma}\right) a_{\mathbf{q}_4\alpha} \\
&= a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_4\alpha} (2\pi)^3\delta(\mathbf{q}_3 - \mathbf{q}_2)\delta_{\alpha\sigma} - a^\dagger_{\mathbf{q}_3\alpha} a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_4\alpha} a_{\mathbf{q}_2\sigma} \\
&= a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_4\alpha} (2\pi)^3\delta(\mathbf{q}_3 - \mathbf{q}_2)\delta_{\alpha\sigma} - a^\dagger_{\mathbf{q}_3\alpha} \left((2\pi)^3\delta(\mathbf{q}_4 - \mathbf{q}_1)\delta_{\alpha\sigma} - a_{\mathbf{q}_4\alpha} a^\dagger_{\mathbf{q}_1\sigma}\right) a_{\mathbf{q}_2\sigma} \\
&= a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_4\sigma} (2\pi)^3\delta(\mathbf{q}_3 - \mathbf{q}_2) - a^\dagger_{\mathbf{q}_3\sigma} a_{\mathbf{q}_2\sigma} (2\pi)^3\delta(\mathbf{q}_4 - \mathbf{q}_1) + a^\dagger_{\mathbf{q}_3\alpha} a_{\mathbf{q}_4\alpha} a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_2\sigma}
\end{aligned} \tag{9.36}$$

We now average

$$\begin{aligned}
\left\langle[a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_2\sigma}, a^\dagger_{\mathbf{q}_3\alpha} a_{\mathbf{q}_4\alpha}]\right\rangle &= \left\langle a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_4\sigma}\right\rangle (2\pi)^3\delta(\mathbf{q}_3 - \mathbf{q}_2) - \left\langle a^\dagger_{\mathbf{q}_3\sigma} a_{\mathbf{q}_2\sigma}\right\rangle (2\pi)^3\delta(\mathbf{q}_4 - \mathbf{q}_1) \\
&= 2(2\pi)^6\delta(\mathbf{q}_3 - \mathbf{q}_2)\delta(\mathbf{q}_1 - \mathbf{q}_4)\left(f_{\mathbf{q}_1} - f_{\mathbf{q}_2}\right)
\end{aligned} \tag{9.37}$$

$$\begin{aligned}
\rho_I(\mathbf{r},t) &= \Psi^\dagger_{0\sigma}(\mathbf{r},t)\Psi_{0\sigma}(\mathbf{r},t) \\
&= \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^6} e^{-i(\mathbf{q}_1-\mathbf{q}_2)\cdot\mathbf{r}} a^\dagger_{0\mathbf{q}_1\sigma}(t) a_{0\mathbf{q}_2\sigma}(t) \\
&= \int \frac{d\mathbf{q}_1 d\mathbf{q}_2}{(2\pi)^6} e^{-i(\mathbf{q}_1-\mathbf{q}_2)\cdot\mathbf{r}} e^{-i\xi_{\mathbf{q}_1}t} e^{i\xi_{\mathbf{q}_2}t} a^\dagger_{\mathbf{q}_1\sigma} a_{\mathbf{q}_2\sigma}
\end{aligned} \tag{9.38}$$

$$\rho_I(0,0) = \int \frac{d\mathbf{q}_3 d\mathbf{q}_4}{(2\pi)^6} a^\dagger_{\mathbf{q}_3\sigma} a_{\mathbf{q}_4\sigma} \tag{9.39}$$

with the free Hamiltonian

$$H_0 = \int \frac{d\mathbf{p}}{(2\pi)^3} \xi_{\mathbf{p}} \hat{a}^\dagger_{\mathbf{p}\alpha} \hat{a}_{\mathbf{p}\alpha} \tag{9.40}$$

where $\xi_{\mathbf{p}} \equiv \frac{\mathbf{p}^2}{2m} - \mu$. We can directly calculate the interacting picture operators:

$$\begin{aligned}
a^\dagger_{0\mathbf{q}\sigma}(t) &= e^{iH_0 t} a^\dagger_{\mathbf{q}\sigma} e^{-iH_0 t} \\
&= \sum_{n=0}^\infty \frac{(it)^n}{n!} [{}^n H_0, a^\dagger_{\mathbf{q}}] \\
&= \sum_{n=0}^\infty \frac{1}{n!} \left(i\xi_{\mathbf{q}} t\right)^n a^\dagger_{\mathbf{q}\sigma} \\
&= e^{-i\xi_{\mathbf{q}} t} a^\dagger_{\mathbf{q}\sigma}
\end{aligned} \tag{9.41}$$

similarly

$$a_{0\mathbf{q}\sigma}(t) = e^{i\xi_{\mathbf{q}} t} a_{\mathbf{q}\sigma} \tag{9.42}$$

Performing a Taylor expansion in the denomenator, we obtain the susceptibility function

$$\chi(\mathbf{q}) = -2e^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{f_{\mathbf{k}-\mathbf{q}/2} - f_{\mathbf{k}+\mathbf{q}/2}}{\hbar^2 \mathbf{k}\cdot\mathbf{q}/m} \tag{9.43}$$

In the small q limit we can make approximation

$$f_{\mathbf{k}+\mathbf{q}/2} = f(\varepsilon(\mathbf{k}+\mathbf{q}/2)) = f(\varepsilon(\mathbf{k})) - \frac{\partial f}{\partial \mu}\frac{\hbar^2}{2m}\mathbf{k}\cdot\mathbf{q} \tag{9.44}$$

and the susceptibility recovers that of TF approximation

$$\chi(\mathbf{q}) = -2e^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial f}{\partial \mu} = -e^2 \frac{\partial n_0}{\partial \mu} \tag{9.45}$$

However, if we set $T = 0$ directly in the Lindhard approxiamtion, we have

$$\begin{aligned}
\chi(\mathbf{q}) &= -2e^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\theta(k_F - |\mathbf{k}-\mathbf{q}/2|) - \theta(k_F - |\mathbf{k}+\mathbf{q}/2|)}{\hbar^2 \mathbf{k}\cdot\mathbf{q}/m} \\
&= -e^2 \frac{m}{(2\pi)^3\hbar^2} \int d^3k \frac{\theta(k_F - |\mathbf{k}-\mathbf{q}/2|) - \theta(k_F - |\mathbf{k}+\mathbf{q}/2|)}{\mathbf{k}\cdot\mathbf{q}/2} \\
&= -e^2 \frac{m}{(2\pi)^2\hbar^2} \int_{-1}^{1} d\cos\theta \int_0^\infty dk k^2 \frac{\theta(k_F - |\mathbf{k}-\mathbf{q}/2|) - \theta(k_F - |\mathbf{k}+\mathbf{q}/2|)}{\mathbf{k}\cdot\mathbf{q}/2} \\
&= -e^2 \left(\frac{mk_F}{\pi^2\hbar^2}\right) \frac{1}{4} \int_{-1}^{1} d\cos\theta \int_0^\infty dp p^2 \frac{\theta(1 - |\mathbf{p}-\mathbf{x}|) - \theta(1 - |\mathbf{p}+\mathbf{x}|)}{\mathbf{p}\cdot\mathbf{x}} \\
&= -e^2 \left(\frac{mk_F}{\pi^2\hbar^2}\right) \frac{1}{4} \int_{-1}^{1} d\cos\theta \int_0^\infty dp \frac{p^2}{\mathbf{p}\cdot\mathbf{x}} \theta(1 - |\mathbf{p}-\mathbf{x}|)\theta(|\mathbf{p}+\mathbf{x}| - 1) \\
&= -e^2 \left(\frac{mk_F}{\pi^2\hbar^2}\right) \frac{1}{4} \int_{0}^{1} d\cos\theta \int_0^\infty dp \frac{p}{x\cos\theta} \theta(1 - \left(p^2 + x^2 - 2px\cos\theta\right))\theta(\left(p^2 + x^2 + 2px\cos\theta\right) - 1) \\
&= -e^2 \left(\frac{mk_F}{\hbar^2\pi^2}\right) \frac{1}{2} \left[\frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right|\right]
\end{aligned} \tag{9.46}$$

(there is an extra factor of 1/2)
where we used $p \equiv \frac{k}{k_F}$, $x \equiv \frac{q}{2k_F}$ and from the third step onward we restrict $\mathbf{p}$, $\mathbf{x}$ to be on the same 2D plane.

We have $|\cos\theta| \le \min\left(\frac{x^2+p^2-1}{2px}, 1\right)$. If $x < 1$, we have $1 - x < p < 1 + x$ and $|\frac{x^2+p^2-1}{2kx}| < \cos\theta < 1$, and the integral evaluate to

$$\begin{aligned}
\frac{1}{2x}\int_{1-x}^{1+x} dpp \int_{|\frac{x^2+p^2-1}{2kx}|}^{1} \frac{d\cos\theta}{\cos\theta} &= \frac{1}{2x}\int_{1-x}^{1+x} dpp \ln\left|\frac{2px}{x^2+p^2-1}\right| \\
&= \frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|
\end{aligned} \tag{9.47}$$

(I didn't do this step, actually)
for $x > 1$ we actually get the same result. So we have

$$\chi(\mathbf{q}) = -e^2 \left(\frac{mk_F}{\hbar^2\pi^2}\right) \left[\frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right|\right] \tag{9.48}$$

with $x = \frac{q}{2k_F}$. In the limit $q \ll k_F$, $x \ll 1$. In the limit $x = 0$ we recover the TF approximation.

10 Electrical Conductivity

In this section we will derive the generalized Ohm's law

$$J_e^\alpha(\mathbf{r}, t) = \int dt' \int d\mathbf{r}' \sum_\beta \sigma^{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') E^\beta(\mathbf{r}', t') \tag{10.1}$$

and give an expression for the conductivity $\sigma^{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t')$ in terms of fluctuations of the equilibrium system, through the Kubo formula. We need the general susceptibility χ^R_{JE}, so we must express δH as a function of E.

To couple a charged-particle to a magnetic field, we use minimal coupling

$$\partial_\mu \to \partial_\mu - ieA_\mu \tag{10.2}$$

(Throughout this expression e is the **charge** of the particle, not the elementary charge.)
where the four vectors are

$$\partial_\mu = \left(\frac{1}{c}\partial_t, \nabla\right), \quad A_\mu = (-\phi/c, \mathbf{A}) \tag{10.3}$$

equivalently,

$$\begin{aligned} i\partial_t &\to i\partial_t - e\phi \\ \nabla &\to \nabla - ie\mathbf{A} \end{aligned} \tag{10.4}$$

If we use the Weyl gauge $\phi = 0$, then we only need to introduce the coupling through a time dependent vector field $\mathbf{A}(\mathbf{r}, t)$, this results in

$$H = \int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{r}) \left(-\frac{(\nabla - ie\mathbf{A}(\mathbf{r},t))^2}{2m}\right) \hat{\Psi}_\alpha(\mathbf{r}) \tag{10.5}$$

In order to do linear response theory, we have to separate out the interaction part δH.

$$\begin{aligned} -(\nabla - ie\mathbf{A}(\mathbf{r},t))^2 &= (i\nabla + e\mathbf{A}(\mathbf{r},t)) \cdot (i\nabla + e\mathbf{A}(\mathbf{r},t)) \\ &= -\nabla^2 + ie\nabla\cdot\mathbf{A}(\mathbf{r},t) + ie\mathbf{A}(\mathbf{r},t)\cdot\nabla + e^2\mathbf{A}^2(r,t) \end{aligned} \tag{10.6}$$

$$\delta H = \frac{1}{2m}\int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{r}) \left(ie\nabla\cdot\mathbf{A}(\mathbf{r},t) + ie\mathbf{A}(\mathbf{r},t)\cdot\nabla + e^2\mathbf{A}^2(r,t)\right) \hat{\Psi}_\alpha(\mathbf{r}) \tag{10.7}$$

The current operator without magnetic field is

$$\mathbf{J}(\mathbf{r}) = \frac{e}{2mi}\left(\psi^\dagger_\sigma(\mathbf{r})\nabla\psi_\sigma(\mathbf{r}) - \psi_\sigma(\mathbf{r})\nabla\psi^\dagger_\sigma(\mathbf{r})\right) \tag{10.8}$$

naively, we would promote it with minimal coupling

$$\begin{aligned} \mathbf{J}^A(\mathbf{r}) &= \frac{e}{2mi}\left(\psi^\dagger_\sigma(\mathbf{r})\left(\nabla - ie\mathbf{A}\right)\psi_\sigma(\mathbf{r}) - \psi_\sigma(\mathbf{r})\left(\nabla - ie\mathbf{A}\right)\psi^\dagger_\sigma(\mathbf{r})\right) \\ &= \mathbf{J}(\mathbf{r}) + \frac{e\mathbf{A}}{2m}\left(\psi^\dagger_\sigma(\mathbf{r})\psi_\sigma(\mathbf{r}) - \psi_\sigma(\mathbf{r})\psi^\dagger_\sigma(\mathbf{r})\right) \\ &= \mathbf{J}(\mathbf{r}) + \frac{e}{m}\mathbf{A}(\mathbf{r},t)\left(\rho(\mathbf{r}) - \frac{\delta(0)}{2}\right) \end{aligned} \tag{10.9}$$

but this introduces an infinity $\delta(0)$. An alternative derivation is from the assumption

$$\delta H = -\int d\mathbf{r}\mathbf{A}(\mathbf{r},t)\cdot\mathbf{J}^A(\mathbf{r}) \tag{10.10}$$

So we have

$$\begin{aligned} \mathbf{J}^A(\mathbf{r}) &= -\frac{\delta H}{\delta\mathbf{A}(\mathbf{r})} \\ &= -\frac{1}{2m}\int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x})\left[ie\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{r}) + ie\delta(\mathbf{x}-\mathbf{r})\nabla_{\mathbf{x}} + e^2 2\mathbf{A}(\mathbf{x})\delta(\mathbf{r}-\mathbf{x})\right]\hat{\Psi}_\alpha(\mathbf{x}) \\ &= -\frac{ie}{2m}\left[\int d^3x \hat{\Psi}^\dagger_\alpha(\mathbf{x})\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{r})\hat{\Psi}_\alpha(\mathbf{x}) + \hat{\Psi}^\dagger_\alpha(\mathbf{r})\nabla_{\mathbf{r}}\hat{\Psi}_\alpha(\mathbf{r})\right] - \frac{e^2}{m}\rho(\mathbf{r})\mathbf{A}(\mathbf{r}) \\ &= \frac{e}{2mi}\left[\int d^3x\left(-\nabla_{\mathbf{r}}\right)\hat{\Psi}^\dagger_\alpha(\mathbf{r})\hat{\Psi}_\alpha(\mathbf{r}) + \hat{\Psi}^\dagger_\alpha(\mathbf{r})\nabla_{\mathbf{r}}\hat{\Psi}_\alpha(\mathbf{r})\right] - \frac{e^2}{m}\rho(\mathbf{r})\mathbf{A}(\mathbf{r}) \\ &= \mathbf{J}(\mathbf{r}) - \frac{e^2}{m}\rho(\mathbf{r})\mathbf{A}(\mathbf{r},t) \end{aligned} \tag{10.11}$$

we will call these two parts: paramagnetic and diamagnetic current

$$\begin{aligned}\mathbf{J}^A(\mathbf{r}) &= \mathbf{J}^P(\mathbf{r}) + \mathbf{J}^D(\mathbf{r}) \\ \mathbf{J}^P(\mathbf{r}) &= \frac{e}{2mi}\left(\psi^\dagger_\sigma(\mathbf{r})\nabla\psi_\sigma(\mathbf{r}) - \psi_\sigma(\mathbf{r})\nabla\psi^\dagger_\sigma(\mathbf{r})\right) \\ \mathbf{J}^D(\mathbf{r}) &= -\frac{e^2}{m}\rho(\mathbf{r})\mathbf{A}(\mathbf{r},t)\end{aligned} \tag{10.12}$$

Now, using the $\delta H = -\int \mathbf{A}\cdot\mathbf{J}^A$ formula and the explicit expression for $\mathbf{J}^A$ above. Consider now the effect of this perturbation to the expectation of $\mathbf{J}^A$, The diamagnetic part is directly proportional to $\mathbf{A}$ and thus we can write (without Kubo formula)

$$\delta\left\langle J^D_j(\mathbf{r},t)\right\rangle = -\frac{e^2}{m}\left\langle\rho(\mathbf{r})\right\rangle A_j(\mathbf{r},t) = \left(-\frac{ne^2}{m}\delta_{ij}\right)A_i(\mathbf{r},t) \tag{10.13}$$

$$\delta\left\langle J^D_j(\mathbf{q},\omega)\right\rangle = \left(-\frac{ne^2}{m}\delta_{ij}\right)A_i(\mathbf{q},\omega) \tag{10.14}$$

For the paramagnetic part, we using linear response theory,

$$\delta\langle J^P_j(\mathbf{q},\omega)\rangle = \chi^R_{J^P_j J^A_i}(\mathbf{q},\omega)A_i(\mathbf{q},\omega) \tag{10.15}$$

$$\chi^R_{J^A_j J^A_i}(\mathbf{r},t;\mathbf{r}',t') = i\theta(t-t')\left\langle\left[J^P_j(\mathbf{r},t), J^A_i(\mathbf{r}',t')\right]\right\rangle \tag{10.16}$$

$$\begin{aligned}\left[J^P_j(\mathbf{r},t), J^A_i(\mathbf{r}',t')\right] &= \left[J_j(\mathbf{r}), J_i(\mathbf{r}') - \frac{e^2}{m}\rho(\mathbf{r}')A_i(\mathbf{r}',t')\right] \\ &= [J_j(\mathbf{r}), J_i(\mathbf{r}')] - \frac{e^2}{m}A_i(\mathbf{r}',t')[J_j(\mathbf{r}),\rho(\mathbf{r}')]\end{aligned} \tag{10.17}$$

To lowest order in A, we keep only the first term, so we have

$$\delta\langle J^P_j(\mathbf{q},\omega)\rangle \approx \chi^R_{J^P_j J^P_i}(\mathbf{q},\omega)A_i(\mathbf{q},\omega) \tag{10.18}$$

if we now relax the gauge condition and add a ϕ field, the interaction is

$$\delta\mathcal{H}(t)_\phi = \int d\mathbf{r}\phi(\mathbf{r},t)\rho(\mathbf{r}) \tag{10.19}$$

$$\delta\left\langle J^A_j(\mathbf{q},\omega)\right\rangle = \chi^R_{J^A_j\rho}(\mathbf{q},\omega)\left(-\phi(\mathbf{q},\omega)\right) \tag{10.20}$$

to lowest order in A and ϕ, $\chi^R_{J^A_j\rho}(\mathbf{q},\omega) \approx \chi^R_{J^P_j\rho}(\mathbf{q},\omega)$. In summary, linear response theory gives, for a general perturbation $\mathbf{A}(\mathbf{r},t),\phi(\mathbf{r},t)$,

$$\delta\left\langle J^A_j(\mathbf{q},\omega)\right\rangle = \left[\chi^R_{J^P_j J^P_i}(\mathbf{q},\omega) - \frac{ne^2}{m}\delta_{ij}\right]A_i(\mathbf{q},\omega) - \chi^R_{J^P_j\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega) \tag{10.21}$$

it is not obvious that this expression is invariant under gauge transformation:

$$\begin{aligned}\mathbf{A}(\mathbf{q},\omega) &\to \mathbf{A}(\mathbf{q},\omega) + i\mathbf{q}\Lambda(\mathbf{q},\omega) \\ \phi(\mathbf{q},\omega) &\to \phi(\mathbf{q},\omega) + i\omega\Lambda(\mathbf{q},\omega)\end{aligned} \tag{10.22}$$

To obtain Ohm's law, write

$$\mathbf{E}(\mathbf{r},t) = -\nabla\phi(\mathbf{r},t) - \partial_t\mathbf{A}(\mathbf{r},t) \to \mathbf{E}(\mathbf{q},\omega) = -i\mathbf{q}\phi(\mathbf{q},\omega) + i(\omega+i\eta)\mathbf{A}(\mathbf{q},\omega) \tag{10.23}$$

where we introduced $\omega + i\eta$, which assumes that the field is adiabatically switched on.
if we choose the Weyl gauge and let $\phi = 0$, we have

$$\delta\left\langle J^A_j(\mathbf{q},\omega)\right\rangle = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{J^P_j J^P_i}(\mathbf{q},\omega) - \frac{ne^2}{m}\delta_{ij}\right]E_i(\mathbf{q},\omega) \tag{10.24}$$

and the conductivity tensor is

$$\sigma_{ji}(\mathbf{q},\omega) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{J^P_j J^P_i}(\mathbf{q},\omega) - \frac{ne^2}{m}\delta_{ij}\right] \tag{10.25}$$

10.1 Transverse conductivity

The electromagnetic fields can be separated into the transverse ($\mathbf{q} \perp \mathbf{E}(\mathbf{q},\omega)$) part and the longitudinal ($\mathbf{q} \parallel \mathbf{E}(\mathbf{q},\omega)$) part. The electric field due to a scalar potential

$$\mathbf{E}(\mathbf{r}) = -\nabla\phi(\mathbf{r}) \rightarrow \mathbf{E}(\mathbf{q}) = -i\mathbf{q}\phi(\mathbf{q}) \tag{10.26}$$

is always longitudinal. On the other hand, the magnetic field

$$\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A} \rightarrow \mathbf{B}(\mathbf{q}) = i\mathbf{q} \times \mathbf{A} \tag{10.27}$$

is always transverse. There is still another part of $\mathbf{E} = -\partial_t \mathbf{A}$. Let us decompose $\mathbf{A}$ into a transverse and a longitudinal part. This is easily done by using the unit vector $\hat{\mathbf{q}} = \mathbf{q}/|\mathbf{q}|$

$$\begin{aligned} \mathbf{A}^L &= \hat{\mathbf{q}}\hat{\mathbf{q}} \cdot \mathbf{A} \\ \mathbf{A}^T &= (I - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \mathbf{A} \end{aligned} \tag{10.28}$$

In the last expression $\hat{\mathbf{q}}\hat{\mathbf{q}}$is called the "dyadic product" representation of the matrix $\left(\hat{\mathbf{q}}\hat{\mathbf{q}}\right)_{ab} = \hat{q}_a\hat{q}_b$. The first $\hat{\mathbf{q}}$acts on the left while the second acts on the right.

The transverse and longitudinal parts of the conductivity tensor are defined as

$$\begin{aligned} \sigma^T(\mathbf{q},\omega) &= (I - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \sigma(\mathbf{q},\omega) \cdot (I - \hat{\mathbf{q}}\hat{\mathbf{q}}) \\ \sigma^L(\mathbf{q},\omega) &= \hat{\mathbf{q}}\hat{\mathbf{q}} \cdot \sigma(\mathbf{q},\omega) \cdot \hat{\mathbf{q}}\hat{\mathbf{q}} \end{aligned} \tag{10.29}$$

for a homogeneous isotropic system with no magnetic field, off-diagonal elements such as $(I - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \sigma(\mathbf{q},\omega) \cdot \hat{\mathbf{q}}\hat{\mathbf{q}}$ vanish and we have $\sigma = \sigma^T + \sigma^L$. This means that fields of a given polarization induce currents of the same polarization.

To simplify the notation, we take the current and applied electric field in the y-direction, and the spatial dependence in the x-direction. This is what happens usually in a wire made of homogeneous and isotropic material in the presence of the **skin effect** (ref Fig. 11-1). Then

$$\sigma_{yy}(q_x,\omega) = \frac{1}{i(\omega + i\eta)}\left[\chi^R_{J_yJ_y}(q_x,\omega) - \frac{ne^2}{m}\right] \tag{10.30}$$

$$\delta\left\langle j_y^A\left(q_x,\omega\right)\right\rangle \equiv \sigma_{yy}\left(q_x,\omega\right) E_y\left(q_x,\omega\right) \tag{10.31}$$

10.2 Longitudinal conductivity

We now consider the longitudinal response. Using the f-sum rule, it is possible to rewrite the expression which involves both scalar and vector potential in a way that makes the response look explicitly invariant under gauge transformations.

Current conservation and gauge invariance are intimately related. In the Hamiltonian, the scalar potential couples to density while the vector potential couples to current

$$\delta H = -\int d\mathbf{r}\mathbf{A}(\mathbf{r},t) \cdot \mathbf{J}^A(\mathbf{r}) + \int d\mathbf{r}\phi(\mathbf{r},t)\rho(\mathbf{r}) \tag{10.32}$$

Noether's theorem states that to each continuous transformation that leaves the action invariant, corresponds a conserved quantity. Using this theorem, gauge invariance leads to current conservation, namely

$$\begin{aligned} \frac{\partial\rho(\mathbf{r},t)}{\partial t} &= -\nabla \cdot \mathbf{J}(\mathbf{r},t) \\ \frac{\partial\rho(\mathbf{q},t)}{\partial t} &= -i\mathbf{q} \cdot \mathbf{J}(\mathbf{q},t) \end{aligned} \tag{10.33}$$

We can use current conservation to replace the $\rho(\mathbf{r})$ in the term describing the response of the scalar potential by a $\mathbf{J}(\mathbf{r})$. Take $\mathbf{q}$ in the x-direction to be more specific. This gives

$$\omega\rho(q_x,\omega) = q_x J_x(q_x,\omega) \tag{10.34}$$

Some gymnastics on the time-dependent susceptibility in terms of commutator and Heaviside function gives,

$$\begin{aligned}\frac{\partial\chi^R_{J_x\rho}(q_x,t)}{\partial t} &= \frac{i}{\hbar}\partial_t\left\{\theta(t)\left\langle[J_x(q_x,0),\rho(-q_x,-t)]\right\rangle\right\}\\ &= \frac{i}{\hbar}\delta(t)\left\langle[J_x(q_x,0),\rho(-q_x,0)]\right\rangle + \frac{i}{\hbar}\theta(t)\left\langle[J_x(q_x,0),\partial_t\rho(-q_x,-t)]\right\rangle\\ &= \frac{i}{\hbar}\delta(t)\left\langle[J_x(q_x,0),\rho(-q_x,0)]\right\rangle + \frac{i}{\hbar}\theta(t)(-iq_x)\left\langle[J_x(q_x,0),J_x(-q_x,-t)]\right\rangle\end{aligned} \tag{10.35}$$

where in the last step we used $\partial_t\rho(-q_x,-t) = -iq_xJ_x(-q_x,-t)$. The equal-time commutator is calculated from the f-sum rule. First use the definition

$$\begin{aligned}\chi^R_{J_x\rho}(q_x,t) &= \frac{1}{2V}\left\langle[J_x(q_x,t),\rho\left(-q_x,0\right)]\right\rangle\\ \chi^R_{J_x\rho}(q_x,0) &= \int\frac{d\omega}{2\pi}\chi^R_{J_x\rho}(q_x,\omega) = \frac{1}{2V}\int\frac{d\omega}{2\pi}\left\langle[J_x(q_x,t),\rho\left(-q_x,0\right)]\right\rangle\end{aligned} \tag{10.36}$$

$$\begin{aligned}\chi^R_{J_x\rho}(q_x,\omega) &= \frac{1}{V}\frac{1}{T_p}\left\langle[J_x(q_x,\omega),\rho\left(-q_x,-\omega\right)]\right\rangle\\ &= \frac{\omega}{q_x}\frac{1}{V}\frac{1}{T_p}\left\langle[\rho(q_x,\omega),\rho\left(-q_x,-\omega\right)]\right\rangle\\ &= \frac{\omega}{q_x}\chi^R_{\rho\rho}(q_x,\omega)\end{aligned} \tag{10.37}$$

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(q_x,\omega) = \frac{nq_x^2}{m} \tag{10.38}$$

$$\begin{aligned}\frac{i}{V}\left\langle[J_x\left(q_x,0\right),\rho\left(-q_x,0\right)]\right\rangle &= 2i\chi^R_{J_x\rho}(q_x,t=0)\\ &= i\int\frac{d\omega}{\pi}\chi^R_{J_x\rho}(q_x,\omega)\\ &= i\int\frac{d\omega}{\pi}\frac{\omega}{q_x}\chi^R_{\rho\rho}(q_x,\omega)\\ &= ie^2\int\frac{d\omega}{\pi}\frac{\omega}{q_x}\chi^R_{nn}(q_x,\omega)\\ &= ie^2\frac{1}{q_x}\frac{nq_x^2}{m}\\ &= iq_x\frac{ne^2}{m}\end{aligned} \tag{10.39}$$

A Fourier Transform of the $\partial_t\chi$ w.r.t $t\to\omega$ gives

$$-i(\omega+i\eta)\chi^R_{J_x\rho}(q_x,\omega) = -iq_x\left[\chi^R_{J_xJ_x}(q_x,\omega) - \frac{ne^2}{m}\right] \tag{10.40}$$

this relates the two susceptibilities $\chi^R_{J_x\rho}$ and $\chi^R_{J_xJ_x}$ in the linear response equation.

$$\begin{aligned}\delta\left\langle J_x^A(\mathbf{q},\omega)\right\rangle &= \left[\chi^R_{J_xJ_x}(\mathbf{q},\omega) - \frac{ne^2}{m}\right]A_x(\mathbf{q},\omega) - \chi^R_{J_x\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega)\\ &= \frac{1}{i(\omega+i\eta)}\left[\chi^R_{J_xJ_x}(\mathbf{q},\omega) - \frac{ne^2}{m}\right]\left\{i(\omega+i\eta)A_x(\mathbf{q},\omega) - iq_x\phi(\mathbf{q},\omega)\right\}\end{aligned} \tag{10.41}$$

the part in $\{\}$ is simply the electric field

$$E_x(q_x,\omega) = i(\omega+i\eta)A_x(q_x,\omega) - iq_x\phi(q_x,\omega) \tag{10.42}$$

so we have Ohm's law independent of gauge choice

$$\delta\left\langle J_x^A(\mathbf{q},\omega)\right\rangle = \sigma_{xx}(q_x,\omega)E_x(q_x,\omega) \tag{10.43}$$

$$\sigma_{xx}\left(q_x,\omega\right) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_xj_x}\left(q_x,\omega\right) - \frac{ne^2}{m}\right] = \left[\frac{1}{iq_x}\chi^R_{j_x\rho}\left(q_x,\omega\right)\right] \tag{10.44}$$

10.2.1 Further consequences

The electric and magnetic fields, as well as all observable quantities are invariant under gauge transformations,

$$\begin{aligned} \mathbf{A} &\to \mathbf{A} + \nabla\Lambda \\ \phi &\to \phi - \tfrac{\partial\Lambda}{\partial t} \end{aligned} \tag{10.45}$$

$$\begin{aligned} A_x &\to A_x + iq_x\Lambda \\ \phi &\to \phi + i\omega\Lambda \end{aligned} \tag{10.46}$$

Now choose the Weyl gauge $\phi = 0$, then

$$\delta\left\langle J_x^A\left(q_x,\omega\right)\right\rangle = \left[\chi^R_{J_xJ_x}\left(q_x,\omega\right) - \frac{ne^2}{m}\right] A_x\left(q_x,\omega\right) \tag{10.47}$$

Doing a gauge transformation with $\Lambda(q_x,\omega) \propto \delta(\omega)$ does not induce a new scalar potential ($\phi = 0$). The response to this pure gauge field through the vector potential $\nabla\Lambda$ should be zero

$$\begin{aligned} 0 &= \left[\chi^R_{J_xJ_x}\left(q_x,\omega\right) - \frac{ne^2}{m}\right] iq_x\Lambda\left(q_x,\omega\right) \\ &= \left[\chi^R_{J_xJ_x}\left(q_x,0\right) - \frac{ne^2}{m}\right] iq_x\Lambda\left(q_x,0\right)\delta(\omega) \end{aligned} \tag{10.48}$$

for any $\Lambda\left(q_x,0\right)$, so we conclude that

$$\left[\chi^R_{J_xJ_x}\left(q_x,\omega=0\right) - \frac{ne^2}{m}\right] = 0 \tag{10.49}$$

This can be proven explicitly using the spectral representation:

$$\chi^R_{J_xJ_x}\left(q_x,\omega=0\right) = \int\frac{d\omega'}{\pi}\frac{\chi''_{J_xJ_x}(q_x,\omega')}{\omega'-i\eta} = \int\frac{d\omega}{\pi}\frac{\chi''_{J_xJ_x}(q_x,\omega)}{\omega} \tag{10.50}$$

where we have used the oddness of χ'' since the system has time-reversal symmetry and J_x, J_x have the same signature under time reversal. Using the conservation of charge,

$$\chi''_{J_xJ_x}(q_x,\omega) = \frac{\omega^2}{q_x^2}\chi''_{\rho\rho}(q_x,\omega) = \frac{\omega^2e^2}{q_x^2}\chi''_{nn}(q_x,\omega) \tag{10.51}$$

$$\chi^R_{J_xJ_x}\left(q_x,\omega=0\right) = \frac{1}{q_x^2}\int\frac{d\omega}{\pi}\omega\chi''_{\rho\rho}(q_x,\omega) = \frac{1}{q_x^2}\int\frac{d\omega}{\pi}\omega\chi''_{\rho\rho}(q_x,\omega) = \frac{e^2}{q_x^2}\frac{nq_x^2}{m} = \frac{ne^2}{m} \tag{10.52}$$

So we have proved explicitly

$$\chi^R_{J_xJ_x}\left(q_x,\omega=0\right) = \int\frac{d\omega}{\pi}\frac{\chi''_{J_xJ_x}(q_x,\omega)}{\omega} = \frac{ne^2}{m} \tag{10.53}$$

this is also a sum rule.

10.2.2 Simplification of Longitudinal Conductivity

The expression for the longitudinal conductivity

$$\sigma_{xx}\left(q_x,\omega\right) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{J_xJ_x}\left(q_x,\omega\right) - \frac{ne^2}{m}\right] \tag{10.54}$$

can be written in an even more convenient manner by using our previous results and the spectral representation for the current-current correlation function

$$\begin{aligned} \sigma_{xx}\left(q_x,\omega\right) &= \frac{1}{i(\omega+i\eta)}\left[\chi^R_{J_xJ_x}\left(q_x,\omega\right) - \chi^R_{J_xJ_x}\left(q_x,\omega=0\right)\right] \\ &= \frac{1}{i(\omega+i\eta)}\left[\int\frac{d\omega'}{\pi}\frac{\chi''_{J_xJ_x}(q_x,\omega')}{\omega'-(\omega+i\eta)} - \int\frac{d\omega'}{\pi}\frac{\chi''_{J_xJ_x}(q_x,\omega')}{\omega'}\right] \\ &= \frac{1}{i(\omega+i\eta)}\int\frac{d\omega'}{\pi}\chi''_{J_xJ_x}(q_x,\omega')\frac{\omega+i\eta}{\omega'\left(\omega'-(\omega+i\eta)\right)} \\ &= \frac{1}{i}\int\frac{d\omega'}{\pi}\frac{\chi''_{J_xJ_x}(q_x,\omega')}{\omega'\left(\omega'-(\omega+i\eta)\right)} \end{aligned} \tag{10.55}$$

From this formula, we easily obtain with the usual identity for principal parts,

$$\Re\sigma_{xx}(q_x,\omega) = \frac{\chi''_{J_xJ_x}(q_x,\omega)}{\omega} \tag{10.56}$$

from which we obtain the conductivity sum rule valid for arbitrary q_x:

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Re\sigma_{xx}(q_x,\omega) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{\chi''_{J_xJ_x}(q_x,\omega)}{\omega}\\ &= \frac{1}{2}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\omega^2e^2}{q_x^2}\frac{\chi''_{nn}(q_x,\omega)}{\omega}\\ &= \frac{ne^2}{2m} = \frac{\varepsilon_0\omega_p^2}{2}\end{aligned} \tag{10.57}$$

In the above expression, ε_0 is the permittivity of the vacuum and ω_p^2 is the plasma frequency, which we will discuss later. Using the fact that the real part of the conductivity is an even function of ω, as follows from the fact that $\chi''_{j_xj_x}(q_x,\omega)$ is odd, the above formula is often written in the form of an integral from 0 to ∞. The case $q_x = 0$ needs a separate discussion, presented in the following section.

11 Drude Weight, Metals, Insulators and Superconductors

All the above considerations about conductivity, correlation functions and sum rules may seem rather formal, and even useless. Let us put what we learned to work. In the present Chapter, we will find some powerful and unexpected results. For example, one can measure the penetration depth, i.e. the distance over which a static magnetic field is expelled by a superconductor, by doing instead a finite frequency conductivity measurement.

If we begin to talk about a superconductor, the first thing that comes to mind is the DC conductivity. Even if in the end we will see that zero resistance or infinite conductivity is not what characterizes a superconductor, this is a legitimate starting point. Suppose we are interested in the DC conductivity. We then need the response for a uniform, or very long wavelength field, i.e. the limit $q_x \to 0$ of our earlier formulae. It is important to notice that this is the proper way to compute the *DC* conductivity: Take the $\mathbf{q} \to 0$ limit, before the $\omega \to 0$ limit. In the opposite limit the response vanishes. Physically, transport probes dynamical quantities. A DC measurement can be seen as the zero frequency limit of a microwave experiment for example. By taking the $\mathbf{q} \to \mathbf{0}$ limit first, we ensure that we are looking at an infinite volume, where energy levels can be arbitrarily close in energy. Then only can we take the zero frequency limit and still get absorption when the state is metallic. Otherwise the discrete nature of the energy states would not allow absorption in the zero frequency limit. By asking questions about the DC conductivity, we are clearly beginning to ask what is the difference between a perfect metal, a superconductor, and an insulator. This is the question we will focus on in this chapter. Many of the answers were given by Kohn. The first step is to define the Drude weight.

11.1 The Drude weight

We start with the conductivity

$$\Re\sigma_{xx}(q_x,\omega) = \frac{\chi''_{j_xj_x}(q_x,\omega)}{\omega} \tag{11.1}$$

In the correct limit $q_x \to 0$ first,

$$\Re\sigma_{xx}(0,\omega) = \frac{\chi''_{j_xj_x}(0,\omega)}{\omega} \tag{11.2}$$

If we take the full expression

$$\begin{aligned}\sigma_{xx}(q_x,\omega) &= \frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_xj_x}(q_x,\omega) - \frac{ne^2}{m}\right]\\ &= \left(\mathcal{P}\frac{1}{i\omega} - \pi\delta(\omega)\right)\left[\chi^R_{j_xj_x}(q_x,\omega) - \frac{ne^2}{m}\right]\\ &= \mathcal{P}\frac{1}{i\omega}\left[\chi^R_{j_xj_x}(q_x,\omega) - \frac{ne^2}{m}\right] - \pi\delta(\omega)\left[\chi^R_{j_xj_x}(q_x,\omega) - \frac{ne^2}{m}\right]\end{aligned} \tag{11.3}$$

$$\Re\left[\sigma_{xx}\left(q_x,\omega\right)\right]=\mathcal{P}\frac{\chi''_{j_xj_x}\left(q_x,\omega\right)}{\omega}-\pi\delta(\omega)\left[\Re[\chi^R_{j_xj_x}\left(q_x,\omega\right)]-\frac{ne^2}{m}\right] \tag{11.4}$$

at $q_x\to 0$,

$$\Re\left[\sigma_{xx}\left(0,\omega\right)\right]=\mathcal{P}\frac{\chi''_{j_xj_x}\left(0,\omega\right)}{\omega}-\pi\delta(\omega)\left[\Re[\chi^R_{j_xj_x}\left(0,\omega\right)]-\frac{ne^2}{m}\right] \tag{11.5}$$

the coefficient of $\delta(\omega)$ at zero frequency is called the **Drude weight** D:

$$D=\pi\lim_{\omega\to 0}\left[\frac{ne^2}{m}-\Re\left[\chi^R_{j_xj_x}\left(0,\omega\right)\right]\right] \tag{11.6}$$

In general

$$\lim_{\omega\to 0}\Re\left[\sigma_{xx}(0,\omega)\right]=D\delta(\omega)+(...) \tag{11.7}$$

Alternatively, it can be written as

$$D=\pi\lim_{\omega\to 0}\omega\Im\left[\sigma_{xx}\left(0,\omega\right)\right] \tag{11.8}$$

where we used the fact that $\lim_{\omega\to 0}\chi''_{j_xj_x}\left(q_x,\omega\right)=0$ since it is odd.

In practice, the delta function in optical experiments is broadened by impurity scattering or scattering due to finite temperature. Whenever there is a peak in the conductivity centered at zero frequency, one refers to it as a Drude peak.

11.2 What is a metal

To understand what is a metal, let us first begin by asking what is the Drude weight for free electrons.

Let the current $\mathbf{J}=ne\mathbf{v}$. Then, using Newton's equation of motion in an electric field we find,

$$\frac{\partial\mathbf{j}(\mathbf{q}=\mathbf{0},t)}{\partial t}=\frac{ne^2}{m}\mathbf{E}(\mathbf{q}=\mathbf{0},t) \tag{11.9}$$

$$\mathbf{j}(\mathbf{q}=\mathbf{0},\omega)=-\frac{1}{i(\omega+i\eta)}\frac{ne^2}{m}\mathbf{E}(\mathbf{q}=\mathbf{0},\omega) \tag{11.10}$$

$$\sigma(\mathbf{q}=0,\omega)=-\frac{1}{i(\omega+i\eta)}\frac{ne^2}{m} \tag{11.11}$$

From this we see that the conductivity has only a Drude contribution (free acceleration).

$$\Re\sigma(\mathbf{q}=\mathbf{0},\omega)=\pi\frac{ne^2}{m}\delta(\omega) \tag{11.12}$$

$$D=\frac{\pi ne^2}{m} \tag{11.13}$$

There is no contribution from the $\pi\lim_{\omega\to 0}\Re\chi^R_{j_xj_x}(0,\omega)$, the current of a single particle is conserved, meaning that $\mathbf{J}(t)=e^{iHt}\mathbf{J}e^{-iHt}=\mathbf{J}$, and $[J,J]=0$. For interacting electrons this is not true, so we do get finite contributions from the susceptibility term. Kohn defined a metal by a finite Drude weight at $T=0$. In the absence of impurities we have a $\delta(\omega)$, leading to infinite conductivity even in the presence of interaction. In the presence of elastic scattering, by impurities for example, the zero-temperature Drude weight is broadened.

At finite temperature or when there is inelastic scattering with some other system, like the phonons, the delta function is also broadened. The conductivity is not infinite at zero frequency, but it has a weight that can be close to the ideal Drude weight if there is not too much broadening.

11.3 What is an insulator

Kohn's criterion for a material to be an insulator is that it has a vanishing DC conductivity, or Drude weight $D=0$. The DC conductivity vanishes whenever

$$\lim_{\omega\to 0}\Re\left[\chi^R_{j_xj_x}(0,\omega)\right]=\lim_{\omega\to 0}\mathcal{P}\int\frac{d\omega'}{\pi}\frac{\chi''_{j_xj_x}\left(0,\omega'\right)}{\omega'-\omega}=\frac{ne^2}{m} \tag{11.14}$$

Recalling the $\chi_{J_x J_x}$ sum rule

$$\chi^R_{J_x J_x}(q_x, \omega = 0) = \int \frac{d\omega}{\pi} \frac{\chi''_{J_x J_x}(q_x, \omega')}{\omega'} = \frac{ne^2}{m} \tag{11.15}$$

this means that when the order of limits can be inverted, the system is an insulator:

$$\lim_{\omega \to 0} \lim_{q_x \to 0} \Re \left[\chi^R_{j_x j_x}(q_x, \omega)\right] = \lim_{q_x \to 0} \lim_{\omega \to 0} \Re \left[\chi^R_{j_x j_x}(q_x, \omega)\right] \tag{11.16}$$

This occurs in particular when there is a gap Δ. In this case, then $\chi''_{j_x j_x}(q_x, \omega) = 0$ for all q_x as long as $\omega < \Delta$. In particular, there can be no contribution from zero frequency since $\chi''_{j_x j_x}(q_x, 0) = 0$ so that the principal part integral and the full integral are equal.

Gapless insulators: The condition of having a gap is sufficient but not necessary to have an insulator. There are examples where there is no gap in the two-particle excitations but there is a vanishing DC conductivity (R. Cote & AMS Tremblay. Spiral magnets as gapless Mott insulators. EPL (Europhysics Letters), 29(1):37, 1995.).

11.4 What is a Superconductor

The superconducting state is a state of matter that is thermodynamically stable. It expels magnetic fields whether the fields are applied at a temperature above or below the superconducting temperature. Magnetic fields are either expelled completely by a superconductor (Type I) or they penetrate in quantized units (Type II).

First, a bit of phenomenology about the **Meissner effect**. London assumed that the response was controlled only by the diamagnetic term:

$$\delta \left\langle j^A_a(\mathbf{q}, 0)^T \right\rangle = -\frac{n_s e^2}{m} A^T_a(\mathbf{q}, 0) \tag{11.17}$$

To simplify the discussion, I take a simple case where the $\mathbf{q}$ dependence of the prefactor n_s can be neglected in the zero-frequency limit, (we keep the zeroth order term in the power series in $\mathbf{q}$). I have written n_s to emphasize that this quantity is in general different from the complete density n. This quantity, n_s is called the **superfluid density**. The above equation is the so-called **London equation**. We take the curl on both sides of the Fourier transformed expression,

$$\nabla \times \delta \langle \mathbf{j}(\mathbf{r}, \omega = 0) \rangle = -\frac{n_s e^2}{m} \mathbf{B}(\mathbf{r}, \omega = 0) \tag{11.18}$$

and then multiply by μ_0, the permeability of the vacuum, and use Maxwell's equation $\nabla \times \mathbf{B}(\mathbf{r}, \omega = 0) = \mu_0 \mathbf{j}(\mathbf{r}, \omega = 0)$ as well as $\nabla \times (\nabla \times \mathbf{B}) = \nabla(\nabla \cdot \mathbf{B}) - \nabla^2 \mathbf{B} = -\nabla^2 \mathbf{B}$. The last equation takes the form,

$$\nabla^2 \mathbf{B} = \frac{n_s e^2}{m} \mu_0 \mathbf{B} \tag{11.19}$$

whose solution in the half-plane geometry is

$$B_y(x) = B_y(0) e^{-x/\lambda_L} \tag{11.20}$$

with London penetration depth

$$\lambda_L^{-2} = \frac{n_s e^2}{m} \mu_0 \tag{11.21}$$

This is perfect diamagnetism.

I now show how the London equation follows from our formalism. First recall the f-sum rule

$$\left[\chi^R_{j_x j_x}(q_x, 0) - \frac{ne^2}{m}\right] = 0 \tag{11.22}$$

Superficially then, it looks as if there can be no $\omega = 0$ response of the current to a pure vector potential. That is a correct assumption, but only for the longitudinal part of the vector potential. Gauge invariance does not force the transverse response to vanish. Indeed, gauge transformations are always longitudinal ($A_x \to A_x + i q_x \Lambda$). Hence, it is possible to have,

$$\left[\chi^R_{j_y j_y}(q_x, 0) - \frac{ne^2}{m}\right] = -\frac{n_s(q_x) e^2}{m} \tag{11.23}$$

where n_s is any density less than n. A superconductor will indeed have such a non-vanishing "**transverse Drude weight**". We will be interested in the long wave length limit short-coherence length limit (that will be defined later) so that the q_x dependence in $n_s(q_x)$ can be neglected. It will be shown that positivity of the dissipation will imply that n_s cannot be larger than n.

Combine this with Kubo formula for the transverse part of conductivity at $\omega = 0$, assuming $\mathbf{A}$ come from a finite magnetic field only,

$$\delta \left\langle j_y^A (q_x, 0)^T \right\rangle = \left[\left(\chi^R_{j_y j_y}(q_x, 0) \right)^T - \frac{ne^2}{m} \right] A_y^T (q_x, 0) . \tag{11.24}$$

and we have the London equation.

Superfluid stiffness: The energy associated with a gradient in the phase of the superconductor, is often written in the form $\frac{1}{2}\rho_s(\nabla\theta)^2$. The quantity ρ_s is known as the superfluid stiffness: $\rho_s \mu_0 = \lambda_L^{-2}$.

Since the magnetic induction $\mathbf{B}$ obeys $\mathbf{B} = \boldsymbol{\mu}_0(\mathbf{H} + \mathbf{M})$, another way to look at this result is that the magnetic field intensity $\mathbf{H}$ is cancelled by the magnetization $\mathbf{M}$ to yield a vanishing magnetic induction $\mathbf{B}$.

Why are the transverse and longitudinal zero-frequency responses different in a superconductor? By comparing the result of the f-sum rule $\left[\chi^R_{j_x j_x}(q_x, 0) - \frac{ne^2}{m} \right] = 0$ with the definition of the transverse Drude weight $\left[\chi^R_{j_y j_y}(q_x, 0) - \frac{ne^2}{m} \right] = -\frac{n_s(q_x)e^2}{m}$ (we can change $x \leftrightarrow y$) this can happen only if

$$\lim_{q_x \to 0} \chi^R_{j_x j_x}(q_x, 0, \omega = 0) \neq \lim_{q_y \to 0} \chi^R_{j_x j_x}(0, q_y, \omega = 0) \tag{11.25}$$

or in other words

$$\lim_{q_x \to 0} \int dt \int d\mathbf{r} e^{-iq_x x} \chi^R_{j_x j_x}(\mathbf{r}, t) \neq \lim_{q_y \to 0} \int dt \int d\mathbf{r} e^{-iq_y y} \chi^R_{j_x j_x}(\mathbf{r}, t) \tag{11.26}$$

That is the true definition of a superconductor. A superconductor can have a finite conductivity in the presence of magnetic flux quanta and have no gap like in a d-wave superconductor. The above two limits cannot be inverted in a superconductor because **long-range order** leads to $\chi^R_{j_x j_x}(\mathbf{r}, \omega = 0)$ that does not decay fast enough for the integral to be uniformly convergent, i.e. independent of the order of limits: $\chi^R_{j_x j_x}(\mathbf{r}, \omega = 0)$ does not decay the same way at infinity for $\mathbf{r}$ along the direction x of the current and perpendicular to it. More on this in a later chapter. In an ordinary metal there is no such long-range order and both limits are identical so that the London penetration depth is infinite, in other words $n_s = 0$ for a metal.

Finally, a superconductor has infinite DC conductivity, namely at $\omega = 0$. While the delta function Drude peak is an idealization in a metal, in a superconductor, the delta function response at $\omega = 0$ is really there. In other words, the full transverse conductivity is

$$\Re\sigma_{yy}(q_x, \omega) = \mathcal{P}\frac{1}{\omega}\left[\chi''_{j_y j_y}(q_x, \omega) \right] - \pi\delta(\omega) \left[\Re\chi^R_{j_y j_y}(q_x, \omega) - \frac{ne^2}{m} \right] \tag{11.27}$$

12 Relation Between Conductivity and Dielectric Constant

The relation between dielectric constant and conductivity is a matter of macroscopic electromagnetism. Hence, since we already know the relation between conductivity and correlation functions, we will be able to relate dielectric constant and correlation functions that we can compute later. The dielectric constant is basic to optical measurements. In infrared spectroscopy for example, one measures the reflectivity or the transmission coefficient, either of which is related to the complex index of refraction which follows from the dielectric constant.

Start from Maxwell's equations. We consider a translationally invariant system, so that it suffices to consider the Fourier-space version

$$\begin{aligned} i\mathbf{q} \cdot \mathbf{E} &= \frac{\rho}{\varepsilon_0} \\ i\mathbf{q} \times \mathbf{E} &= i(\omega + i\eta)\mathbf{B} \\ i\mathbf{q} \cdot \mathbf{B} &= 0 \\ i\mathbf{q} \times \mathbf{B} &= \mu_0 \mathbf{j} - \frac{i(\omega + i\eta)}{c^2}\mathbf{E} \end{aligned} \tag{12.1}$$

where $\varepsilon_0 = 8.85 \times 10^{-12}$ farad/meter is the permittivity of vacuum and μ_0 its permeability is given by $\mu_0 = 4\pi \times 10^{-7}$ henry/meter. The speed of light is related to these quantities by $\varepsilon_0 \mu_0 = 1/c^2$.

12.1 Transverse dielectric constant

Now assume only transverse electric field $\mathbf{q}\cdot\mathbf{E}=0$, which results in $\mathbf{q}\cdot\mathbf{j}=0$ also, here we have

$$\mathbf{j}=\sigma^T\mathbf{E} \tag{12.2}$$

the last of Maxwell's equations now reads,

$$i\mathbf{q}\times\mathbf{B}=\mu_0\sigma^T\cdot\mathbf{E}-\frac{i(\omega+i\eta)}{c^2}\mathbf{E} \tag{12.3}$$

from the second Maxwell equation $i\mathbf{q}\times\mathbf{E}=i(\omega+i\eta)\mathbf{B}$ and that $\mathbf{q}\times(\mathbf{q}\times\mathbf{E})=\mathbf{q}(\mathbf{q}\cdot\mathbf{E})-q^2\mathbf{E}=-q^2\mathbf{E}$, we have

$$q^2\mathbf{E}=i(\omega+i\eta)\mu_0\sigma^T\cdot\mathbf{E}+\frac{(\omega+i\eta)^2}{c^2}\mathbf{E}\equiv\frac{(\omega+i\eta)^2}{c^2}\frac{\epsilon^T}{\varepsilon_0}\mathbf{E} \tag{12.4}$$

where the last equality is the definition of the dielectric tensor ϵ^T. We have dispersion relation (where ϵ is some diagonal term of ϵ^T)

$$\omega=\pm\sqrt{\frac{\varepsilon_0}{\epsilon}}cq \tag{12.5}$$

If there was no coupling to matter, the electric field would have the usual pole for light $\omega=cq$ and $\epsilon^T=\varepsilon_0$. If $\epsilon<0$, we will have $\omega=\pm i\sqrt{\frac{\varepsilon_0}{-\epsilon}}cq$. The component $E(\omega,\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}}e^{-i\omega t}$ then will contain exponentially decaying terms, which means that the given EM mode cannot propagate.

In general,

$$\begin{aligned}\epsilon^T&=\varepsilon_0\left[1+\frac{i\sigma^T/\varepsilon_0}{\omega+i\eta}\right]\\&=\varepsilon_0+\frac{i\sigma^T}{\omega+i\eta}\end{aligned} \tag{12.6}$$

In the simple case where the dielectric tensor is diagonal, it is related to the dielectric constant n and the attenuation constant κ through $\sqrt{\epsilon}=n+i\kappa$. Using the Kubo formula for the conductivity in terms of response function

$$\sigma_{yy}\left(q_x,\omega\right)=\frac{1}{i(\omega+i\eta)}\left[\chi^R_{J_yJ_y}\left(q_x,\omega\right)-\frac{ne^2}{m}\right] \tag{12.7}$$

we have that

$$\begin{aligned}\epsilon^T&=\varepsilon_0+\frac{1}{(\omega+i\eta)^2}\left[\left[\chi^R_{\mathbf{jj}}\left(\mathbf{q},\omega\right)\right]^T-\omega_p^2\varepsilon_0\right]\\&=\varepsilon_0\left(1-\frac{\omega_p^2}{(\omega+i\eta)^2}\right)+\frac{1}{(\omega+i\eta)^2}\left[\chi^R_{\mathbf{jj}}\left(\mathbf{q},\omega\right)\right]^T\end{aligned} \tag{12.8}$$

where we used plasma frequency $\omega_{\mathrm{p}}=\sqrt{\frac{ne^2}{m\varepsilon_0}}$. If we ignore the $\chi^R_{\mathbf{jj}}$ term, the first part is negative when $\omega<\omega_p$, so no propagation is allowed below plasma frequency.

12.2 Longitudinal dielectric constant

Let the system be subjected to some external charge $\rho_e(\mathbf{q},\omega)$. The electric field depends on the total charge, including the induced one

$$i\mathbf{q}\cdot\mathbf{E}=\frac{(\rho_e+\delta\langle\rho\rangle)}{\varepsilon_0} \tag{12.9}$$

The longitudinal dielectric constant is defined by

$$i\mathbf{q}\cdot\epsilon^L\cdot\mathbf{E}=\rho_e \tag{12.10}$$

where $\epsilon^L(\mathbf{q},\omega)$ is a retarded response function. The ration between these two equations give

$$\frac{1}{\epsilon^L}=\frac{\rho_e+\delta\langle\rho\rangle}{\varepsilon_0\rho_e} \tag{12.11}$$

In the Landau gauge, where $\nabla \cdot \mathbf{A} = 0$ so $i\mathbf{q} \cdot \mathbf{A} = 0$, the electric field $\mathbf{E} = -\partial_t \mathbf{A}$ will then be transverse. So the only longitudinal contribution comes from $\mathbf{E} = -\nabla\phi$, this leads to Poisson's equation:

$$\phi_e(\mathbf{q}, \omega) = \frac{1}{\varepsilon_0 q^2} \rho_e(\mathbf{q}, \omega) \tag{12.12}$$

As above, linear response to

$$\delta\mathcal{H}(t) = \int d\mathbf{r} \rho(\mathbf{r}) \phi_e(\mathbf{r}, t) \tag{12.13}$$

is given by

$$\delta \langle \rho(\mathbf{q}, \omega) \rangle = -\chi^R_{\rho\rho}(\mathbf{q}, \omega) \phi_e(\mathbf{q}, \omega) \tag{12.14}$$

so we have

$$\frac{1}{\epsilon^L} = \frac{1}{\varepsilon_0} \left[1 - \frac{1}{\varepsilon_0 q^2} \chi^R_{\rho\rho}(\mathbf{q}, \omega) \right] \tag{12.15}$$

The longitudinal dielectric constant is simply related to the cross section for inelastic electron scattering. Indeed, the fluctuation-dissipation theorem gives us

$$S_{\rho\rho}(\mathbf{q}, \omega) = \frac{2\hbar}{1 - e^{-\beta\hbar\omega}} \Im \left[\chi^R_{\rho\rho}(\mathbf{q}, \omega) \right] = -\frac{2\hbar}{1 - e^{-\beta\hbar\omega}} q^2 \Im \left[\frac{\varepsilon_0^2}{\epsilon^L(\mathbf{q}, \omega)} \right] \tag{12.16}$$

(in the book there is only a single power of ε_0)

Part III
Green's function in single-particle quantum mechanics

13 Definitions

13.1 Preliminaries

For a while we work with the continuum normalization for the position $|\mathbf{r}\rangle$ and momentum $|\mathbf{k}\rangle$ eigenstates.

$$\begin{aligned} \int d\mathbf{r}|\mathbf{r}\rangle\langle\mathbf{r}| &= 1 \\ \langle\mathbf{r} \mid \mathbf{r}'\rangle &= \delta(\mathbf{r}-\mathbf{r}') \end{aligned} \tag{13.1}$$

momentum eigenstates are **not normalized**

$$\langle\mathbf{r} \mid \mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} \tag{13.2}$$

$$\begin{aligned} \int \frac{d\mathbf{k}}{(2\pi)^3}|\mathbf{k}\rangle\langle\mathbf{k}| &= 1 \\ \langle\mathbf{k} \mid \mathbf{k}'\rangle &= (2\pi)^3\delta(\mathbf{k}-\mathbf{k}') \end{aligned} \tag{13.3}$$

13.2 Definition of the Green's function

Previously, we needed to know how an operator, such as charge for example, was correlated with another one at another time. The generalization of this idea for a one-body wave function is to know how it correlates with itself at different times. That is also useful because the main idea of perturbation theory is to prepare a state $\Psi_0(\mathbf{r}', t')$ and to let it evolve adiabatically in the presence of the perturbation into the new eigenstate $\Psi(\mathbf{r}, t)$.

According to Shrodinger equation

$$\begin{aligned} i\partial_t|\psi(t)\rangle &= \hat{H}|\psi(t)\rangle \\ |\psi(t)\rangle &= e^{-i\hat{H}t}|\psi(0)\rangle \end{aligned} \tag{13.4}$$

now suppose we make a measurement which result in the system in a definite state $|\psi(0)\rangle$. This measurement is a perturbation which propagate forward as $e^{-i\hat{H}t}$ and cannot propagate backwards, nor can $t<0$ wavefunction propagate forward. Therefore, after a measurement, we must restrict to $t>0$, this is done by adding a $\theta(t)$ in the Shrodinger's equation

$$|\psi(t)\rangle\,\theta(t) = e^{-i\hat{H}t}\theta(t)|\psi(0)\rangle \equiv i\hat{G}^R(t)|\psi(0)\rangle \tag{13.5}$$

so the propagator should be

$$\hat{G}^R(t) = -ie^{-i\hat{H}t}\theta(t) \tag{13.6}$$

Notice that, unlike the harmonic oscillator, the Shrodinger equation does not have linear combination of response which starts at different time, but only a single perturbation at $t=0$.

The differential equation satisfied by the propagator $\hat{G}^R(t)$ is

$$\left(i\frac{\partial}{\partial t} - \hat{H}\right)\hat{G}^R(t) = \delta(t) \tag{13.7}$$

we have

$$\langle\mathbf{r} \mid \Psi(t)\rangle\theta(t) = i\int d\mathbf{r}'\left\langle\mathbf{r}\left|\widehat{G}^R(t)\right|\mathbf{r}'\right\rangle\langle\mathbf{r}' \mid \Psi(0)\rangle \tag{13.8}$$

If $\Psi(0) = |\mathbf{r}''\rangle$, then

$$\Psi(\mathbf{r}, t)\theta(t) = i\left\langle\mathbf{r}\left|\widehat{G}^R(t)\right|\mathbf{r}''\right\rangle \tag{13.9}$$

we define $G^R(\mathbf{r},\mathbf{r}',t) \equiv \left\langle \mathbf{r} \left| \widehat{G}^R(t) \right| \mathbf{r}'' \right\rangle$. To obtain a differential equation for $G^R(\mathbf{r},\mathbf{r}',t)$,

$$\begin{aligned} \int d\mathbf{r}' \left\langle \mathbf{r} \right| \left(i\frac{\partial}{\partial t} - \hat{H} \right) \left| \mathbf{r}' \right\rangle \left\langle \mathbf{r}' \right| \hat{G}^R(t) \left| \mathbf{r}'' \right\rangle &= \delta(t) \left\langle \mathbf{r} \right| \left. \mathbf{r}'' \right\rangle \\ \int d\mathbf{r}' \left(i\frac{\partial}{\partial t}\delta(\mathbf{r}-\mathbf{r}') - \left\langle \mathbf{r} \right| H \left| \mathbf{r}' \right\rangle \right) G^R(\mathbf{r}',\mathbf{r}'',t) &= \delta(t)\delta(\mathbf{r}-\mathbf{r}'') \\ \left(i\frac{\partial}{\partial t} - H_{\mathbf{r}} \right) G^R(\mathbf{r},\mathbf{r}'',t) &= \delta(t)\delta(\mathbf{r}-\mathbf{r}'') \end{aligned} \tag{13.10}$$

since $\left\langle \mathbf{r} \right| H \left| \psi \right\rangle = H_{\mathbf{r}} \left\langle \mathbf{r} \right| \left. \psi \right\rangle = H_{\mathbf{r}}\psi(\mathbf{r})$.
Formally, we can invert the equation for the Green's function as follows:

$$\hat{G}^R(t) = \left(i\frac{\partial}{\partial t} - \hat{H} \right)^{-1} \delta(t) \tag{13.11}$$

and thus $\hat{G}^R(t)$ can be thought of as the response to a delta function $\delta(t)$. The inverse is taken in matrix language.

14 Properties of Green's function

14.1 Representation in frequency space and Lehmann representation

We define Fourier Transform

$$G^R(\mathbf{r},\mathbf{r}';\omega) = -i\int_0^\infty dt e^{i(\omega+i\eta)t} \left\langle \mathbf{r} \left| e^{-iHt} \right| \mathbf{r}' \right\rangle \tag{14.1}$$

In this expression, I have used the $\theta(t)$ and the corresponding $\omega + i\eta$ in Fourier space to insure causality. Insert in this equation a complete set of energy eigenstates

$$\begin{aligned} H|n\rangle &= E_n|n\rangle \\ \left\langle n \left| e^{-iHt} \right| m \right\rangle &= e^{-iE_n t}\delta_{n,m} \end{aligned} \tag{14.2}$$

$$\begin{aligned} G^R(\mathbf{r},\mathbf{r}';\omega) &= \sum_n \frac{\langle \mathbf{r} \mid n\rangle \langle n \mid \mathbf{r}'\rangle}{\omega + i\eta - E_n} = \sum_n \frac{\Psi_n(\mathbf{r})\Psi_n^*(\mathbf{r}')}{\omega + i\eta - E_n} \\ &= \langle \mathbf{r}| \frac{1}{\omega + i\eta - \hat{H}} |\mathbf{r}'\rangle \end{aligned} \tag{14.3}$$

Define spectral weight

$$A(\mathbf{r},\mathbf{r}';\omega) \equiv -2\Im G^R(\mathbf{r},\mathbf{r}';\omega) = \sum_n \Psi_n(\mathbf{r})\Psi_n^*(\mathbf{r}')2\pi\delta(\omega - E_n) \tag{14.4}$$

we can thus write

$$\hat{G}^R(\omega) = \frac{1}{\omega + i\eta - \hat{H}} \tag{14.5}$$

this is called the **resolvent operator**. We have $G^R(\mathbf{r},\mathbf{r}';\omega) = \left\langle \mathbf{r} \left| \widehat{G}^R(\omega) \right| \mathbf{r}' \right\rangle$.

$$\hat{A}(\omega) = -2\Im\hat{G}^R(\omega) = 2\pi\delta(\omega - \hat{H}) \tag{14.6}$$

$$\begin{aligned} A(\mathbf{r},\mathbf{r}';\omega) &= \langle \mathbf{r}| 2\pi\delta(\omega - \hat{H}) |\mathbf{r}'\rangle \\ &= \sum_n \langle \mathbf{r}| 2\pi\delta(\omega - E_n) |n\rangle \langle n| |\mathbf{r}'\rangle \\ &= \sum_n \Psi_n(\mathbf{r})\Psi_n^*(\mathbf{r}')2\pi\delta(\omega - E_n) \end{aligned} \tag{14.7}$$

We thus see more clearly what is meant by the inverse operator. This could be generalized to

$$G^R_{ab} = \langle a| \frac{1}{\omega + i\eta - \hat{H}} |b\rangle \tag{14.8}$$

where $|a\rangle, |b\rangle$ are two vectors from a set of basis. Take a free particle with momentum eigenstates $H|\mathbf{k}\rangle = \varepsilon_{\mathbf{k}}|\mathbf{k}\rangle$, we have

$$\left\langle \mathbf{k} \left| \widehat{G}^R(\omega) \right| \mathbf{k}' \right\rangle = \left\langle \mathbf{k} \left| \frac{1}{\omega + i\eta - \hat{H}} \right| \mathbf{k}' \right\rangle = \frac{\langle \mathbf{k} \mid \mathbf{k}' \rangle}{\omega + i\eta - \varepsilon_{\mathbf{k}}} \tag{14.9}$$

We see that

1. The poles of $G^R(\mathbf{r}, \mathbf{r}', \omega)$ are at the eigenenergies.
2. The residue at the pole is related to the corresponding energy eigenstate.
3. This is the analog of a Lehmann representation, that we will encounter later.

We can also define an advanced propagator

$$\widehat{G}^A(t) = ie^{-iHt}\theta(-t) \tag{14.10}$$

with its resolvent

$$\widehat{G}^A(\omega) = \frac{1}{\omega - i\eta - \hat{H}} \tag{14.11}$$

14.2 Relations to Physical Observables

For an arbitrary state that has evolved from a given initial condition, we can use the relation between Green's function and wave function to build any time-dependent expectation value using the usual rules of quantum mechanics.

We define the local density of states

$$\rho(\mathbf{r}, \omega) = \frac{1}{2\pi} A(\mathbf{r}, \mathbf{r}; \omega) = \sum_n \Psi_n(\mathbf{r}) \Psi_n^* (\mathbf{r}) \, \delta (\omega - E_n) \tag{14.12}$$

as **local density of states**, a quantity relevant in particular when there is no translational invariance. If we have a tip whose density of states is structureless, to a good approximation, the local density of states is what is measured by scanning tunneling microscopes. The local density of states can be interpreted as the probability that an electron in an eigenstate of energy $\omega = E_n$ is at position $\mathbf{r}$, namely $\Psi_n(\mathbf{r})\Psi_n^*(\mathbf{r})$ summed over all eigenstates with the same energy.

Integrating over all positions, we obtain the **density of states**

$$\begin{aligned}
\rho(\omega) &= \int d\mathbf{r} \rho(\mathbf{r}, \omega) \\
&= \int d\mathbf{r} \sum_n \langle \mathbf{r} |n\rangle \langle n| \mathbf{r}\rangle \delta (\omega - E_n) \\
&= \sum_n \delta (\omega - E_n) \\
&= \mathrm{Tr} \left[\delta \left(\omega - \hat{H} \right) \right] \\
&= -\frac{1}{\pi} \mathrm{Tr} \left[\Im \frac{1}{\omega - \hat{H} + i\eta} \right] \\
&= -\frac{1}{\pi} \mathrm{Tr} \left[\Im \widehat{G}^R(\omega) \right]
\end{aligned} \tag{14.13}$$

where we have extended

$$\frac{1}{\omega - i\eta} = \mathcal{P} \frac{1}{\omega} + i\pi\delta(\omega) \tag{14.14}$$

to operator form. In summary, the density of states can be expressed in a basis-independent form in terms of the resolvent:

$$\rho(\omega) = -\frac{1}{\pi}\,\mathrm{Tr}\left[\Im \hat{G}^R(\omega)\right] \tag{14.15}$$

This procedure can be used for any other observable. Take operator $\hat{K}$, if we wish to find its expectation in eigenstate $|n\rangle$. First notice

$$\delta(\omega - \hat{H}) = \delta(\omega - \sum_n E_n |n\rangle \langle n|) = \sum_n \delta(\omega - E_n) |n\rangle \langle n| \tag{14.16}$$

this can be seen from the fact that $\delta(\omega - \hat{H})|n\rangle = \delta(\omega - E_n)|n\rangle$ is satisfied for LHS and RHS. Second, there is a way to restrict $\delta(\omega - \hat{H})$ to a single eigenstate suspace:

$$\int_{E_n-\varepsilon}^{E_n+\varepsilon} d\omega \delta(\omega - \hat{H}) = \int_{E_n-\varepsilon}^{E_n+\varepsilon} d\omega \delta(\omega - E_n) |n\rangle \langle n| = |n\rangle \langle n| \tag{14.17}$$

Second, there is a way to restrict the Hamiltonian to a single eigenstate. Since $\hat{A}(\omega) = 2\pi\delta(\omega - \hat{H})$, if we restrict $\omega \in [E_n - \varepsilon, E_n + \varepsilon]$,

$$\begin{aligned} K_n &= \langle n| \hat{K} |n\rangle = \mathrm{Tr}\left(|n\rangle \langle n| \hat{K}\right) \\ &= \int_{E_n-\varepsilon}^{E_n+\varepsilon} d\omega\, \mathrm{Tr}\left(\delta(\omega - \hat{H})\hat{K}\right) \\ &= \int_{E_n-\varepsilon}^{E_n+\varepsilon} \frac{d\omega}{2\pi}\, \mathrm{Tr}\left(\hat{A}(\omega)\hat{K}\right) \end{aligned} \tag{14.18}$$

in position space, for a local operator $\langle \mathbf{r}| \hat{K} |\psi\rangle = K_{\mathbf{r}}\psi(\mathbf{r})$. In particular, take $K_{\mathbf{r}} = -\frac{\nabla_{\mathbf{r}}^2}{2m}$, we have

$$\begin{aligned} K_n &= \int_{E_n-\varepsilon}^{E_n+\varepsilon} \frac{d\omega}{2\pi} \int d\mathbf{r} d\mathbf{r}' \langle \mathbf{r}| \hat{A}(\omega) |\mathbf{r}'\rangle \langle \mathbf{r}'| \hat{K}(\omega) |\mathbf{r}\rangle \\ &= \int_{E_n-\varepsilon}^{E_n+\varepsilon} \frac{d\omega}{2\pi} \int d\mathbf{r} d\mathbf{r}' A(\mathbf{r}, \mathbf{r}'; \omega) K_{\mathbf{r}'} \delta(\mathbf{r} - \mathbf{r}') \\ &= \int_{E_n-\varepsilon}^{E_n+\varepsilon} \frac{d\omega}{2\pi} \int d\mathbf{r} \left[-\frac{\nabla_{\mathbf{r}}^2}{2m} A(\mathbf{r}, \mathbf{r}'; \omega)\right]_{\mathbf{r}'=\mathbf{r}} \end{aligned} \tag{14.19}$$

similarily, for $\hat{V}|\mathbf{r}\rangle = V(\mathbf{r})|\mathbf{r}\rangle$, we have

$$\begin{aligned} V_n &= \int_{E_n-\varepsilon}^{E_n+\varepsilon} \frac{d\omega}{2\pi}\, \mathrm{Tr}\left(\hat{A}(\omega)\hat{V}\right) \\ &= \int_{E_n-\varepsilon}^{E_n+\varepsilon} \frac{d\omega}{2\pi} \int d\mathbf{r} V(\mathbf{r}) A(\mathbf{r}, \mathbf{r}; \omega) \end{aligned} \tag{14.20}$$

14.3 Spectral Representation

Green's functions are response functions for the wave function, hence they have many formal properties that are analogous to those of response functions that we saw earlier. We discuss some of them here.

14.3.1 Spectral representation and Kramers-Kronig relations

Since $G^R$is retarded, we automatically have the inverse of the imaginary operator on G^R:

$$\begin{aligned} \hat{A}(\omega) &= -2\Im \hat{G}^R(\omega) \\ \hat{G}^R(\omega) &= \int d\frac{\omega'}{2\pi} \frac{\hat{A}(\omega')}{\omega + i\eta - \omega'} \end{aligned} \tag{14.21}$$

in position space

$$\begin{aligned} A(\mathbf{r}, \mathbf{r}'; \omega) &= \sum_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}') 2\pi\delta(\omega - E_n) \\ G^R(\mathbf{r}, \mathbf{r}'; \omega) &= \sum_n \frac{\Psi_n(\mathbf{r})\Psi_n^*(\mathbf{r}')}{\omega + i\eta - E_n} = \int d\frac{\omega'}{2\pi} \frac{\hat{A}(\mathbf{r}, \mathbf{r}'; \omega')}{\omega + i\eta - \omega'} \end{aligned} \tag{14.22}$$

for translationally-invariant system, $|\mathbf{k}\rangle$ is an eigenstate so $\hat{G}^R |\mathbf{k}\rangle = \hat{G}^R(\mathbf{k}) |\mathbf{k}\rangle$ and similarly for $A(\mathbf{k})$, so we can apply $\langle \mathbf{k}| ... |\mathbf{k}\rangle$ to $\hat{G}^R$ and get

$$G^R(\mathbf{k};\omega) = \int \frac{d\omega'}{2\pi} \frac{A(\mathbf{k};\omega')}{\omega + i\eta - \omega'} \tag{14.23}$$

14.3.2 Sum rules

We now show sum rules for $A(\mathbf{r},\mathbf{r}';\omega)$

$$\begin{aligned} \int d(\mathbf{r}-\mathbf{r}') \int \frac{d\omega}{2\pi} A(\mathbf{r},\mathbf{r}';\omega) &= \int d(\mathbf{r}-\mathbf{r}') \int \frac{d\omega}{2\pi} \sum_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}') \, 2\pi\delta(\omega - E_n) \\ &= \int d(\mathbf{r}-\mathbf{r}') \sum_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}') \\ &= \int d(\mathbf{r}-\mathbf{r}') \delta(\mathbf{r}-\mathbf{r}') \\ &= 1 \end{aligned} \tag{14.24}$$

therefore,

$$\begin{aligned} \int d\mathbf{r} \int \frac{d\omega}{2\pi} A(\mathbf{r},\mathbf{r};\omega)\,\omega &= \int d\mathbf{r} \int \frac{d\omega}{2\pi} \sum_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}) 2\pi\delta(\omega - E_n)\,\omega \\ &= \int d\mathbf{r} \sum_n \Psi_n(\mathbf{r}) \Psi_n^*(\mathbf{r}) E_n \\ &= \int d\mathbf{r} \langle \mathbf{r}| \hat{H} |\mathbf{r}\rangle \end{aligned} \tag{14.25}$$

in operator form , the above results are trivial

$$\int \frac{d\omega}{2\pi} \omega^n \operatorname{Tr}\left(\hat{A}(\omega)\right) = \int d\omega \omega^n \operatorname{Tr}\left(\delta(\omega - \hat{H})\right) = \operatorname{Tr}\left(\hat{H}^n\right) \tag{14.26}$$

evaluating the trace in position space,

$$\begin{aligned} \int \frac{d\omega}{2\pi} \omega^n \int d\mathbf{r} \hat{A}(\mathbf{r},\mathbf{r},\omega) &= \int d\mathbf{r} \langle \mathbf{r}| \hat{H}^n |\mathbf{r}\rangle \\ \int \frac{d\omega}{2\pi} \omega^n \int \frac{d\mathbf{k}}{(2\pi)^3} \hat{A}(\mathbf{k},\omega) &= \int \frac{d\mathbf{k}}{(2\pi)^3} \langle \mathbf{k}| \hat{H}^n |\mathbf{k}\rangle \end{aligned} \tag{14.27}$$

14.3.3 High frequency expansion

Sum rules can help us do high frequency expansions. Consider the spectral representation

$$G^R(\mathbf{k};\omega) = \int \frac{d\omega'}{2\pi} \frac{A(\mathbf{k};\omega')}{\omega + i\eta - \omega'} \tag{14.28}$$

For ω sufficiently large, $A(\mathbf{k};\omega') = 0$, the Green's function becomes purely real and one can expand the denominator so that at asymptotically large frequencies,

$$G^R(\mathbf{k};\omega) = \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d\omega'}{2\pi} (\omega')^n A(\mathbf{k};\omega') \tag{14.29}$$

integrating both sides and using the sum rules,

$$\begin{aligned} \int \frac{d\mathbf{k}}{(2\pi)^3} G^R(\mathbf{k};\omega) &= \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d\mathbf{k}}{(2\pi)^3} \int \frac{d\omega'}{2\pi} \omega'^n A(\mathbf{k};\omega') \\ &= \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \int \frac{d\mathbf{k}}{(2\pi)^3} \langle \mathbf{k}| \hat{H}^n |\mathbf{k}\rangle \end{aligned} \tag{14.30}$$

in operator form

$$\mathrm{Tr}\left(\hat{G}^R(\omega)\right) \approx \mathrm{Tr}\left(\frac{1}{\omega - \hat{H}}\right) = \sum_{n=0}^{\infty} \frac{1}{\omega^{n+1}} \mathrm{Tr}\left(\hat{H}^n\right) \tag{14.31}$$

Part IV
Green's function at finite temperature

In this chapter we follow Andre's book chapter IV.

15 Retarded Green's function

In the section on linear response theory, we have the retarded response function

$$\chi^R_{BA}\left(\mathbf{r}, t; \mathbf{r}', t'\right) \equiv i\theta\left(t - t'\right) \left\langle [B(t), A\left(t'\right)] \right\rangle \tag{15.1}$$

If A, B are field operators, the retarded response is called the retarded Green's function. Specifically, they are defined as

$$G^R\left(\mathbf{r}, t; \mathbf{r}', t'\right) = -i \left\langle \left\{ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t') \right\} \right\rangle \theta\left(t - t'\right), \quad \text{fermions} \tag{15.2}$$

$$G^R\left(\mathbf{r}, t; \mathbf{r}', t'\right) = -i \left\langle \left[\psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t') \right] \right\rangle \theta\left(t - t'\right), \quad \text{bosons} \tag{15.3}$$

$$\begin{aligned} \psi(\mathbf{r}, t) &\equiv e^{itH} \psi_S(\mathbf{r}) e^{-itH} \\ \psi^\dagger(\mathbf{r}, t) &\equiv e^{itH} \psi_S^\dagger(\mathbf{r}) e^{-itH} \end{aligned} \tag{15.4}$$

or, if we are using grand-canonical ensemble,

$$\begin{aligned} K &= H - \mu N \\ \psi(\mathbf{r}, t) &\equiv e^{itK} \psi_S(\mathbf{r}) e^{-itK} \\ \psi^\dagger(\mathbf{r}, t) &\equiv e^{itK} \psi_S^\dagger(\mathbf{r}) e^{-itK} \end{aligned} \tag{15.5}$$

The Fourier transform $\mathbf{r} \to \mathbf{k}$ of G^R is (for fermions, with translation symmetry)

$$\begin{aligned} G^R\left(\mathbf{k}, t\right) &= \int d(\mathbf{r} - \mathbf{r}') e^{-i\mathbf{k}\cdot(\mathbf{r} - \mathbf{r}')} G^R\left(\mathbf{r} - \mathbf{r}', t - t'\right) \\ &= \frac{1}{V} \int d\mathbf{r} e^{-i\mathbf{k}\cdot r} \int d\mathbf{r}' e^{+i\mathbf{k}\cdot r'} G^R\left(\mathbf{r} - \mathbf{r}', t - t'\right) \\ &= -i \left\langle \left\{ c_{\mathbf{k}}(t), c_{\mathbf{k}}^\dagger(t') \right\} \right\rangle \theta\left(t - t'\right) \end{aligned} \tag{15.6}$$

where we used the field operator transformation

$$\begin{aligned} c_{\mathbf{k}} &= \frac{1}{\sqrt{V}} \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} \psi(\mathbf{r}) \\ c_{\mathbf{k}}^\dagger &= \frac{1}{\sqrt{V}} \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \psi^\dagger(\mathbf{r}) \end{aligned} \tag{15.7}$$

so the Fourier Transform $\mathbf{r} \to \mathbf{k}$ give $G^R(\mathbf{k}, t)$, which is also $G^R_{c_{\mathbf{k}} c_{\mathbf{k}}^\dagger}$ for operators $c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger$.

As an example, for a quadratic Hamiltonian $H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$, we have

$$\begin{aligned} G^R(\mathbf{k}, t) &= -i \left\langle \left\{ c_{\mathbf{k}}(t), c_{\mathbf{k}}^\dagger \right\} \right\rangle \theta\left(t\right) \\ &= -ie^{-i\epsilon_{\mathbf{k}} t} \left\langle \left\{ c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger \right\} \right\rangle \theta\left(t\right) \\ &= -ie^{-i\epsilon_{\mathbf{k}} t} \theta\left(t\right) \end{aligned} \tag{15.8}$$

Its Fourier transform gives

$$G^R(\mathbf{k}, t) = \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\eta} \tag{15.9}$$

15.1 Spectral representation of G^R

By analogy with what we have done previously for response functions χ, it is useful to introduce the spectral representation for the retarded Green's function. Starting with definition

$$G^R(\mathbf{r},\mathbf{r}';t) = -i\left\langle\left\{\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',0)\right\}\right\rangle\theta(t) \tag{15.10}$$

We now proceed by analogy with the response functions. On the left we show the definitions for response functions, and on the right the analogous definitions for response functions. Let

$$G^R(\mathbf{r},\mathbf{r}';t) = -iA(\mathbf{r},\mathbf{r}';t)\,\theta(t) \quad ; \quad \chi^R_{ij}(t) = 2i\chi''_{ij}(t)\theta(t) \tag{15.11}$$

$$A(\mathbf{r},\mathbf{r}';t) \equiv \left\langle\left\{\psi(\mathbf{r},t),\psi^+(\mathbf{r}',0)\right\}\right\rangle \quad ; \quad \chi''_{ij}(t) = \frac{1}{2}\left\langle[A_i(\mathbf{r},t),A_j(\mathbf{r}',0)]\right\rangle \tag{15.12}$$

$$G^R(\mathbf{r},\mathbf{r}';\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A(\mathbf{r},\mathbf{r}';\omega')}{\omega+i\eta-\omega'} \quad ; \quad \chi^R_{ij}(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''_{ij}(\omega')}{\omega'-(\omega+i\eta)} \tag{15.13}$$

$$\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}A(\mathbf{r},\mathbf{r}';\omega') = \left\langle\left\{\psi(\mathbf{r},0),\psi^+(\mathbf{r}',0)\right\}\right\rangle = \delta(\mathbf{r}-\mathbf{r}') \tag{15.14}$$

16 Imaginary Time Pictures

Let

$$H = H_0 + V \tag{16.1}$$

With $K = H-\mu N$, $\quad K_0 = H_0-\mu N$, we define the imaginary time Heisenberg picture

$$\begin{aligned} Q_{\mathrm{H}}(\tau) &= \mathrm{e}^{K\tau}Q_{\mathrm{S}}\mathrm{e}^{-K\tau} \\ Q_{\mathrm{I}}(\tau) &= \mathrm{e}^{K_0\tau}Q_{\mathrm{S}}\mathrm{e}^{-K_0\tau} \end{aligned} \tag{16.2}$$

in particular, the field operators in Heisenberg picture (we usually ignore the index H, here for clarity we add it in)

$$\begin{aligned} \psi_H(\mathbf{r},\tau) &\equiv e^{\tau K}\psi_S(\mathbf{r})e^{-\tau K} \\ \psi^\dagger_H(\mathbf{r},\tau) &\equiv e^{\tau K}\psi^\dagger_S(\mathbf{r})e^{-\tau K} \end{aligned} \tag{16.3}$$

we can relate Q_H and Q_I

$$\begin{aligned} Q_{\mathrm{H}}(\tau) &= \mathrm{e}^{K\tau}\mathrm{e}^{-K_0\tau}Q_{\mathrm{I}}(\tau)\mathrm{e}^{K_0\tau}\mathrm{e}^{-K\tau} \\ &= U_I(0,\tau)Q_{\mathrm{I}}(\tau)U_I(\tau,0) \end{aligned} \tag{16.4}$$

this defines the imaginary evolution operator

$$\begin{aligned} U_I(\tau_1,\tau_2) &= \mathrm{e}^{K_0\tau_1}\mathrm{e}^{-K(\tau_1-\tau_2)}\mathrm{e}^{-K_0\tau_2} \\ U_I(\tau,0) &= \mathrm{e}^{K_0\tau}\mathrm{e}^{-K\tau} \end{aligned} \tag{16.5}$$

here U is no unitary, but we still have transitivity

$$\begin{aligned} U_I(\tau_1,\tau_2)\,U_I(\tau_2,\tau_3) &= U_I(\tau_1,\tau_3) \\ U_I(\tau_1,\tau_1) &= 1 \end{aligned} \tag{16.6}$$

the equation of motion can be obtained from $\partial_{\tau_1}U_I(\tau_1,\tau_2)$:

$$\partial_\tau U_I(\tau,0) = -V_I(\tau)U_I(\tau,0) \tag{16.7}$$

with a formal solution

$$U_I(\tau,0) = T_\tau\exp\left[-\int_0^\tau \mathrm{d}\tau_1 V_{\mathrm{I}}(\tau_1)\right] \tag{16.8}$$

to first order

$$U_I(\tau,0) = 1-\int_0^\tau \mathrm{d}\tau_1 V_{\mathrm{I}}(\tau_1)+\mathcal{O}(V_I^2) \tag{16.9}$$

The partition function

$$\begin{aligned} Z = e^{-\beta\Omega} &= \mathrm{Tr}\left(e^{-\beta K}\right) \\ &= \mathrm{Tr}\left(e^{-\beta K_0} U_I(\beta, 0)\right) \end{aligned} \tag{16.10}$$

notice that here Z is also dependent on the interaction V.
we can now calculate the expectation value of any Heisenberg operator $A_H(\tau)$

$$\begin{aligned} \langle A_H(\tau)\rangle &= \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta K} A_H(\tau)\right) \\ &= \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta K_0} U_I(\beta,0) U_I(0,\tau) A_{\mathrm{I}}(\tau) U_I(\tau,0)\right) \\ &= \frac{1}{Z}\mathrm{Tr}\left(e^{-\beta K_0} U_I(\beta,\tau) A_{\mathrm{I}}(\tau) U_I(\tau,0)\right) \\ &= \frac{\mathrm{Tr}\left(e^{-\beta K_0}\mathcal{T}_\tau\left[U_I(\beta,0) A_{\mathrm{I}}(\tau)\right]\right)}{\mathrm{Tr}\left(e^{-\beta K_0} U_I(\beta,0)\right)} \end{aligned} \tag{16.11}$$

So we can rewrite this as

$$\langle A_H(\tau)\rangle = \frac{\langle \mathcal{T}_\tau\left[U_I(\beta,0) A_{\mathrm{I}}(\tau)\right]\rangle_0}{\langle U_I(\beta,0)\rangle_0} \tag{16.12}$$

similarly

$$\langle T_\tau[A_H(\tau_1) B_H(\tau_2)]\rangle = \frac{\langle T_\tau\left[A_{\mathrm{I}}(\tau_1) B_{\mathrm{I}}(\tau_2) U(\beta\hbar, 0)\right]\rangle_0}{\langle U(\beta\hbar,0)\rangle_0} \tag{16.13}$$

Using Wick's theorem (which we will prove later), we can write RHS as a connected average

$$\langle T_\tau[A_H(\tau_1) B_H(\tau_2)]\rangle = \langle T_\tau\left[A_{\mathrm{I}}(\tau_1) B_{\mathrm{I}}(\tau_2) U(\beta\hbar, 0)\right]\rangle_{0c} \tag{16.14}$$

17 The Matsubara susceptibility

In thermodynamic equilibrium the time evolution operator as well as the density matrix are exponentials of H times a complex number. To evaluate these operators perturbatively, one needs to calculate time-ordered products along a contour in the complex time domain that is relatively complicated, as we saw in the previous section. To simplify the calculation, we introduce a new Green's function called **Matsubara Green's function**, which is itself a time-ordered product but along the imaginary time axis only. This simplifies the calculation since the integration contour is now simple.

In a sense, we take advantage of the fact that we are free to define Green's functions as we wish, as long as we connect them to observable quantities at the end of the calculation. This is similar to what we did for correlation function. All the information about the system was in $\chi''(\mathbf{k},\omega)$, now it is all in the spectral weight $A(\mathbf{k},\omega)$, so that as long as we can extract the single-particle spectral weight we do not lose information.

What makes this Green function extremely useful for calculations is the fact that

1. Perturbation theory prefer time-ordered products. (It helps simplify Wick's theorem)
2. For thermodynamic quantities, only equal-time correlation functions are needed. Evaluation in imaginary time or in real time should be equivalent since only $t = 0$ is relevant.
3. More generally, for time-dependent correlation functions in frequency space, the analytic continuation to the retarded function is trivial (only when the calculation is done analytically).

17.1 Definition for Fermions

The Matsubara Green's function is defined by

$$\begin{aligned} \mathcal{G}(\mathbf{r},\mathbf{r}';\tau-\tau') &= -\left\langle T_\tau \psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',\tau')\right\rangle \\ &= -\left\langle \psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',\tau')\right\rangle \theta(\tau-\tau') + \left\langle \psi^\dagger(\mathbf{r}',\tau')\psi(\mathbf{r},\tau)\right\rangle \theta(\tau'-\tau) \end{aligned} \tag{17.1}$$

We still need to specify a few things. First, the thermodynamic average is in the grand-canonical ensemble

$$\langle\mathcal{O}\rangle \equiv \frac{\mathrm{Tr}\left[e^{-\beta(H-\mu N)}\mathcal{O}\right]}{\mathrm{Tr}\left[e^{-\beta(H-\mu N)}\right]} \tag{17.2}$$

with μ the chemical potential and N is the total number of particle operator. Define

$$K \equiv H - \mu N, \quad K_0 \equiv H_0 - \mu N \tag{17.3}$$

the time evolution of the operators is defined by

$$\begin{aligned} \psi(\mathbf{r},\tau) &\equiv e^{\tau K}\psi_S(\mathbf{r})e^{-\tau K} \\ \psi^\dagger(\mathbf{r},\tau) &\equiv e^{\tau K}\psi_S^\dagger(\mathbf{r})e^{-\tau K} \end{aligned} \tag{17.4}$$

we have a corresponding equation of motion for Heisenberg operators in imaginary time

$$\begin{aligned} \mathcal{O}_H(\tau) &\equiv e^{\tau K}\mathcal{O}_S e^{-\tau K} \\ \partial_\tau \mathcal{O}_H &= [K, \mathcal{O}_H] \end{aligned} \tag{17.5}$$

Several points should attract our attention:

1. The correspondence with the real-time evolution operators e^{-iHt} is done by noting that

$$\tau = it \tag{17.6}$$

2. In particular, evolution of the density matrix, or in general of an operator in imaginary time is easily deduced by doing the above replacement in our previous results. For example,

$$e^{-\beta K} = U(-i\beta, 0) = e^{-iK_0(-i\beta)}U_I(-i\beta, 0) = e^{-\beta K_0}U_I(-i\beta, 0) \tag{17.7}$$

3. Strictly speaking, we should use $\psi(\mathbf{r}, -i\tau)$ if we want the symbol $\psi(\mathbf{r}, t)$ for t complex to mean the same thing as before. We will stick with $\psi(\mathbf{r}, \tau)$ since this lack of rigor does not usually lead to confusion.

4. $\psi^\dagger(\mathbf{r}, \tau)$ is not the adjoint of $\psi(\mathbf{r}, \tau)$. However, its analytic continuation $\tau \to it$ is the adjoint of $\psi(\mathbf{r}, t)$.

5. It suffices to define the Matsubara Green's function $\mathcal{G}(\mathbf{r}, \mathbf{r}'; \tau)$ in the interval $-\beta \leq \tau \leq \beta$. We do not need it outside of this interval. The perturbation expansion of $U_I(-i\beta, 0) = \mathcal{T}_\tau\left[\exp\left(-\int_C d\tau V_I(\tau)\right)\right]$ evidently necessitates that we study at least the interval $0 \leq \tau \leq \beta$ but the other part of the interval, namely $-\beta \leq \tau \leq 0$ is also necessary if we want the time ordering operator to lead to both of the possible orders of ψ and $\psi^\dagger$, since G^R has both cases. However, antiperiodicity allows us to trivially take into account what happens in the interval $-\beta \leq \tau \leq 0$ if we know what happens in the interval $0 \leq \tau \leq \beta$.

6. To evaluate $U_I(-i\beta, 0) = \mathcal{T}_\tau\left[\exp\left(-\int_C d\tau V_I(\tau)\right)\right]$ the time-ordering operator $\mathcal{T}_\tau$ orders along the contour $(\Im(t) = -\beta) > (\Im(t') = \beta)$ which corresponds to $(\tau = \beta) > (\tau' = -\beta)$. The present contour is illustrated in Ref. Fig.(29-1).

Similar to the retarded Green's function, since

$$\begin{aligned} c_{\mathbf{k}} &= \frac{1}{\sqrt{V}}\int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}}\psi(\mathbf{r}) \\ c_{\mathbf{k}}^\dagger &= \frac{1}{\sqrt{V}}\int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}}\psi^\dagger(\mathbf{r}) \end{aligned} \tag{17.8}$$

for translation-invariant system, the Fourier Transform of $\mathcal{G}(\mathbf{r} - \mathbf{r}'; \tau - \tau')$ is simply given by

$$\mathcal{G}(\mathbf{k}; \tau - \tau') = -\left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger(\tau')\right\rangle \tag{17.9}$$

17.2 Time ordered product in practice

Suppose I want to compute the following quantity for fermions:

$$\left\langle T_\tau \psi(\tau_1)\psi^\dagger(\tau_3)\psi(\tau_2)\psi^\dagger(\tau_4)\right\rangle \tag{17.10}$$

We drop space indices to unclutter the equations. The time ordered product for fermions keeps tract of permutations, so if I exchange the first two operators for example, I find

$$\left\langle T_\tau \psi(\tau_1)\psi^\dagger(\tau_3)\psi(\tau_2)\psi^\dagger(\tau_4)\right\rangle = -\left\langle T_\tau \psi^\dagger(\tau_3)\psi(\tau_1)\psi(\tau_2)\psi^\dagger(\tau_4)\right\rangle \tag{17.11}$$

We cannot, however, have two of the times equal for a ψ and a $\psi^\dagger$. We have to specify that one is infinitesimally larger or smaller than the other to know in which order to place the operators since they do not commute or anticommute.

Another interesting property of the time-ordered product is that we can differentiate exponentials with respect to parameters appearing in the argument as if it was an ordinary exponential. For example note how the derivative below is done

$$\begin{aligned}&\frac{\partial}{\partial\alpha}\left\langle T_\tau e^{\alpha\left(\psi(\tau_5)\psi^\dagger(\tau_6)\right)}\psi\left(\tau_1\right)\psi^\dagger\left(\tau_3\right)\psi\left(\tau_2\right)\psi^\dagger\left(\tau_4\right)\right\rangle\\&=\left\langle T_\tau e^{\alpha\left(\psi(\tau_5)\psi^\dagger(\tau_6)\right)}\psi\left(\tau_5\right)\psi^\dagger\left(\tau_6\right)\psi\left(\tau_1\right)\psi^\dagger\left(\tau_3\right)\psi\left(\tau_2\right)\psi^\dagger\left(\tau_4\right)\right\rangle\end{aligned} \tag{17.12}$$

This can be understood as follows. The exponential is defined by its power series. One can thus do the expansion, differentiate term by term and re-exponentiate without worrying about the imaginary times appearing in the argument since the time-ordering operator will take care of that when the correlation function needs to be evaluated for a particular set of imaginary times.

17.3 Antiperiodicity and Fourier expansion (Matsubara frequencies)

Suppose $-\beta<\tau<0$, we can relate it to $\mathcal{G}$ at $0<\tau+\beta<\beta$:

$$\begin{aligned}\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)&=\left\langle\psi^\dagger\left(\mathbf{r}',0\right)\psi(\mathbf{r},\tau)\right\rangle\\&=\frac{1}{Z}\operatorname{Tr}\left(e^{-\beta K}\psi^\dagger\left(\mathbf{r}',0\right)\psi(\mathbf{r},\tau)\right)\\&=\frac{1}{Z}\operatorname{Tr}\left(e^{\tau K}\psi(\mathbf{r},0)e^{-\tau K}e^{-\beta K}\psi^\dagger(\mathbf{r}',0)\right)\\&=\frac{1}{Z}\operatorname{Tr}\left(e^{-\beta K}e^{(\tau+\beta)K}\psi(\mathbf{r},0)e^{-(\tau+\beta)K}\psi^\dagger(\mathbf{r}',0)\right)\\&=\left\langle\psi(\mathbf{r},\tau+\beta)\psi^\dagger\left(\mathbf{r}',0\right)\right\rangle\\&=-\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau+\beta\right)\end{aligned} \tag{17.13}$$

This boundary condition is sometimes known as the **Kubo-Martin-Schwinger (KMS) boundary condition**. For $0<\tau<\beta$ we have a similar experssion. In summary,

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)=\begin{cases}-\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau+\beta\right) & -\beta<\tau<0\\-\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau-\beta\right) & +\beta>\tau>0\end{cases} \tag{17.14}$$

While $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau+\beta\right)$ for $\tau>0$ is well defined, we never need this function. So we restrict ourselves to the interval $-\beta\leq\tau\leq\beta$ described in the previous section.

For a function $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)$ restricted in $-\beta\leq\tau\leq\beta$, we can expand it in Fourier Series. Taking advantage of the antiperiodicity condition, we use the $0\leq\tau\leq\beta$ domain only and write

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}e^{-ik_n\tau}\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) \tag{17.15}$$

$$k_n=(2n+1)\pi T=\frac{(2n+1)\pi}{\beta},\quad n\in\mathbb{Z} \tag{17.16}$$

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right)=\int_0^\beta d\tau e^{ik_n\tau}\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) \tag{17.17}$$

k_n are called **fermionic Matsubara frequencies**. From now on, we have taken Boltzmann's constant k_B to be equal to unity.

In defining the Fourier Transform, we have actually taken changed the definition of $\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right),\tau\in[-\beta,\beta]$ and make it repeat for $\tau\in\mathbb{R}$. The resulting function is not $-\left\langle T_\tau\psi(\mathbf{r},\tau)\psi^\dagger\left(\mathbf{r}',\tau'\right)\right\rangle$ anymore. Correspondingly, all functions must be periodic in 2β in the imaginary time formalism.

17.4 G^R and $\mathcal{G}$ are related by contour integration

To establish the relation between the Matsubara Green's function and the retarded one, and by the same token establish the spectral representation for $\mathcal{G}$, we can show explicitly the analytic continuation in the complex real plane. Begin with the definitions

$$\mathcal{G}(\mathbf{r},\mathbf{r}';\tau) = -\left\langle \psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',0)\right\rangle \theta(\tau) + \left\langle \psi^\dagger(\mathbf{r}',0)\,\psi(\mathbf{r},\tau)\right\rangle \theta(-\tau) \tag{17.18}$$

$$\begin{aligned}\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) &= \int_0^\beta d\tau e^{ik_n\tau}\mathcal{G}(\mathbf{r},\mathbf{r}';\tau)\\ &= \int_0^\beta d\tau e^{ik_n\tau}\left[-\left\langle \psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',0)\right\rangle\right]\end{aligned} \tag{17.19}$$

Assume that $k_n > 0$. We now define $t \equiv -i\tau$ and thus $\tau = it$, and let τ, t be in general complex. Then, as illustrated in Ref. Fig.(29-2), setting up the axis $(x,y) = (\Re(t), \Im(t)) = (\Im(\tau), -\Re(\tau))$, we see that the integral for $\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n)$ is taken along t-path $[0,-i\beta]$. The contour can be deormed to t-path $[0,\infty]$, $[\infty,\infty-i\beta]$ and then $[\infty-i\beta,-i\beta]$. This requires the analyticity of $\mathcal{G}(\mathbf{r},\mathbf{r}';\tau)$ in $\tau\in[0,\beta]$, which we can prove in Lehmann representation in the next section. The limit $t\to\infty$ is $\tau\to i\infty$ and $e^{ik_n\tau}\to 0$, so the integral along $[\infty,\infty-i\beta]$ vanishes due to a vanishing integrand. We are left with

$$\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) = \int_{t=0}^{t=\infty} d(it)\left[-\left\langle\psi(\mathbf{r},t)\psi^\dagger(\mathbf{r}')\right\rangle\right]e^{ik_n(it)} + \int_{t=\infty}^{t=0} d(it)\left[-\left\langle\psi(\mathbf{r},t-i\beta)\psi^+(\mathbf{r}')\right\rangle\right]e^{(ik_n)i(t-i\beta)} \tag{17.20}$$

we have identity $e^{(ik_n)i(-i\beta)} = e^{(ik_n)\beta} = -1$ and

$$\begin{aligned}\left\langle\psi(\mathbf{r},t-i\beta)\psi^\dagger(\mathbf{r}',0)\right\rangle &= Z^{-1}\,\mathrm{Tr}\left(e^{-\beta K}e^{iK(t-i\beta)}\psi_S(\mathbf{r})e^{-iK(t-i\beta)}\psi_S^\dagger(\mathbf{r}')\right)\\ &= Z^{-1}\,\mathrm{Tr}\left(e^{iKt}\psi_S(\mathbf{r})e^{-iKt}e^{-\beta K}\psi_S^\dagger(\mathbf{r}')\right)\\ &= Z^{-1}\,\mathrm{Tr}\left(e^{-\beta K}\psi_S^\dagger(\mathbf{r}')e^{iKt}\psi_S(\mathbf{r})e^{-iKt}\right)\\ &= \left\langle\psi^\dagger(\mathbf{r}',0)\psi(\mathbf{r},t)\right\rangle\end{aligned} \tag{17.21}$$

the second integral can thus be written as

$$\begin{aligned}&\int_{t=\infty}^{t=0} d(it)\left[-\left\langle\psi(\mathbf{r},t-i\beta)\psi^+(\mathbf{r}')\right\rangle\right]e^{(ik_n)i(t-i\beta)}\\ =&-i\int_0^\infty dt\left\langle\psi^\dagger(\mathbf{r}',0)\psi(\mathbf{r},t)\right\rangle e^{i(ik_n)t}\end{aligned} \tag{17.22}$$

combining this with the first integral, we see that

$$\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) = -i\int_0^\infty dt\left\langle\left\{\psi(\mathbf{r},t),\psi^\dagger(\mathbf{r}',0)\right\}\right\rangle e^{i(ik_n)t} \tag{17.23}$$

and we have

$$G^R(\mathbf{r},\mathbf{r}';\omega) = \lim_{ik_n\to\omega+i\eta}\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) \tag{17.24}$$

If we had started with $k_n<0$, analytic continuation $ik_n\to\omega-i\eta$ would lead to the advanced Green's function.

17.5 Lehmann Representation

For a general correlation function, not necessarily a Green's function, one establishes the connection between Matsubara functions and retarded functions by using the Lehmann representation. This representation is also

extremely useful to extract the physical significance of the poles of correlation functions.

$$\begin{aligned} A\left(\mathbf{r},\mathbf{r}';t\right) \equiv & \left\langle\left\{\psi(\mathbf{r},t),\psi^{\dagger}\left(\mathbf{r}',0\right)\right\}\right\rangle \\ = & e^{\beta\Omega}\sum_{m,n}\left[\left\langle n\left|e^{-\beta K}e^{iKt}\psi_{S}(\mathbf{r})e^{-iKt}\right|m\right\rangle\left\langle m\left|\psi_{S}^{\dagger}\left(\mathbf{r}'\right)\right|n\right\rangle\right. \\ & \left.+\left\langle n\left|e^{-\beta K}\psi_{S}^{\dagger}\left(\mathbf{r}'\right)\right|m\right\rangle\left\langle m\left|e^{iKt}\psi_{S}(\mathbf{r})e^{-iKt}\right|n\right\rangle\right] \\ = & e^{\beta\Omega}\sum_{m,n}\left[e^{-\beta K_{n}}e^{i\left(K_{n}-K_{m}\right)t}\left\langle n\left|\psi_{S}(\mathbf{r})\right|m\right\rangle\left\langle m\left|\psi_{S}^{\dagger}\left(\mathbf{r}'\right)\right|n\right\rangle\right. \\ & \left.+e^{-\beta K_{n}}e^{i\left(K_{m}-K_{n}\right)t}\left\langle n\left|\psi_{S}^{\dagger}\left(\mathbf{r}'\right)\right|m\right\rangle\left\langle m\left|\psi_{S}(\mathbf{r})\right|n\right\rangle\right] \end{aligned} \tag{17.25}$$

using F.T. of translationally-invariant function, $\mathbf{r}\to\mathbf{k},\mathbf{r}'\to-\mathbf{k}$, but since $c_{\mathbf{k}}^{\dagger}$ transform like an inverse Fourier Transform of $c_{\mathbf{k}}$, we have $\psi(\mathbf{r}),\psi^{\dagger}(\mathbf{r})\to c_{\mathbf{k}},c_{\mathbf{k}}^{\dagger}$ and so

$$A(\mathbf{k};t)=\left\langle\left\{c_{\mathbf{k}}(t),c_{\mathbf{k}}^{\dagger}(0)\right\}\right\rangle \tag{17.26}$$

We now use $e^{-iKt}|n\rangle=e^{-iK_{n}t}|n\rangle$ with $K_{n}=E_{n}-\mu N_{n}$ if there are N_{n} particles in the initial state $|n\rangle$. In the first term above, $|n\rangle$ has one less particle than $|m\rangle$ while the reverse is true for the second term. We have

$$K_{m}-K_{n}=E_{m}-E_{n}+\mu\left(N_{m}-N_{n}\right)=\begin{cases}E_{m}-E_{n}+\mu & \text{first term}\\ E_{m}-E_{n}-\mu & \text{second term}\end{cases} \tag{17.27}$$

Taking the Fourier transform $\int dte^{i\omega t}$ we have

$$\begin{aligned} A\left(\mathbf{r},\mathbf{r}';\omega\right) = & e^{\beta\Omega}\sum_{m,n}e^{-\beta K_{n}}[\left\langle n\left|\psi_{S}(\mathbf{r})\right|m\right\rangle\left\langle m\left|\psi_{S}^{\dagger}\left(\mathbf{r}'\right)\right|n\right\rangle(2\pi)\delta(\omega+K_{n}-K_{m}) \\ & +\left\langle n\left|\psi_{S}^{\dagger}\left(\mathbf{r}'\right)\right|m\right\rangle\left\langle m\left|\psi_{S}(\mathbf{r})\right|n\right\rangle(2\pi)\delta(\omega+K_{m}-K_{n})] \\ = & e^{\beta\Omega}\sum_{m,n}\left(e^{-\beta K_{n}}+e^{-\beta K_{m}}\right)\left\langle n\left|\psi_{S}(\mathbf{r})\right|m\right\rangle\left\langle m\left|\psi_{S}^{\dagger}\left(\mathbf{r}'\right)\right|n\right\rangle(2\pi)\delta(\omega-(K_{m}-K_{n})) \end{aligned} \tag{17.28}$$

We can also perform the Fourier Transform now to obtain the spectral function in momentum space

$$\begin{aligned} A\left(\mathbf{k},\omega'\right) = & e^{\beta\Omega}\sum_{m,n}\left(e^{-\beta K_{n}}+e^{-\beta K_{m}}\right)\left\langle n\left|c_{\mathbf{k}}\right|m\right\rangle\left\langle m\left|c_{-\mathbf{k}}\right|n\right\rangle(2\pi)\delta(\omega-(K_{m}-K_{n})) \\ = & e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_{n}}+e^{-\beta K_{m}}\right)\left|\left\langle n\left|c_{\mathbf{k}}\right|m\right\rangle\right|^{2}2\pi\delta\left(\omega'-(K_{m}-K_{n})\right) \end{aligned} \tag{17.29}$$

we can show that it integrates to unity

$$\int\frac{d\omega'}{2\pi}A(\mathbf{k},\omega')=A(\mathbf{k},t=0)=\left\langle\left\{c_{\mathbf{k}},c_{\mathbf{k}}^{\dagger}\right\}\right\rangle=1 \tag{17.30}$$

One can interpret physically the spectral weight as follows. It has two pieces, the first one for excited states with one more particle, and the second one for excited states with one more hole. Photoemission experiments (See Einstein's Nobel prize) access this last piece of the spectral weight, while Bremsstrahlung inverse spectroscopy (BIS) experiments measure the first piece. Excited particle states contribute to positive frequencies ω if their excitation energy is larger than the chemical potential, $E_{m}-E_{n}>\mu$ and to negative frequencies otherwise. Zero frequency means that the excitation energy is equal to the chemical potential. In other words, every excited single-particle or single-hole state corresponds to a delta function in the spectral weight whose weight depends on the overlap between initial states with one more particle at $\mathbf{r}'$ or one more hole at $\mathbf{r}$, and the true excited states.

We have already shown that spectral representation works for the retarded Green's function

$$G^{R}\left(\mathbf{r},\mathbf{r}';\omega\right)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A(\mathbf{r},\mathbf{r}';\omega')}{\omega+i\eta-\omega'} \tag{17.31}$$

from the analytic continuity we should have

$$\begin{aligned}\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) &= G^R\left(\mathbf{r},\mathbf{r}';\omega+i\eta\to ik_n\right)\\ &= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A(\mathbf{r},\mathbf{r}';\omega')}{ik_n-\omega'}\end{aligned} \tag{17.32}$$

we can derive this explicitly from Lehmann representation. For $\tau\in[0,\beta]$,

$$\begin{aligned}\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right) &= -\left\langle\psi(\mathbf{r},\tau)\psi^\dagger\left(\mathbf{r}',0\right)\right\rangle\\ &= -e^{\beta\Omega}\sum_{m,n}\left\langle n\right|e^{-\beta K}e^{\tau K}\psi_S(\mathbf{r})e^{-\tau K}\left|m\right\rangle\left\langle m\right|\psi_S^\dagger(\mathbf{r}')\left|n\right\rangle\\ &= -e^{\beta\Omega}\sum_{m,n}e^{-\beta K_n}e^{\tau(K_n-K_m)}\left\langle n\right|\psi_S(\mathbf{r})\left|m\right\rangle\left\langle m\right|\psi_S^\dagger(\mathbf{r}')\left|n\right\rangle\end{aligned} \tag{17.33}$$

$$\begin{aligned}\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) &= \int_0^\beta d\tau e^{ik_n\tau}\mathcal{G}\left(\mathbf{r},\mathbf{r}';\tau\right)\\ &= -e^{\beta\Omega}\sum_{m,n}e^{-\beta K_n}\left\langle n\right|\psi_S(\mathbf{r})\left|m\right\rangle\left\langle m\right|\psi_S^\dagger(\mathbf{r}')\left|n\right\rangle\int_0^\beta d\tau e^{ik_n\tau}e^{\tau(K_n-K_m)}\\ &= e^{\beta\Omega}\sum_{m,n}\left\langle n\right|\psi_S(\mathbf{r})\left|m\right\rangle\left\langle m\right|\psi_S^\dagger(\mathbf{r}')\left|n\right\rangle\frac{e^{-\beta K_m}+e^{-\beta K_n}}{ik_n+K_n-K_m}\end{aligned} \tag{17.34}$$

This is the Lehmann representation of the Matsubara Green's function. Comparing this with the Lehmann representation of the spectral function $A\left(\mathbf{r},\mathbf{r}';\omega\right)$, we have

$$\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A\left(\mathbf{r},\mathbf{r}';\omega'\right)}{ik_n-\omega'} \tag{17.35}$$

which agrees with the result obtained from analytic continuity.

17.6 Spectral weight and rules for analytical continuation

The Matsubara Green's function and the retarded functions are special cases of a more general function defined in the complex frequency plane by

$$G\left(\mathbf{r},\mathbf{r}';z\right) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A\left(\mathbf{r},\mathbf{r}';\omega'\right)}{z-\omega'} \tag{17.36}$$

This function is analytic everywhere except on the real axis. Physically interesting special cases are

$$\begin{aligned}\mathcal{G}\left(\mathbf{r},\mathbf{r}';ik_n\right) &= G\left(\mathbf{r},\mathbf{r}';ik_n\right)\\ G^R\left(\mathbf{r},\mathbf{r}';\omega\right) &= \lim_{\eta\to0}G\left(\mathbf{r},\mathbf{r}';\omega+i\eta\right)\\ G^A\left(\mathbf{r},\mathbf{r}';\omega\right) &= \lim_{\eta\to0}G\left(\mathbf{r},\mathbf{r}';\omega-i\eta\right)\end{aligned} \tag{17.37}$$

The function G has a jump on the real axis given by

$$\begin{aligned}A\left(\mathbf{r},\mathbf{r}';\omega\right) &= i\lim_{\eta\to0}\left[G\left(\mathbf{r},\mathbf{r}';\omega+i\eta\right)-G\left(\mathbf{r},\mathbf{r}';\omega-i\eta\right)\right]\\ &= i\left[G^R\left(\mathbf{r},\mathbf{r}';\omega\right)-G^A\left(\mathbf{r},\mathbf{r}';\omega\right)\right]\end{aligned} \tag{17.38}$$

In the special case where A is real (for example when $\mathbf{r}=\mathbf{r}'$ or $\mathbf{k}=\mathbf{k}'$, and using Lehmann rep), we have

$$A(\omega) = -2\Im G^R(\omega) \tag{17.39}$$

The previous results are summarized in Ref. Fig.(29-3) which displays the analytic structure of $G\left(\mathbf{r},\mathbf{r}';z\right)$. This function is analytical everywhere except on the real axis where it has a branch cut leading to a jump in the value of the function described by the spectral function A. The limit as we come from the upper half-plane is equal to $G^R\left(\mathbf{r},\mathbf{r}';\omega\right)$ whereas from the lower half-plane it is equal to $G^A\left(\mathbf{r},\mathbf{r}';\omega\right)$. The Matsubara Green's function is defined only on a discrete but infinite set of points along the imaginary frequency axis.

The problem of finding $G^R(\mathbf{r},\mathbf{r}';\omega)$ along the real-freq axis from the knowledge of the Matsubara Green's function is a problem of analytical continuation. Unfortunately, $G(z=ik_n)$ does not have a unique analytical continuation because there is an infinite number of analytical functions that have the same value along this discrete set of points. For example, suppose we know $G(z=ik_n)$, then $G(z)\left(1+\left(e^{\beta z}+1\right)\right)$ has the same value as $G(z)$ for all points $z=ik_n$ because $e^{ik_n\beta}+1=0$. Baym and Mermin, using results from the theory of complex functions, have obtained the following Theorem:

Theroem: If

1. $G(z)$ is analytic in the upper half plane
2. $G(z)=\mathcal{G}(ik_n)$ for all Matsubara frequencies
3. $\lim_{z\to\infty} zG(z)=\text{const}$

then the analytical continuation is unique and

$$G^R(\mathbf{r},\mathbf{r}';\omega)=\lim_{ik_n\to\omega+i\eta}\mathcal{G}(\mathbf{r},\mathbf{r}';ik_n) \tag{17.40}$$

Numerical calculations are often done in Matsubara frequency, or in imaginary time. This is much easir to handle than oscillating functions. The analytic continuation however is much more problematic. One can use PadÈ approximants if the data has very high precision, or Maximum Entropy analytic continuation[1] if it is less accurate. Software is available on the internet for these tasks[2].

17.7 Matsubara Green's function for non-interacting system

We can get used to the Matsubara Green's function in the non-interacting case. We will derive the results in at least two very different ways: from the definition and from the equations of motion.

17.7.1 From spectral representation

Consider the quadratic Hamiltonian

$$K_0=\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}}-\mu)c^\dagger_{\mathbf{k}}c_{\mathbf{k}}\equiv\sum_{\mathbf{k}}\zeta_{\mathbf{k}}c^\dagger_{\mathbf{k}}c_{\mathbf{k}} \tag{17.41}$$

remember the retarded Green's function

$$G^R(\mathbf{k};\omega)=\frac{1}{\omega+i\eta-\zeta_{\mathbf{k}}} \tag{17.42}$$

$$A(\mathbf{k},\omega)=-2\Im G^R(\mathbf{k};\omega)=2\pi\delta(\omega-\zeta_{\mathbf{k}}) \tag{17.43}$$

and

$$G(\mathbf{k},z)=\int\frac{d\omega}{2\pi}\frac{A(\mathbf{k},\omega)}{z-\omega}=\int\frac{d\omega}{2\pi}\frac{2\pi\delta(\omega-\zeta_{\mathbf{k}})}{z-\omega}=\frac{1}{z-\zeta_{\mathbf{k}}} \tag{17.44}$$

so we have

$$\mathcal{G}(\mathbf{k},z)=G(\mathbf{k},z=ik_n)=\frac{1}{ik_n-\zeta_{\mathbf{k}}} \tag{17.45}$$

17.7.2 From definition

For a quadratic diagonal Hamiltonian we have

$$c_{\mathbf{k}}(\tau)=e^{\tau K}c_{\mathbf{k}}e^{-\tau K}=e^{-\zeta_{\mathbf{k}}\tau}c_{\mathbf{k}} \tag{17.46}$$

from definition

[1] Mark Jarrell and J.E. Gubernatis. Bayesian inference and the analytic con- tinuation of imaginary-time quantum monte carlo data. Physics Reports, 269(3):133 ñ195, 1996.

[2] Dominic Bergeron and A.-M. S. Tremblay. Algorithms for optimized maxi- mum entropy and diagnostic tools for analytic continuation. Phys. Rev. E, 94:023303, Aug 2016.

$$\begin{aligned}
\mathcal{G}_0(\mathbf{k};\tau) &= -\left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger \right\rangle \\
&= -\left\langle c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger \right\rangle \theta(\tau) + \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}}(\tau) \right\rangle \theta(-\tau) \\
&= -e^{-\zeta_{\mathbf{k}}\tau} \left\langle c_{\mathbf{k}} c_{\mathbf{k}}^\dagger \right\rangle \theta(\tau) + e^{-\zeta_{\mathbf{k}}\tau} \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle \theta(-\tau) \\
&= -e^{-\zeta_{\mathbf{k}}\tau} \left[(1 - f(\zeta_{\mathbf{k}}))\theta(\tau) - f(\zeta_{\mathbf{k}})\theta(-\tau) \right]
\end{aligned} \tag{17.47}$$

To expand the Fourier series $\tau \to k_n$, we need only the $\tau > 0$ part,

$$\begin{aligned}
\mathcal{G}_0(\mathbf{k}, ik_n) &= \int_0^\beta d\tau e^{ik_n\tau} \mathcal{G}_0(\mathbf{k};\tau) \\
&= -(1 - f(\zeta_{\mathbf{k}})) \int_0^\beta d\tau e^{(ik_n - \zeta_{\mathbf{k}})\tau} \\
&= (1 - f(\zeta_{\mathbf{k}})) \frac{e^{-\beta\zeta_{\mathbf{k}}} + 1}{ik_n - \zeta_{\mathbf{k}}} \\
&= \frac{1}{ik_n - \zeta_{\mathbf{k}}}
\end{aligned} \tag{17.48}$$

17.7.3 From the equations of motion

$$\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{G}_0(\mathbf{k};\tau) &= -\frac{\partial}{\partial\tau}\left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger \right\rangle \\
&= -\delta(\tau)\left\langle \left\{ c_{\mathbf{k}}(\tau), c_{\mathbf{k}}^\dagger \right\} \right\rangle - \left\langle T_\tau \left(\frac{\partial}{\partial\tau} c_{\mathbf{k}}(\tau) \right) c_{\mathbf{k}}^\dagger \right\rangle
\end{aligned} \tag{17.49}$$

Using the expression for $c_{\mathbf{k}}(\tau)$, we have

$$\frac{\partial}{\partial\tau}\mathcal{G}_0(\mathbf{k};\tau) = -\delta(\tau) + \zeta_{\mathbf{k}}\left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger \right\rangle \tag{17.50}$$

so the equation of motion for the Matsubara propagator is

$$\left(\frac{\partial}{\partial\tau} + \zeta_{\mathbf{k}} \right) \mathcal{G}_0(\mathbf{k};\tau) = -\delta(\tau) \tag{17.51}$$

now Fourier Transform both sides, but with Matsubara frequencies

$$\begin{aligned}
\int_0^\beta d\tau e^{ik_n\tau} \left(\frac{\partial}{\partial\tau} + \zeta_{\mathbf{k}} \right) \mathcal{G}_0(\mathbf{k};\tau) &= -\int_0^\beta d\tau e^{ik_n\tau}\delta(\tau) \\
\left[e^{ik_n\tau}\mathcal{G}_0(\mathbf{k};\tau) \right]_{\tau=0}^{\tau=\beta} + \int_0^\beta d\tau \left(-ik_n + \zeta_{\mathbf{k}} \right) e^{ik_n\tau}\mathcal{G}_0(\mathbf{k};\tau) &= -\beta \\
\left[-\mathcal{G}_0(\mathbf{k};\tau=\beta) - \mathcal{G}_0(\mathbf{k};\tau=0) \right] + \beta \left(-ik_n + \zeta_{\mathbf{k}} \right) \mathcal{G}_0(\mathbf{k};\tau) &= -\beta \\
\mathcal{G}_0(\mathbf{k};\tau) &= \frac{1}{ik_n - \zeta_{\mathbf{k}}}
\end{aligned} \tag{17.52}$$

where we used the antiperiodicity condition: $\mathcal{G}_0(\mathbf{k};\tau=\beta) + \mathcal{G}_0(\mathbf{k};\tau=0) = 0$.
The inverse Fourier Transform gives

$$\mathcal{G}_0(\mathbf{k};\tau) = \frac{1}{\beta}\sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} \tag{17.53}$$

and now we wish to recover the value $-e^{-\zeta_{\mathbf{k}}\tau}\left[(1 - f(\zeta_{\mathbf{k}}))\theta(\tau) - f(\zeta_{\mathbf{k}})\theta(-\tau)\right]$ from this summation.

17.8 Sums over Matsubara frequencies

In this section, we will show the following important identity in evaluating Matsubara summation

$$\begin{aligned} T\sum_n \frac{e^{ik_n 0^+}}{ik_n - \xi} &= n_F(\xi) \\ T\sum_n \frac{e^{iq_n 0^+}}{iq_n - \xi} &= -n_B(\xi) \end{aligned} \tag{17.54}$$

for fermionic k_n and bosonic q_n.

17.8.1 Fermionic summation

In the derivation above, we went from imaginary-time to Matsubara frequencies. We can also do the reverse, from Matsubara frequencies to imaginary time. So you need to learn about sums over Matsubara frequencies. This will be necessary in doing practical calculations even when we are not trying to go back to imaginary time. When we have products of Green's functions, we will use contour integration tricks that are the same as those in this section. Also, we may use partial fractions in such a way that the only sums to evaluate will basically look like

$$T\sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{17.55}$$

where $T = \beta^{-1}$, for odd frequencies $k_n = (2n+1)\pi T$.

To reconstruct the imaginary-time Green's function, we need to evaluate the sum

$$\mathcal{G}_0(\mathbf{k};\tau) = T\sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} \tag{17.56}$$

however, there is an ambiguity as $\tau \to 0$,

$$\begin{aligned} \lim_{\tau\to 0^+} \mathcal{G}_0(\mathbf{k},\tau) &= -\lim_{\tau\to 0^+} \left\langle c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^\dagger \right\rangle = -\left\langle c_{\mathbf{k}} c_{\mathbf{k}}^\dagger \right\rangle \\ \lim_{\tau\to 0^-} \mathcal{G}_0(\mathbf{k},\tau) &= \lim_{\tau\to 0^-} \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}}(\tau) \right\rangle = \left\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \right\rangle \end{aligned} \tag{17.57}$$

the jump has magnitude 1:

$$\lim_{\tau\to 0^-} \mathcal{G}_0(\mathbf{k},\tau) - \lim_{\tau\to 0^+} \mathcal{G}_0(\mathbf{k},\tau) = \left\langle \{c_{\mathbf{k}}^\dagger, c_{\mathbf{k}}\} \right\rangle = 1 \tag{17.58}$$

Therefore, the summation

$$T\sum_n \frac{e^{-ik_n 0^-}}{ik_n - \zeta_{\mathbf{k}}} \neq T\sum_n \frac{e^{-ik_n 0^+}}{ik_n - \zeta_{\mathbf{k}}} \neq T\sum_n \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{17.59}$$

The sum does not converge uniformly in the interval including $\tau = 0$ because $1/n$ decreases too slow. Even if we can obtain a finite limit for the last sum by combining positive and negative Matsubara frequencies, what makes physical sense is only one or the other of the two limits $\tau \to 0^\pm$.

Let us evaluate the Matsubara frequency sums. Considering again the case of fermions I will show as special cases that

$$\begin{aligned} T\sum_n \frac{e^{-ik_n 0^-}}{ik_n - \zeta_{\mathbf{k}}} &= \frac{1}{e^{\beta\zeta_{\mathbf{k}}}+1} = f(\zeta_{\mathbf{k}}) = \mathcal{G}_0\left(\mathbf{k}; 0^-\right) \\ T\sum_n \frac{e^{-ik_n 0^+}}{ik_n - \zeta_{\mathbf{k}}} &= \frac{-1}{e^{-\beta\zeta_{\mathbf{k}}}+1} = -1 + f(\zeta_{\mathbf{k}}) = \mathcal{G}_0\left(\mathbf{k}; 0^+\right) \end{aligned} \tag{17.60}$$

To perform the sum over Matsubara frequencies, the standard trick is to go to the complex plane. The following function

$$-\beta \frac{1}{e^{\beta z}+1} \tag{17.61}$$

has poles for z equal to any fermionic Matsubara frequency: $z = ik_n$. Its residue at these poles is unity since for

$$z = ik_n + \delta z \tag{17.62}$$

$$\lim_{\delta z \to 0} \delta z \left[-\beta \frac{1}{e^{\beta z} + 1} \right] = \lim_{\delta z \to 0} \delta z \left[-\beta \frac{1}{-e^{\beta \delta z} + 1} \right] = 1 \tag{17.63}$$

Similarly another function $\beta \frac{1}{e^{-\beta z}+1}$ has the same property

$$\lim_{\delta z \to 0} \delta z \left[\beta \frac{1}{e^{-\beta z} + 1} \right] = \lim_{\delta z \to 0} \delta z \left[\beta \frac{1}{-e^{-\beta \delta z} + 1} \right] = 1 \tag{17.64}$$

(See Ref. Fig 29-7)

To evaluate the $\tau < 0$ case by contour integration, we use the residue theorem on the contour C_1, which is a sum of circles going counterclockwise around the points where z is equal to the Matsubara frequencies. We can establish the equality

$$\sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} = \int_{C_1} \frac{dz}{2\pi i} \frac{-\beta}{e^{\beta z} + 1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}} \tag{17.65}$$

This contour can then be deformed into C_1' and then $C_2 + C_3$. The integrand vanishes at $\Re z \to \pm\infty$.

$$\frac{1}{e^{\beta z} + 1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}} \to \begin{cases} z^{-1} e^{-z(\tau+\beta)} < z^{-1} e^{-z0^+} & \Re z \to \infty \\ z^{-1} e^{-z\tau} < z^{-1} e^{z0^+} & \Re z \to -\infty \end{cases} \tag{17.66}$$

so there is no contribution from the integral at infinity. So we are left with the residue at $z = \zeta_{\mathbf{k}}$ only:

$$\begin{aligned} \frac{1}{\beta} \sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} &= \mathrm{Res}[\frac{1}{e^{\beta z} + 1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}}, z = \zeta_{\mathbf{k}}] \\ &= \frac{e^{-\zeta_{\mathbf{k}}\tau}}{e^{\beta\zeta_{\mathbf{k}}} + 1} = e^{-\zeta_{\mathbf{k}}\tau} f(\zeta_{\mathbf{k}}) \end{aligned} \tag{17.67}$$

this agrees with the value of $\mathcal{G}_0(\mathbf{k}; \tau)$ for $\tau < 0$. In particular, for $\tau = 0^-$ the sum evaluates to $f(\zeta_{\mathbf{k}})$, proving our early statement.

For the $\tau > 0$ integral we use the same contour but with the other form of auxiliary function $\beta \frac{1}{e^{-\beta z}+1}$:

$$\sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} = \int_{C_1} \frac{dz}{2\pi i} \frac{\beta}{e^{-\beta z} + 1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}} \tag{17.68}$$

the integrand also vanishes at $\Re z \to \pm\infty$ (since we have chosen the right functions).

$$\frac{1}{e^{-\beta z} + 1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}} \to \begin{cases} z^{-1} e^{-z\tau} < z^{-1} e^{-z0^+} & \Re z \to \infty \\ z^{-1} e^{-z(\tau-\beta)} < z^{-1} e^{z0^+} & \Re z \to -\infty \end{cases} \tag{17.69}$$

we then have

$$\begin{aligned} \frac{1}{\beta} \sum_n \frac{e^{-ik_n\tau}}{ik_n - \zeta_{\mathbf{k}}} &= \mathrm{Res}[\frac{-1}{e^{-\beta z} + 1} \frac{e^{-z\tau}}{z - \zeta_{\mathbf{k}}}, z = \zeta_{\mathbf{k}}] \\ &= \frac{-e^{-\zeta_{\mathbf{k}}\tau}}{e^{-\beta\zeta_{\mathbf{k}}} + 1} = -e^{-\zeta_{\mathbf{k}}\tau}(1 - f(\zeta_{\mathbf{k}})) \end{aligned} \tag{17.70}$$

this agrees with the value of $\mathcal{G}_0(\mathbf{k}; \tau)$ for $\tau > 0$. In particular, for $\tau = 0^+$ the sum evaluates to $-1 + f(\zeta_{\mathbf{k}})$, proving our early statement.

17.8.2 General Matsubara Summation

We will show how a general Matsubara summation in either bosonic or fermionic frequencies can be evaluated through a transformation by contour integral. For a summation

$$S = \sum_{\omega_n} h(\omega_n) \tag{17.71}$$

where $h(\omega_n) \propto e^{i\omega_n 0^+}$.

$$\omega_n = \begin{cases} q_n = 2n\pi T & \text{bosonic} \\ k_n = (2n+1)\pi T & \text{fermionic} \end{cases} \tag{17.72}$$

we introduce an auxiliary function $g(z)$ which has simple poles at $i\omega_n$. There are many choices, we focus on a common choice

$$g(z) = \frac{\zeta\beta}{e^{\beta z} - \zeta} = \begin{cases} \frac{\beta}{e^{\beta z}-1} & \text{bosonic} \\ \frac{-\beta}{e^{\beta z}+1} & \text{fermionic} \end{cases} \tag{17.73}$$

we can check that they have residues 1 at each $z = i\omega_n$. We use the contour integral in Altland Fig. 4.2,

$$\begin{aligned} S &= \sum_{\omega_n} h(\omega_n) = \sum_{\omega_n} \operatorname{Res}\left[g(z)h(-iz), z = i\omega_n\right] = \oint_{\gamma_1} \frac{dz}{2\pi i} g(z)h(-iz) \\ &= \oint_{\gamma_2} \frac{dz}{2\pi i} g(z)h(-iz) = 0 - \sum_k \operatorname{Res}\left[g(z)h(-iz), z = i\omega_k\right] \end{aligned} \tag{17.74}$$

where ω_k are poles of function $h(\omega)$. If there are only a finite number of ω_k , then it is advantageous to do this transformation. We have also assumed that $gh \to 0$ sufficiently fast as $|z| \to \infty$ in any direction. More specifically,

$$\lim_{|z|\to\infty} |g(z)h(-iz)| < \frac{1}{|z|} \tag{17.75}$$

Suppose h have only a single pole

$$h(\omega_n) = \frac{Te^{i\omega_n 0^+}}{i\omega_n - \xi}, \qquad h(-iz) = \frac{Te^{z0^+}}{z - \xi} \tag{17.76}$$

we have

$$g(z)h(-iz) \sim \frac{1}{e^{\beta z} - \zeta} \frac{e^{z0^+}}{z - \xi} \tag{17.77}$$

for $\Re z \to \infty$, we have $e^{-\beta z}$, for $\Re z \to -\infty$ we have e^{z0^+}, so the boundary term is indeed zero. In this case, we have

$$S = T\sum_{\omega_n} \frac{e^{i\omega_n 0^+}}{i\omega_n - \xi} = -\operatorname{Res}\left[g(z)h(-iz), z = \xi\right] = -Tg(\xi) = \frac{-\zeta}{e^{\beta z} - \zeta} \tag{17.78}$$

In summary, for fermions and bosons,

$$\begin{aligned} T\sum_n \frac{e^{i\omega_n 0^+}}{i\omega_n - \xi} = \frac{-\zeta}{e^{\beta\xi} - \zeta} &= \begin{cases} -\zeta n_B(\xi) & i\omega_n \text{bosonic} \\ -\zeta n_F(\xi) & i\omega_n \text{fermionic} \end{cases} \\ \zeta &= \begin{cases} 1 & \text{boson} \\ -1 & \text{fermion} \end{cases} \end{aligned} \tag{17.79}$$

$$n_F(\epsilon) = \frac{1}{e^{\beta\epsilon} + 1}, \qquad n_B(\epsilon) = \frac{1}{e^{\beta\epsilon} - 1} \tag{17.80}$$

separately

$$\begin{aligned} T\sum_n \frac{e^{ik_n 0^+}}{ik_n - \xi} &= n_F(\xi) \\ T\sum_n \frac{e^{iq_n 0^+}}{iq_n - \xi} &= -n_B(\xi) \end{aligned} \tag{17.81}$$

18 Linear Response in imaginary time

Susceptibilities are also defined in Matsubara space. As in the fermionic case, analytic continuation suffices to obtain the retarded response. Knowing this, linear response takes a simple form in imaginary time that I will explain.

18.1 Matsubara frequencies for the susceptibility, as bosonic correlation function

Recall that all the information that we need for the susceptibility is in the spectral function χ''. To do actual calculations of correlation functions at finite temperature, whether by numerical or analytical means, it turns out that it is much easier to compute a function that is different from the retarded response function. By analogy with the fermionic case, that function is defined as follows

$$\begin{aligned}\chi_{A_iA_j}(\tau) &= \langle \mathcal{T}_\tau A_i(\tau) A_j \rangle \\ &= \langle A_i(\tau) A_j \rangle \, \theta(\tau) + \langle A_j A_i(\tau) \rangle \, \theta(-\tau)\end{aligned} \tag{18.1}$$

$$A_i(\tau) = e^{\tau K} A_i e^{-\tau K} \tag{18.2}$$

Notice that here $\mathcal{T}_\tau$ is the time ordering operator for bosonic operators, which does not have the extra minus sign when the order is exchanged inside the time ordering. As long as we can extract the spectral function χ'' from the Matsubara susceptibility, we can obtain all the information we need.

We shall define $\chi_{A_iA_j}(\tau)$ in the interval $-\beta < \tau < \beta$ only and find its Fourier Series. There is also a periodic condition for $\chi_{A_iA_j}(\tau)$. Take $-\beta < \tau < 0$, we have

$$\begin{aligned}\chi_{A_iA_j}(\tau) &= Z^{-1} \operatorname{Tr}\left(e^{-\beta K} A_j A_i(\tau)\right) \\ &= Z^{-1} \operatorname{Tr}\left(e^{-\beta K} A_j e^{\tau K} A_i e^{-\tau K}\right) \\ &= Z^{-1} \operatorname{Tr}\left(e^{-\beta K} e^{(\beta+\tau)K} A_i e^{-(\beta+\tau)K} A_j\right) \\ &= \langle A_i(\tau+\beta) A_j \rangle \\ &= \chi_{A_iA_j}(\tau+\beta)\end{aligned} \tag{18.3}$$

therefore $\chi_{A_iA_j}(\tau)$ has period β, and we can restrict to $\tau \in [0, \beta]$ and perform a Fourier series expansion

$$\chi_{A_iA_j}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-iq_n\tau} \chi_{A_iA_j}(iq_n) \tag{18.4}$$

in order to satisfy the periodic boundary condition, the **bosonic Matsubara frequencies** are defined by

$$q_n = 2n\pi k_B T = \frac{2n\pi}{\beta} \quad ; \quad n \in \mathbb{Z} \tag{18.5}$$

the inverse transform is

$$\chi_{A_iA_j}(iq_n) = \int_0^\beta d\tau e^{iq_n\tau} \chi_{A_iA_j}(\tau) \tag{18.6}$$

Using the Lehmann representation, we can find a spectral representation for the Fourier coefficients $\chi_{A_iA_j}(iq_n)$:

$$\begin{aligned}\chi_{A_iA_j}(iq_n) &= \int_0^\beta d\tau e^{iq_n\tau} \langle A_i(\tau) A_j \rangle \\ &= \frac{1}{Z} \sum_{m,n} e^{-\beta K_n} \langle n | A_i | m \rangle \langle m | A_j | n \rangle \int_0^\beta d\tau e^{iq_n\tau} e^{\tau(K_n - K_m)} \\ &= \frac{1}{Z} \sum_{m,n} \langle n | A_i | m \rangle \langle m | A_j | n \rangle \frac{e^{-\beta K_n} - e^{-\beta K_m}}{-iq_n + K_m - K_n}\end{aligned} \tag{18.7}$$

notice that since we are considering bosonic operators of the type A_i, A_j with $\psi^\dagger\psi$, the number of particles is the same between $|m\rangle, |n\rangle$ for non-zero matrix elements, so $K_n - K_m = E_n - E_m$. Recall the Lehmann representation of $\chi''_{A_iA_j}(\omega)$

$$\chi''_{A_iA_j}(\omega) = \frac{1}{Z} \sum_{n,m} \langle n | A_i | m \rangle \langle m | A_j | n \rangle \left(e^{-\beta E_n} - e^{-\beta E_m}\right) \pi\delta(\omega - (E_m - E_n)) \tag{18.8}$$

$$\int \frac{d\omega'}{\pi} \pi \frac{\delta(\omega' - (E_m - E_n))}{-iq_n + \omega'} = \frac{1}{-iq_n + K_m - K_n} \tag{18.9}$$

we can write

$$\chi_{A_iA_j}(iq_n) = \int \frac{d\omega'}{\pi} \frac{\chi''_{A_iA_j}(\omega')}{\omega' - iq_n} \tag{18.10}$$

comparing this with our definition of the spectral function

$$\chi_{A_iA_j}(z) = \int \frac{d\omega'}{\pi} \frac{\chi''_{A_iA_j}(\omega')}{\omega' - z} \tag{18.11}$$

it is clear that

$$\begin{aligned} \chi_{A_iA_j}(z = iq_n) &= \chi_{A_iA_j}(iq_n) \\ \chi_{A_iA_j}(z = \omega + i\eta) &= \chi^R_{A_iA_j}(\omega) \end{aligned} \tag{18.12}$$

and that they are the same function defined in the real and imaginary axis. If we know the analytic form of $\chi_{A_iA_j}(iq_n)$, we can then easily obtain $\chi^R_{A_iA_j}(\omega)$ which is represent physical quantities directly.

18.2 Linear Response in imaginary time

Knowing that retarded responses can be obtained from analytical continuation, it is clear that there is a formulation of linear response in imaginary time. The interacting in Shrodinger picture is now written as

$$H = H_0 + \delta\mathcal{H}(\tau) \tag{18.13}$$

$$\delta\mathcal{H}(\tau) = -\int d^3 r A_i(\mathbf{r}) a_i(\mathbf{r}, \tau) \tag{18.14}$$

where t has been replaced with τ. The classical field $a_i(\mathbf{r}, \tau)$ in imaginary time does not make sense physically, but we can nevertheless imagine adding such a Hamiltonian $\delta\mathcal{H}(\tau)$ to H_0 and forming a new Hamiltonian. So far, τ is only a free variable here.

$$\langle B_{\mathrm{H}}(\mathbf{r}, \tau)\rangle = \frac{\langle \mathcal{T}_\tau \left[U_I(\beta, 0) B_{\mathrm{I}}(\mathbf{r}, \tau)\right]\rangle_0}{\langle U_I(\beta, 0)\rangle_0} \tag{18.15}$$

we approximate U_I to first order in the numerator and zero order in the denomenator

$$\begin{aligned} \langle B_H(\mathbf{r}, \tau)\rangle &\approx \langle B_I(\mathbf{r}, \tau)\rangle - \int_0^\tau \mathrm{d}\tau' \left\langle \mathcal{T}_\tau \left[\mathcal{H}_{\mathrm{I}}(\tau') B_{\mathrm{I}}(\mathbf{r}, \tau)\right]\right\rangle_0 \\ &= \langle B_I(\mathbf{r}, \tau)\rangle + \int d^3 r' \int_0^\tau \mathrm{d}\tau' a_i(\mathbf{r}', \tau') \left\langle \mathcal{T}_\tau \left[A_i(\mathbf{r}', \tau') B_{\mathrm{I}}(\mathbf{r}, \tau)\right]\right\rangle_0 \end{aligned} \tag{18.16}$$

We have

$$\begin{aligned} \delta \langle B(\mathbf{r}, t)\rangle &= \int d^3 r' \int_0^\tau \mathrm{d}\tau' \chi^R_{BA_i}(\mathbf{r}, \tau; \mathbf{r}', \tau') a_i(\mathbf{r}', \tau') \\ \chi_{BA_i}(\mathbf{r}, \tau; \mathbf{r}', \tau') &\equiv \langle \mathcal{T}_\tau \left[A_i(\mathbf{r}', \tau') B_{\mathrm{I}}(\mathbf{r}, \tau)\right]\rangle \end{aligned} \tag{18.17}$$

in momentum-frequency space (assume translation invariance)

$$\delta \langle B(\mathbf{q}, iq_n)\rangle = \chi^R_{BA_i}(\mathbf{q}, iq_n) a_i(\mathbf{q}, iq_n) \tag{18.18}$$

with

$$\chi_{BA_i}(\mathbf{q}, iq_n) = \int_0^\beta d\tau \int d\mathbf{r} e^{iq_n(\tau - \tau')} e^{-i\mathbf{k}\cdot(\mathbf{r} - \mathbf{r}')} \chi_{BA_i}(\mathbf{r} - \mathbf{r}', \tau - \tau') \tag{18.19}$$

so we have derived explicitly the linear response function in imaginary time. Later, the perturbations will be put into the system in the form of imaginary operators $\delta\mathcal{H}(\tau)$, and calculate the corresponding imaginary response function $\chi(iq_n)$.

19 Quasiparticles and Spectral Weight

19.1 Probabilistic interpretation of the spectral weight

In non-interacting particles

$$\mathcal{G}_0(k) = \frac{1}{ik_n - \zeta_{\mathbf{k}}}, \qquad G_0^R(\mathbf{k},\omega) = \frac{1}{\omega - \zeta_{\mathbf{k}} + i\eta} \tag{19.1}$$

$$A_0(\omega) = -2\Im G^R(\omega) = 2\pi\delta(\omega - \zeta_{\mathbf{k}}) \tag{19.2}$$

In physical terms, this tells us that for non-interacting particles in a translationally invariant system, a single excited particle or hole of momentum $\mathbf{k}$ added to an eigenstate is a true excited eigenstate located at an energy $\omega = \zeta_{\mathbf{k}}$ above or below the Fermi level. In the interacting case, the Lehmann representation will show us clearly that what we just said is the correct interpretation.

For a different representation, for example for momentum,

$$A(\mathbf{k},\omega') = e^{\beta\Omega}\sum_{mn}\left(e^{-\beta K_n} + e^{-\beta K_m}\right)\left|\langle n\left|c_{\mathbf{k}}\right|m\rangle\right|^2 2\pi\delta\left(\omega' - (K_m - K_n)\right) \tag{19.3}$$

The overlap matrix element $\left|\langle n\left|c_{\mathbf{k}}\right|m\rangle\right|^2$ that gives the magnitude of the delta function contribution to the spectral weight represents the overlap between the initial state with one more particle or hole in a momentum eigenstate and the true excited one-particle or one-hole state. The last equation clearly shows that $A(\mathbf{k},\omega')/(2\pi)$ is positive and we already know that it is normalized to unity,

$$\int \frac{d\omega'}{2\pi} A(\mathbf{k},\omega') = \left\langle \left\{ c_{\mathbf{k}}, c_{\mathbf{k}}^\dagger \right\} \right\rangle = 1 \tag{19.4}$$

The probability interpretation of $A(\mathbf{k},\omega')$ is as follows: Suppose we are in the non-interacting system, adding a particle with momentum $\mathbf{k}$ would take many-body ground state $|n\rangle$ to $|m\rangle$, with energy change $\omega = K_m - K_n = \zeta_{\mathbf{k}}$. For an interacting system, when we add a particle with momentum $\mathbf{k}$, we ask the same question whether it takes some eigenstate state $|n\rangle$ to $|m\rangle$, but now in general $c_{\mathbf{k}}^\dagger|n\rangle$ is not an eigenstate, so we can at best ask the probability amplitude of such transitions. Hence $A(\mathbf{k},\omega')$ is the probability that a state formed from a true eigenstate $|n\rangle$ by adding a particle in a single-particle state $\mathbf{k}$, namely $c_{\mathbf{k}}^\dagger|n\rangle$, is a true eigenstate whose energy is ω above or below the chemical potential. In the interacting case, many energy eigenstates will have a non-zero overlap with the state formed by simply adding a particle or a hole in a momentum eigenstate. While particle-like excitations will overlap mostly with eigenstates that are reached by adding positive ω, they can also overlap eigenstates that are reached by adding negative ω. In an analogous manner, hole-like eigenstates will be mostly at negative ω. Let us see how this manifests itself in a specific experiment.

19.2 ARPES experiment

In a photoemission experiment, a photon ejects an electron from a solid. This is nothing but the old familiar photoelectric effect. In the angle-resolved version of this experiment (ARPES), the energy and the direction of the outgoing electron are measured. This is illustrated in Fig.(26-1). The outgoing electron energy can be measured. Because it is a free electron, this measurement gives the value of the wave vector through $k^2/2m$. Using energy conservation, the energy of the outgoing electron is equal to the energy of the incident photon E_{ph}, minus the work function W plus the energy of the electron in the system, ω, measured relative to the Fermi level

$$E_{\rm ph} + (\omega + \mu) - W = \frac{k^2}{2m} \tag{19.5}$$

The energy of the electron in the system ω will be mostly negative. The value of $\mathbf{k}_\parallel$ may be extracted by simple geometric considerations from the value of k. Since in this experiment there is translational invariance only in the direction parallel to the plane, this means that in fact it is only the value of $\mathbf{k}_\parallel$ that is conserved. Hence, it is only for layered systems that we really have access to both energy ω and total momentum $\mathbf{k}_\parallel$ of the electron when it was in the system.

The scattering cross-section is given by the fermi function $f(\omega)$ and the in-plane modes of the spectral weight $A(\mathbf{k}_\parallel,\omega)$

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto f(\omega)A\left(\mathbf{k}_\parallel,\omega\right) \tag{19.6}$$

The state of technology and historical coincidences have conspired so that the first class of layered (quasi-two-dimensional) compounds that became available for ARPES study around 1990 were high temperature superconductors. These materials have properties that make them non-conventional materials that are not yet understood using standard approaches of solid-state Physics. Hence, people started to look for two-dimensional materials that would behave as expected from standard models. Such a material, semimetallic $TiTe_2$ was finally found around 1992. For our purposes, quasi-two-dimensional just means here that the Fermi velocity perpendicular to the planes is much smaller than the Fermi velocity in the planes. The results of this experiment[3] appear in Ref. Fig.(31-1).

The incident photon energy is 21.2eV while the variation of ω is on a scale of 200meV so that, for all practical purposes, the magnitude of the momentum vector k is a fixed quantity. Hence, the angle with respect to the incident photon suffices to define the value of $\mathbf{k}_\parallel$. Each curve in Fig.(31-1) is for a given $\mathbf{k}_\parallel$, in other words for a given angle measured from the direction of incidence of the photon. The intensity is plotted as a function of the energy of the outgoing electron. Hence these plots are often called **EDC** (**energy distribution curves**). The zero corresponds to an electron extracted from the Fermi level. Electrons with a smaller kinetic energy come from states with larger binding energy. In other words, each of the curves above is basically a plot of the hole-like part of $A(\mathbf{k}_\parallel, \omega)$, or if you want $f(\omega)A(\mathbf{k}_\parallel, \omega)$. From band structure calculations, one knows that the angle $\theta = 14.75^0$ corresponds to the Fermi level (marked k_F on the plot) of a $Ti - 3d$ derived band. It is for this scattering angle that the agreement between experiment and Fermi liquid theory is best (see Sec.(31.5) below). The plots for angles $\theta < 14.75^0$ correspond to wave vectors above the Fermi level. There, the intensity is much smaller than for the other peaks. For $\theta = 13^0$, the experimental results are scaled up by a factor 16 .

The energy resolution is $35meV$: Nevertheless, it is clear that the line shapes are larger than the energy resolution: Clearly the spectral weight is not a delta function and the electrons in the system are not free particles. Nevertheless, there is a definite maximum in the spectra whose position changes with $\mathbf{k}_\parallel$: It is tempting to associate the width of the line to a lifetime. In other words, a natural explanation of these spectra is that the electrons inside the system are quasiparticles whose energy disperses with wave vector and that have a lifetime. We try to make these concepts more precise below.

One can also make plots of the probability of having a certain momentum at the Fermi level $\omega = 0$: This is usually represented by a color plot called MDC(**momentum distribution curve**). A spectacular case, shown in Fig. (31.3) is that of strontium ruthenate Sr_2RuO_4[4], also interesting because it was proposed to be a topological superconductor.

Fig. (31-2) shows some beautiful experimental and theoretical recent work on this compound. [228] On the left is the Fermi surface and on the right various MDCs at energies below the Fermi surface. This should be contrasted with high-temperature superconductors in Fig. 31.3. The Fermi surface seems to vanish in thin air ([157]). Getting back to strontium ruthenate [228], Fig. (31-3) shows some detailed comparisons between experiment and theory. The theory is based on density-functional theory, augmented by dynamical mean-field calculations, topics we will address in subsequent chapters. The calculation shows that the effect of spin-orbit interactions is crucial. The red dots are the measurements and the color curves the calculations.

19.3 Quasiparticles

The intuitive notions we may have about lifetime and effective mass of an electron caused by interactions in a solid can all be extracted from the **self-energy**. For a general interacting system, the one-particle retarded Green's function takes the form

$$G^R(\mathbf{k}, \omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}} - \Sigma^R(\mathbf{k}, \omega)} \tag{19.7}$$

We can drop in since $\Im\Sigma^R(\mathbf{k}, \omega)$ is negative to preserve causality and always larger than $i\eta$ that should anyway be taken to zero at the end. The spectral weight is then

$$\begin{aligned} A(\mathbf{k}, \omega) &= -2\Im G^R(\mathbf{k}, \omega) \\ &= \frac{-2\Im\Sigma^R(\mathbf{k}, \omega)}{\left(\omega - \zeta_{\mathbf{k}} - \Re\Sigma^R(\mathbf{k}, \omega)\right)^2 + \left(\Im\Sigma^R(\mathbf{k}, \omega)\right)^2} \end{aligned} \tag{19.8}$$

If the imaginary part of the self-energy, the scattering rate, is not too large and varies smoothly with frequency, conditions I will refine when I discuss Fermi liquids soon, the spectral weight will have a maximum whenever, at

[3] R. Claessen, R.O. Anderson, J.W. Allen, C.G. Olson, C. Janowitz, W.P. Ellis, S. Harm, M. Kalning, R. Manzke, and M. Skibowski, Phys. Rev. Lett 69, 808 (1992).

[4] A. Damascelli, D. H. Lu, K. M. Shen, N. P. Armitage, F. Ronning, D. L. Feng, C. Kim, Z.-X. Shen, T. Kimura, Y. Tokura, Z. Q. Mao, and Y. Maeno. Fermi surface, surface states, and surface reconstruction in sr2ruo4. Phys. Rev. Lett., 85:5194ñ5197, Dec 2000.

fixed $\mathbf{k}$, there is a value of ω that satisfies

$$\omega - \zeta_{\mathbf{k}} - \Re\Sigma^R(\mathbf{k},\omega) = 0 \tag{19.9}$$

We assume the solution of this equation exists. Let $E_{\mathbf{k}} - \mu$ be the value of ω for which this equation is satisfied:

$$E_{\mathbf{k}} - \mu - \zeta_{\mathbf{k}} - \Re\Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu) = 0 \tag{19.10}$$

$E_{\mathbf{k}}$ is the so-called **quasiparticle energy**. This energy is clearly in general different from the results of band structure calculations that are usually obtained by neglecting the frequency dependence of the self-energy. Expanding $\omega - \zeta_{\mathbf{k}} - \Re\Sigma^R(\mathbf{k},\omega)$ around $\omega = E_{\mathbf{k}} - \mu$ where $A(\mathbf{k},\omega)$ is a maximum, we find

$$\begin{aligned}
\omega - \zeta_{\mathbf{k}} - \Re\Sigma^R(\mathbf{k},\omega) &\approx 0 + \frac{\partial}{\partial\omega}\left[\omega - \zeta_{\mathbf{k}} - \Re\Sigma^R(\mathbf{k},\omega)\right]_{\omega=E_{\mathbf{k}}-\mu}(\omega - E_{\mathbf{k}} + \mu) + \dots \\
&\approx \left(1 - \left.\frac{\partial\Re\Sigma^R(\mathbf{k},\omega)}{\partial\omega}\right|_{\omega=E_{\mathbf{k}}-\mu}\right)(\omega - E_{\mathbf{k}} + \mu) + \dots \\
&= \frac{\omega - E_{\mathbf{k}} + \mu}{Z_{\mathbf{k}}}
\end{aligned} \tag{19.11}$$

where we define the **quasiparticle weight** or square of the wave function renormalization by

$$Z_{\mathbf{k}} = \frac{1}{1 - \frac{\partial}{\partial\omega}\Re\Sigma^R(\mathbf{k},\omega)\big|_{\omega=E_{\mathbf{k}}-\mu}} \tag{19.12}$$

then in the vicinity of the maximum, the spectral weight takes the form

$$\begin{aligned}
A(\mathbf{k},\omega) &= \frac{-2\Im\Sigma^R(\mathbf{k},\omega)}{Z_{\mathbf{k}}^{-2}\left(\omega - E_{\mathbf{k}} + \mu\right)^2 + \left(\Im\Sigma^R(\mathbf{k},\omega)\right)^2} + inc \\
&= 2\pi Z_{\mathbf{k}}\frac{1}{\pi}\frac{-Z_{\mathbf{k}}\Im\Sigma^R(\mathbf{k},\omega)}{\left(\omega - E_{\mathbf{k}} + \mu\right)^2 + \left(Z_{\mathbf{k}}\Im\Sigma^R(\mathbf{k},\omega)\right)^2} + inc \\
&= 2\pi Z_{\mathbf{k}}\left[\frac{1}{\pi}\frac{\Gamma_{\mathbf{k}}(\omega)}{\left(\omega - E_{\mathbf{k}} + \mu\right)^2 + \left(\Gamma_{\mathbf{k}}(\omega)\right)^2}\right] + inc
\end{aligned} \tag{19.13}$$

where we've defined the scattering rate

$$\Gamma_{\mathbf{k}}(\omega) = -Z_{\mathbf{k}}\Im\Sigma^R(\mathbf{k},\omega) \tag{19.14}$$

If we neglect the frequency dependence of $\Gamma_{\mathbf{k}}(\omega)$, the bracket is then a Lorentzian function centered at the quasiparticle energy $E_{\mathbf{k}} - \mu$ with width $\Gamma_{\mathbf{k}}$.

The integral over frequency of the square bracket is unity. Since $A(\mathbf{k},\omega)/2\pi$ is normalized to unity, this means both that

$$Z_{\mathbf{k}} \leq 1 \tag{19.15}$$

and that there are additional contributions to the spectral weight that we have denoted *inc* in accord with the usual terminology of incoherent background. The equality in the last equation holds only if the real part of the self-energy is frequency independent.

It is also natural to ask how the quasiparticle disperses, in other words, what is its effective Fermi velocity compared with that of the bare particle. Let us define the bare velocity by

$$v_{\mathbf{k}} = \nabla_{\mathbf{k}}\zeta_{\mathbf{k}} \tag{19.16}$$

and the **renormalized velocity** by

$$v^*_{\mathbf{k}} = \nabla_{\mathbf{k}}E_{\mathbf{k}} \tag{19.17}$$

the relation between them is given by taking the gradient of the quasiparticle equation

$$\begin{aligned}
\nabla_{\mathbf{k}}\left[E_{\mathbf{k}} - \mu - \zeta_{\mathbf{k}} - \Re\Sigma^R\left(\mathbf{k}, E_{\mathbf{k}} - \mu\right)\right] &= 0 \\
v^*_{\mathbf{k}} - v_{\mathbf{k}} - \frac{\partial\Re\Sigma^R\left(\mathbf{k}, E_{\mathbf{k}} - \mu\right)}{\partial\mathbf{k}} - \left.\frac{\partial\Re\Sigma^R(\mathbf{k},\omega)}{\partial\omega}\right|_{E_{\mathbf{k}}-\mu} v^*_{\mathbf{k}} &= 0
\end{aligned} \tag{19.18}$$

The last equation is easily solved if we can write the $\mathbf{k}$ dependence of Σ^R as a function of $\zeta_{\mathbf{k}}$ instead, something that is always possible for spherical Fermi surfaces. In such a case, $\nabla_{\mathbf{k}} \to (\nabla_{\mathbf{k}}\zeta_{\mathbf{k}})\,\partial/\partial\zeta_{\mathbf{k}}$ as we can see for example when $\zeta_{\mathbf{k}} = \mathbf{k}^2/2m$ and we have

$$\frac{v^*_{\mathbf{k}}}{v_{\mathbf{k}}} = \frac{1 + \frac{\partial}{\partial\zeta_{\mathbf{k}}}\Re\Sigma^R\left(\mathbf{k}, E_{\mathbf{k}} - \mu\right)}{1 - \frac{\partial}{\partial\omega}\Re\Sigma^R(\mathbf{k},\omega)\big|_{\omega=E_{\mathbf{k}}-\mu=0}} \tag{19.19}$$

In cases where the electronic (band) structure has correctly treated the $\mathbf{k}$-dependence of the self-energy, or when the latter is negligible, then the renormalized Fermi velocity differs from the bare one only through the famous **quasiparticle renormalization factor**. In other words, $v^*_{\mathbf{k}} = Z_{\mathbf{k}} v_{\mathbf{k}}$. The equation for the renormalized velocity is also often written in terms of a mass renormalization instead. Indeed, we will discuss later the fact that the Fermi wave vector k_F is unmodified by interactions for spherical Fermi surfaces (Luttinger's theorem). Defining then $m^* v^*_{k_F} = k_F = m v_{k_F}$ means that our equation for the renormalized velocity gives us

$$\frac{m}{m^*} = \lim_{\mathbf{k}\to\mathbf{k}_F} \frac{1 + \frac{\partial}{\partial\zeta_{\mathbf{k}}}\Re\Sigma^R\left(\mathbf{k}, E_{\mathbf{k}} - \mu\right)}{1 - \frac{\partial}{\partial\omega}\Re\Sigma^R(\mathbf{k},\omega)\big|_{\omega=E_{\mathbf{k}}-\mu}} \tag{19.20}$$

19.4 Fermi liquid interpretation of ARPES

Let us see how to interpret the experiments of the previous subsection in light of the quasiparticle model just described. First of all, the wave vectors studied are all close to the Fermi surface as measured on the scale of k_F. Hence, every quantity appearing in the quasiparticle spectral weight $A(\mathbf{k},\omega)$ that depends on the self-energy is evaluated at the Fermi wave vector, which can however be angle dependent. The frequency dependence of the self-energy then is most important. The experiments were carried out at $T = 20K$ where the resistivity has a T^2 temperature dependence. This is the regime dominated by electron-electron interactions, where so-called Fermi liquid theory applies.

We have already discussed the main ingredients in Fermi liquid theory which allows for the description of electrons in a metal as quasiparticles, basically that the phase space available for scattering vanishes near the Fermi surface. One way to allow this is for the self energy $\Sigma(\mathbf{k},\omega)$ near the Fermi surface in the limit of zero temperature to be

1. Analytic
2. Has an imaginary part that vanishes at zero frequency

The latter result follows from general considerations on the Pauli exclusion principle and available phase space that are briefly summarized in Fig. (31-4). I will give an alternate derivation in the section on the electron-gas.

Let us define real and imaginary parts of the retarded self-energy by

$$\Sigma^R = \Sigma' + i\Sigma'' \tag{19.21}$$

our hypothesis imply that the imaginary part should have a Taylor expansion in ω as

$$\Sigma''\left(\mathbf{k}_F;\omega\right) = \alpha\omega - \gamma\omega^2 + \ldots \tag{19.22}$$

The imaginary part of the retarded self-energy must be **negative** to insure that the retarded Green's function has poles in the lower half-plane, as is clear from

$$G^R(\mathbf{k},\omega) = \frac{1}{\omega + i\eta - \zeta_{\mathbf{k}} - \Sigma^R(\mathbf{k},\omega)} \tag{19.23}$$

This means that we must have $\alpha = 0$ and $\gamma > 0$. Fermi liquid theory keeps only the leading term

$$\Sigma'' = -\gamma\omega^2 \tag{19.24}$$

We will verify for simple models that this quadratic frequency dependence is essentially correct in $d \geq 3$. We know that the imaginary part of the self-energy must vanish at infinite frequency where free-particle behavior is expected, as in the harmonic oscillator case. We thus take the following smooth cutoff model, neglecting impurity scattering and temperature

$$\Sigma''(\omega) = \begin{cases} -s\frac{\omega^2}{\omega^{*2}} & \text{for } \omega < \omega^* \\ -sF(\frac{\omega}{\omega^*}) & \text{for } \omega > \omega^* \end{cases} \tag{19.25}$$

where ω^* is the frequency at which ω^2 behavior stops, $2s$ is the electron-electron scattering rate (in units $\hbar = 1$) without many-body effects, and the cutoff function $F(y)$ takes the value unity at $y = 1$ and then decreases monotonically to zero afterwards. A more realistic model, as we will see, crosses over from ω^2 behavior while continuing to increase in absolute value before decreasing. But that does not modify the result.

The real part is then obtained from the Kramers-Kronig relation

$$\begin{aligned}\Sigma'(\mathbf{k}_F;\omega) - \Sigma'(\mathbf{k}_F;\infty) &= \mathcal{P}\int \frac{d\omega'}{\pi}\frac{\Sigma''(\mathbf{k}_F;\omega')}{\omega'-\omega} \\ &= -\frac{s}{(\omega^*)^2}\mathcal{P}\int_{-\omega^*}^{\omega^*}\frac{d\omega'}{\pi}\frac{(\omega')^2}{\omega'-\omega} - 2s\mathcal{P}\int_{\omega^*}^{\infty}\frac{d\omega'}{\pi}\frac{F(\omega'/\omega^*)}{\omega'-\omega}\end{aligned} \tag{19.26}$$

Where we make the additional assumption that $\Sigma''(\omega)$ is even in frequency. Another way to state that is that we assume particle-hole symmetry.

The first integral gives

$$-\frac{s}{(\omega^*)^2}\mathcal{P}\int_{-\omega^*}^{\omega^*}\frac{d\omega'}{\pi}\frac{(\omega')^2}{\omega'-\omega} = -\frac{s}{\pi}\left[2(\omega/\omega^*) + (\omega/\omega^*)^2\ln\left|\frac{1-(\omega/\omega^*)}{1+(\omega/\omega^*)}\right|\right] \tag{19.27}$$

we will set $\Sigma'(\mathbf{k}_F;\infty) = -\frac{s}{\pi}$, related to the renormalization of the chemical potential.

$$\begin{aligned}\Sigma'(\mathbf{k}_F;\omega) &= -\frac{s}{\pi}\left[1 + 2(\omega/\omega^*) + (\omega/\omega^*)^2\ln\left|\frac{1-(\omega/\omega^*)}{1+(\omega/\omega^*)}\right|\right] \\ &= -\frac{s}{\pi}\left[1 + 2x + x^2\ln\left|\frac{1-x}{1+x}\right|\right] \\ \lim_{x\ll 1}\Sigma'(\mathbf{k}_F;\omega) &= -\frac{s}{\pi}\left[1 + 2x - 2x^3\right]\end{aligned} \tag{19.28}$$

where we defined $x \equiv \omega/\omega^*$ and used the fact $\ln\frac{1-x}{1+x} \sim -2x$ for small x. The remaining terms involving $F(x)$ can also be Taylor expanded

$$-2s\int_{\omega^*}^{\infty}\frac{d\omega'}{\pi}\frac{F(\omega'/\omega^*)}{\omega'}\sum_{n=0}^{\infty}(\frac{\omega}{\omega'})^{2n+1} \tag{19.29}$$

the linear in ω term is $n = 0$, we can find an upper bound

$$-2s\int_{\omega^*}^{\infty}\frac{d\omega'}{\pi}\frac{F(\omega'/\omega^*)}{\omega'}(\frac{\omega}{\omega'}) \le -2s\int_{\omega^*}^{\infty}\frac{d\omega'}{\pi}\frac{1}{\omega'}(\frac{\omega}{\omega'}) = -\frac{2s}{\pi}\frac{\omega}{\omega^*} \tag{19.30}$$

so the overall Σ' up to first order is

$$\begin{aligned}\Sigma' \equiv -\frac{s}{\pi}\left[1 + 2\zeta x\right] &\le -\frac{s}{\pi}\left[1 + 4x\right] \\ \zeta &\le 2\end{aligned} \tag{19.31}$$

We then have

$$\frac{\partial}{\partial\omega}\Sigma'(\mathbf{k}_F,\omega)\Big|_{\omega=0} = -\frac{2s\zeta}{\pi\omega^*} < 0 \tag{19.32}$$

This in turn means that the corresponding value of Z_{k_F} is less than unity. In summary, the analyticity hypothesis along with the vanishing of $\Sigma''(\omega = 0)$ implies the existence of quasiparticles.

The solid lines in Fig.(31-1) are two-parameter fits that also take into account the wave vector and energy resolution of the experiment. One parameter is $E_k - \mu$ while the other one is γ', a quantity defined by substituting the Fermi liquid approximation in the equation for damping

$$\Gamma_{k_F}(\omega) = Z_{k_F}\gamma\omega^2 = \gamma'\omega^2 \tag{19.33}$$

19.5 Momentum distribution in an interacting system

In an interacting system, momentum is not a good quantum number so $\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle \neq f(\zeta_{\mathbf{k}})$. It should instead be computer by the spectral function $A(\mathbf{k}, \omega')$. To see this, recall that

$$\begin{aligned} \mathcal{G}(\mathbf{k}; \tau - \tau') &= -\left\langle T_\tau c_{\mathbf{k}}(\tau) c_{\mathbf{k}}^{\dagger}(\tau') \right\rangle \\ \mathcal{G}\left(\mathbf{k}; \tau = 0^-\right) &= \left\langle c_{\mathbf{k}}^{\dagger}(0) c_{\mathbf{k}}(0^-) \right\rangle = \left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle \end{aligned} \tag{19.34}$$

$$\mathcal{G}(\mathbf{k}; ik_n) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(\mathbf{k}; \omega')}{ik_n - \omega'} \tag{19.35}$$

$$\begin{aligned} \mathcal{G}\left(\mathbf{k}; \tau = 0^-\right) &= T \sum_{ik_n} e^{ik_n 0^+} \mathcal{G}(\mathbf{r}, \mathbf{r}'; ik_n) \\ &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') \, T \sum_{ik_n} e^{ik_n 0^+} \frac{1}{ik_n - \omega'} \\ &= \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k}; \omega') \, f(\omega') \end{aligned} \tag{19.36}$$

so we have the momentum distribution from the spectral function

$$\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} f(\omega') A(\mathbf{k}, \omega') \tag{19.37}$$

this follows from a Fermi-Dirac distribution only when A is a delta function in ω', which happens in non-interacting case

$$\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} f(\omega') 2\pi \delta(\omega' - \zeta_{\mathbf{k}}) = f(\zeta_{\mathbf{k}}) \tag{19.38}$$

in the general case, we still have a jump at $k = k_F$ for $T = 0$ this can be seen from the $T = 0$ limit

$$\begin{aligned} \left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle &= \int_{-\infty}^{0} \frac{d\omega'}{2\pi} A(\mathbf{k}, \omega') \\ &= Z_{\mathbf{k}} \int_{-\infty}^{0} d\omega' \left[\frac{1}{\pi} \frac{\Gamma_{\mathbf{k}}(\omega')}{\left(\omega' - E_{\mathbf{k}} + \mu\right)^2 + \left(\Gamma_{\mathbf{k}}(\omega')\right)^2} \right] + \int_{-\infty}^{0} \frac{d\omega'}{2\pi} inc(\mathbf{k}, \omega') \end{aligned} \tag{19.39}$$

the incoherent part is smooth and does not provide a jump. The coherent part, on the other hand

$$\lim_{k \to k_F} \frac{1}{\pi} \frac{\Gamma_{\mathbf{k}}(\omega)}{\left(\omega - E_{\mathbf{k}} + \mu\right)^2 + \left(\Gamma_{\mathbf{k}}(\omega)\right)^2} = \frac{1}{\pi} \frac{\gamma' \omega^2}{\omega^2 + (\gamma' \omega^2)^2} \to \delta(\omega) \tag{19.40}$$

as $\omega \to 0$, we see that $\Gamma_{\mathbf{k}}(\omega) \sim \omega^2$ but $\omega - E_{\mathbf{k}} + \mu \sim \omega$, so we first obtain a delta function in $\delta(\omega)$,

$$\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle \to Z_{\mathbf{k}} \int_{-\infty}^{0} d\omega' \delta(\omega) = Z_{\mathbf{k}} \theta(\omega) + inc \tag{19.41}$$

20 Wick's Theorem

Wick's theorem allows us to compute expectation values of creation-annihilation operators such as,

$$\left\langle a_i(\tau_i)a_j(\tau_j)a_k^\dagger(\tau_k)a_l^\dagger(\tau_l)\right\rangle_0 \tag{20.1}$$

for $e^{-\beta H_0}$ where H_0 is a quadratic Hamiltonian. Note that since quadratic Hamiltonians conserve the number of particles, expectation values vanish when the number of creation operators does not match the number of destruction operators.

As an simple example, for $H_0 = \varepsilon_1 a_1^\dagger a_1 + \varepsilon_2 a_2^\dagger a_2$ we have

$$\left\langle a_1 a_1^\dagger a_2 a_2^\dagger\right\rangle = \left\langle a_1 a_1^\dagger\right\rangle \left\langle a_2 a_2^\dagger\right\rangle \tag{20.2}$$

Proof: For a single fermion state

$$\begin{aligned}\left\langle a_1 a_1^\dagger\right\rangle &= \frac{\mathrm{Tr}\left[e^{-\beta H_0} a_1 a_1^\dagger\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} \\ &= \frac{\langle 0| e^{-\beta H_0} a_1 a_1^\dagger |0\rangle + \langle 1| e^{-\beta H_0} a_1 a_1^\dagger |1\rangle}{\langle 0| e^{-\beta H_0} |0\rangle + \langle 1| e^{-\beta H_0} a_1 a_1^\dagger |1\rangle} \\ &= \frac{1}{1+e^{-\beta\varepsilon_1}}\end{aligned} \tag{20.3}$$

for two fermion states we have basis

$$|0\rangle|0\rangle, \quad a_1^\dagger|0\rangle|0\rangle, \quad |0\rangle a_2^\dagger|0\rangle, \quad a_1^\dagger|0\rangle a_2^\dagger|0\rangle \tag{20.4}$$

so that

$$\left\langle a_1 a_1^\dagger\right\rangle = \frac{1}{1+e^{-\beta\epsilon_1}} \frac{1+e^{-\beta\epsilon_2}}{1+e^{-\beta\epsilon_2}} = \frac{1}{1+e^{-\beta\epsilon_1}} \tag{20.5}$$

The easiest way to understand the last result is to recall that $\left(1+a_1^\dagger\right)\left(1+a_2^\dagger\right)|0\rangle$ will generate the trace so that we can factor each subspace. The last result will remain true for an arbitrary number of fermion states, in other words

$$\left\langle a_1 a_1^\dagger\right\rangle = \frac{1}{1+e^{-\beta\epsilon_1}} \frac{\prod_{m\neq 1} 1+e^{-\beta\epsilon_m}}{\prod_{m\neq 1} 1+e^{-\beta\epsilon_m}} = \frac{1}{1+e^{-\beta\epsilon_1}}. \tag{20.6}$$

Furthermore,

$$\begin{aligned}\left\langle a_1 a_1^\dagger a_2 a_2^\dagger\right\rangle &= \frac{1}{1+e^{-\beta\epsilon_1}} \frac{1}{1+e^{-\beta\epsilon_2}} \frac{\prod_{m\neq 1,2} 1+e^{-\beta\epsilon_m}}{\prod_{m\neq 1,2} 1+e^{-\beta\epsilon_m}} \\ &= \frac{1}{1+e^{-\beta\epsilon_1}} \frac{1}{1+e^{-\beta\epsilon_2}} \\ &= \left\langle a_1 a_1^\dagger\right\rangle \left\langle a_2 a_2^\dagger\right\rangle\end{aligned} \tag{20.7}$$

Theorem: Any expectation value such as $\left\langle a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l)\right\rangle_0$ calculated with a density matrix $e^{-\beta K_0}$ that is quadratic in field operators can be computed as the sum of all possible products of the type $\left\langle a_j(\tau_j)\, a_k^\dagger(\tau_k)\right\rangle_0 \left\langle a_i(\tau_i)\, a_l^\dagger(\tau_l)\right\rangle$ that can be formed by pairing creation and annihilation operators. For a given term on the right-hand side, there is a minus sign if the order of the operators is an odd permutation of the order of operators on the left-hand side.

A simple case: We first prove a simple special case where we can see everything that happens. The trick to prove the theorem is to transform the operators to the basis where H_0 is diagonal, to evaluate the expectation values, then to transform back to the original basis. Let Greek letters stand for the basis where H_0 is diagonal. Using the formula for basis changes, we have, (with an implicit sum over Greek indices)

$$\left\langle a_i(\tau_i)\, a_j(\tau_j)\, a_k^\dagger(\tau_k)\, a_l^\dagger(\tau_l)\right\rangle_0 = \langle i \mid \alpha\rangle\langle j \mid \beta\rangle \left\langle a_\alpha(\tau_i)\, a_\beta(\tau_j)\, a_\gamma^\dagger(\tau_k)\, a_\delta^\dagger(\tau_l)\right\rangle_0 \langle\gamma \mid k\rangle\langle\delta \mid l\rangle \tag{20.8}$$

in these basis the operators evolve only in phase

$$a_\alpha(\tau_i) = e^{-\zeta_\alpha \tau_i} a_\alpha \quad ; \quad a_\alpha^\dagger(\tau_i) = a_\alpha^\dagger e^{\zeta_\alpha \tau_i} \tag{20.9}$$

we have

$$\left\langle a_\alpha\left(\tau_i\right) a_\beta\left(\tau_j\right) a_\gamma^\dagger\left(\tau_k\right) a_\delta^\dagger\left(\tau_l\right)\right\rangle_0 = e^{-\zeta_\alpha \tau_i} e^{-\zeta_\beta \tau_j}\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0 e^{\zeta_\gamma \tau_k} e^{\zeta_\delta \tau_l} \tag{20.10}$$

What we need to evaluate then are expectation values of the type

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0 \tag{20.11}$$

Evaluating the trace in the diagonal basis, we see that we will obtain a non- zero value only if indices of creation and annihilation operators match two-by-two or are all equal. Suppose $\alpha=\delta\neq\beta=\gamma$, we then have

$$\left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger\right\rangle_0 = \left\langle a_\alpha a_\alpha^\dagger\right\rangle_0\left\langle a_\beta a_\beta^\dagger\right\rangle_0 \tag{20.12}$$

suppose $\alpha=\gamma\neq\beta=\delta$, then

$$\left\langle a_\alpha a_\beta a_\alpha^\dagger a_\beta^\dagger\right\rangle_0 = -\left\langle a_\alpha a_\beta a_\beta^\dagger a_\alpha^\dagger\right\rangle_0 = -\left\langle a_\alpha a_\alpha^\dagger\right\rangle_0\left\langle a_\beta a_\beta^\dagger\right\rangle_0 . \tag{20.13}$$

suppose $\alpha=\delta=\beta=\gamma$

$$\left\langle a_\alpha a_\alpha a_\alpha^\dagger a_\alpha^\dagger\right\rangle_0 = 0 \tag{20.14}$$

these results can be combined to give

$$\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0 = \left\langle a_\alpha a_\delta^\dagger\right\rangle_0\left\langle a_\beta a_\gamma^\dagger\right\rangle_0 - \left\langle a_\alpha a_\gamma^\dagger\right\rangle_0\left\langle a_\beta a_\delta^\dagger\right\rangle_0 \tag{20.15}$$

in other words, all possible pairs of creation and annihilation operators must be paired (ìcontractedî) in all possible ways. There is a minus sign if an odd number of operator exchanges (transpositions) is necessary to bring the contracted operators next to each other on the right-hand side (In practice, just count one minus sign every time two operators are permuted).

Using the expression for $\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0$, we can write

$$\begin{aligned}\left\langle a_\alpha\left(\tau_i\right) a_\beta\left(\tau_j\right) a_\gamma^\dagger\left(\tau_k\right) a_\delta^\dagger\left(\tau_l\right)\right\rangle_0 &= e^{-\zeta_\alpha \tau_i} e^{-\zeta_\beta \tau_j}\left\langle a_\alpha a_\beta a_\gamma^\dagger a_\delta^\dagger\right\rangle_0 e^{\zeta_\gamma \tau_k} e^{\zeta_\delta \tau_l} \\ &= \left\langle a_\alpha(\tau_i) a_\delta^\dagger(\tau_l)\right\rangle_0\left\langle a_\beta(\tau_j) a_\gamma^\dagger(\tau_k)\right\rangle_0 - \left\langle a_\alpha(\tau_i) a_\gamma^\dagger(\tau_k)\right\rangle_0\left\langle a_\beta(\tau_j) a_\delta^\dagger(\tau_l)\right\rangle_0\end{aligned} \tag{20.16}$$

$$\begin{aligned}\left\langle a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right\rangle_0 &= \langle i \mid \alpha\rangle\langle j \mid \beta\rangle\left\langle a_\alpha\left(\tau_i\right) a_\beta\left(\tau_j\right) a_\gamma^\dagger\left(\tau_k\right) a_\delta^\dagger\left(\tau_l\right)\right\rangle_0\langle\gamma \mid k\rangle\langle\delta \mid l\rangle \\ &= \left\langle a_i(\tau_i) a_l^\dagger(\tau_l)\right\rangle_0\left\langle a_j(\tau_j) a_k^\dagger(\tau_k)\right\rangle_0 - \left\langle a_i(\tau_i) a_k^\dagger(\tau_k)\right\rangle_0\left\langle a_j(\tau_j) a_l^\dagger(\tau_l)\right\rangle_0\end{aligned} \tag{20.17}$$

In the context of Wick's theorem, we call each factor $\left\langle a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0$ on the right-hand side a "contraction".

Since Wick's theorem is valid for an arbitrary time ordering, it is also valid for time-ordered products so that, for example

$$\begin{aligned}&\left\langle T_\tau\left[a_i\left(\tau_i\right) a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right) a_l^\dagger\left(\tau_l\right)\right]\right\rangle_0 \\ =&\left\langle T_\tau\left[a_i\left(\tau_i\right) a_l^\dagger\left(\tau_l\right)\right]\right\rangle_0\left\langle T_\tau\left[a_j\left(\tau_j\right) a_k^\dagger\left(\tau_k\right)\right]\right\rangle_0 - \left\langle T_\tau\left[a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right]\right\rangle_0\left\langle T_\tau\left[a_j\left(\tau_j\right) a_l^\dagger\left(\tau_l\right)\right]\right\rangle_0\end{aligned} \tag{20.18}$$

The only simplification that occurs with time-ordered products is the following. Note that, given the definition of time-ordered product, we have

$$\left\langle T_\tau\left[a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right]\right\rangle_0 = -\left\langle T_\tau\left[a_k^\dagger\left(\tau_k\right) a_i\left(\tau_i\right)\right]\right\rangle_0 \tag{20.19}$$

operators can be permuted at will inside a time-ordered product, in particular inside a contraction, as long as we take care of the minus-signs associated with permutations. This is true for time-ordered products of an arbitrary number of operators and for an arbitrary density matrix. On the other hand, if we apply Wickís theorem to a product that is not time ordered, then we have to remember that

$$\left\langle a_i\left(\tau_i\right) a_k^\dagger\left(\tau_k\right)\right\rangle_0 \neq -\left\langle a_k^\dagger\left(\tau_k\right) a_i\left(\tau_i\right)\right\rangle_0 \tag{20.20}$$

as we can easily check by the case $\tau_i=\tau_k$.

21 Linked Cluster Theorem

In evaluating the Green's function, there is a cancellation of the denominator which removes all the disconnected diagrams. This is a very general problem that forces us to introduce the notion of connected graphs. A generalization of this problem also occurs if we want to compute the free-energy from

$$\begin{aligned}\ln Z &= \ln\left(\mathrm{Tr}\left[e^{-\beta H_0}U_I(\beta,0)\right]\right) = \ln\left(Z_0\left\langle U_I(\beta,0)\right\rangle_0\right)\\ &= \ln\left(\left\langle T_\tau\left[\exp\left(-\int_0^\beta d\tau_1 V_I\left(\tau_1\right)\right)\right]\right\rangle_0\right) + \ln Z_0\end{aligned} \tag{21.1}$$

In probability theory this is like computing the **cumulant expansion** of the characteristic function. These problems are special cases of much more general problems in the theory of random variables which do not even refer to specific Feynman diagrams or to quantum mechanics. The theorems, and their corollary that we prove below, are amongst the most important theorems used in many-body Physics or Statistical Mechanics in general. Linked cluster theorems lead to observables that are expressed in terms of connected diagrams.

21.1 Linked cluster theorem for normalized averages

Suppose we have some multivariate probability distribution function for the variables collectively represented by $\mathbf{x}$, denote $\langle g(\mathbf{x})\rangle$ as the expectation of the function $g(\mathbf{x})$ in this distribution. We will prove the following relation

$$\frac{\left\langle e^{-f(\mathbf{x})}A(\mathbf{x})\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle} = \left\langle e^{-f(\mathbf{x})}A(\mathbf{x})\right\rangle_c \tag{21.2}$$

where all three exponentials should be Taylor expanded, with each term corresponding to a given diagram:

$$\left\langle f^n A\right\rangle, \left\langle f^n\right\rangle, \left\langle f^n A\right\rangle_c \tag{21.3}$$

If $\langle AB\rangle = \langle A\rangle\langle B\rangle$, then in the diagram A and B are unconnected. We will show that $\langle f^n A\rangle_c$ are "**connected**", defined as

1. The diagrams $\{\langle f^n A\rangle_c\}$ form a subset of diagrams $\{\langle f^n A\rangle\}$
2. A connected diagram $\langle f^n A\rangle_c$ cannot be broken down into $\langle f^m A\rangle_c\langle f^{n-m}\rangle$ where $m<n$

We start by defining the connected expectation of a function $\langle f^n(\mathbf{x})\rangle_c$ by

$$\ln\left\langle e^{-f(\mathbf{x})}\right\rangle = \sum_{n=1}^{\infty}\frac{1}{n!}\left\langle(-f(\mathbf{x}))^n\right\rangle_c = \left\langle e^{-f(\mathbf{x})}\right\rangle_c - 1 \tag{21.4}$$

for any function $f(\mathbf{x})$. (In perturbation theory, $\left(-\int_0^\beta d\tau V_I(\tau)\right)$ play the role of $-f(\mathbf{x})$). To obtain $\langle f^n(\mathbf{x})\rangle_c$ explicitly, let $f(\mathbf{x})\to\lambda f(\mathbf{x})$, which is also an arbitrary function, define the generating function $H(\lambda), G(\lambda)$

$$\begin{aligned}G(\lambda) &\equiv \left\langle e^{-\lambda f(\mathbf{x})}\right\rangle\\ H(\lambda) &\equiv \ln G(\lambda) = \ln\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle\end{aligned} \tag{21.5}$$

now perform $(-1)^n\frac{d^n}{d\lambda^n}\left[...\right]_{\lambda=0}, \quad n>1$ on both sides, we have

$$\begin{aligned}\left\langle f^n(\mathbf{x})\right\rangle &= (-1)^n\left[\frac{d^n G}{d\lambda^n}\right]_{\lambda=0} \equiv G^{(n)}\\ \left\langle f^n(\mathbf{x})\right\rangle_c &= (-1)^n\left[\frac{d^n H}{d\lambda^n}\right]_{\lambda=0} \equiv H^{(n)}\end{aligned} \tag{21.6}$$

$$H(\lambda) \approx \left(-\left\langle f\right\rangle\right)\lambda + \left(\frac{1}{2}\left\langle f^2\right\rangle - \frac{1}{2}\left\langle f\right\rangle^2\right)\lambda^2 + \left(-\frac{1}{6}\left\langle f^3\right\rangle + \frac{1}{2}\left\langle f\right\rangle\left\langle f^2\right\rangle - \frac{1}{3}\left\langle f^3\right\rangle\right)\lambda^3 + ... \tag{21.7}$$

so we obtain

$$\begin{aligned}
\langle f\rangle_c &= \langle f\rangle \\
\left\langle f^2\right\rangle_c &= \left\langle f^2\right\rangle - \langle f\rangle^2 \\
\left\langle f^3\right\rangle_c &= \left\langle f^3\right\rangle - 3\left\langle f^2\right\rangle\langle f\rangle + 2\langle f\rangle^3 \\
\left\langle f^4\right\rangle_c &= ...
\end{aligned} \tag{21.8}$$

We now prove a nice property about connected expectation:

$$\left\langle e^{-f(\mathbf{x})}A(\mathbf{x})\right\rangle_c = \frac{\left\langle e^{-f(\mathbf{x})}A(\mathbf{x})\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle} \tag{21.9}$$

Letting $-f(\mathbf{x}) \to -f(\mathbf{x}) + \lambda A(\mathbf{x})$,

$$\begin{aligned}
\ln\left\langle e^{-f(\mathbf{x})+\lambda A(\mathbf{x})}\right\rangle &= \left\langle e^{-f(\mathbf{x})+\lambda A(\mathbf{x})}\right\rangle_c - 1 \\
\frac{d}{d\lambda}\ln\left\langle e^{-f(\mathbf{x})+\lambda A(\mathbf{x})}\right\rangle &= \frac{d}{d\lambda}\left[\left\langle e^{-f(\mathbf{x})+\lambda A(\mathbf{x})}\right\rangle_c - 1\right] \\
\frac{\left\langle e^{-f(\mathbf{x})+\lambda A(\mathbf{x})}A(\mathbf{x})\right\rangle}{\left\langle e^{-f(\mathbf{x})+\lambda A(\mathbf{x})}\right\rangle} &= \left\langle e^{-f(\mathbf{x})+\lambda A(\mathbf{x})}A(\mathbf{x})\right\rangle_c \\
\frac{\left\langle e^{-f(\mathbf{x})}A(\mathbf{x})\right\rangle}{\left\langle e^{-f(\mathbf{x})}\right\rangle} &= \left\langle e^{-f(\mathbf{x})}A(\mathbf{x})\right\rangle_c
\end{aligned} \tag{21.10}$$

we now use this to prove another expansion, first write

$$\left\langle e^{-\lambda f(\mathbf{x})}A(\mathbf{x})\right\rangle = \left\langle e^{-\lambda f(\mathbf{x})}A(\mathbf{x})\right\rangle_c \left\langle e^{-\lambda f(\mathbf{x})}\right\rangle \tag{21.11}$$

then $(-1)^n \frac{d^n}{d\lambda^n}[...]_{\lambda=0}$ both hand side, using Leibniz rule, we have

$$\begin{aligned}
\langle f^n(\mathbf{x})A(\mathbf{x})\rangle &= (-1)^n \frac{d^n}{d\lambda^n}\left[\left\langle e^{-\lambda f(\mathbf{x})}A(\mathbf{x})\right\rangle_c \left\langle e^{-\lambda f(\mathbf{x})}\right\rangle\right]_{\lambda=0} \\
&= \sum_{k=0}^{n}\frac{n!}{k!(n-k)!}\left((-1)^k\frac{d^k}{d\lambda^k}\left\langle e^{-\lambda f(\mathbf{x})}A(\mathbf{x})\right\rangle_c\right)_{\lambda=0}\left((-1)^{n-k}\frac{d^{n-k}}{d\lambda^{n-k}}\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle\right)_{\lambda=0} \\
&= \sum_{l=0}^{\infty}\sum_{k=0}^{\infty}\delta_{n,l+k}\frac{n!}{k!l!}\left((-1)^k\frac{d^k}{d\lambda^k}\left\langle e^{-\lambda f(\mathbf{x})}A(\mathbf{x})\right\rangle_c\right)_{\lambda=0}\left((-1)^l\frac{d^l}{d\lambda^l}\left\langle e^{-\lambda f(\mathbf{x})}\right\rangle\right)_{\lambda=0} \\
&= \sum_{l=0}^{\infty}\sum_{k=0}^{\infty}\delta_{n,l+k}\frac{n!}{k!l!}\left\langle f^k(\mathbf{x})A(\mathbf{x})\right\rangle_c\left\langle f^l(\mathbf{x})\right\rangle \\
&= \sum_{k=0}^{n}\binom{n}{k}\left\langle f^k(\mathbf{x})A(\mathbf{x})\right\rangle_c\left\langle f^{n-k}(\mathbf{x})\right\rangle
\end{aligned} \tag{21.12}$$

treating $\langle f^n(\mathbf{x})A(\mathbf{x})\rangle$ as a combination of terms like $\left\langle f^k(\mathbf{x})A(\mathbf{x})\right\rangle_c\left\langle f^{n-k}(\mathbf{x})\right\rangle$, we see that $\left\langle f^k(\mathbf{x})A(\mathbf{x})\right\rangle_c$ is just a special case with $k=n$. This corresponds to the statement that "connected diagrams are only a subset of all diagrams".

We now show that $\left\langle f^k(\mathbf{x})A(\mathbf{x})\right\rangle_c$ cannot in general be expanded further into $\left\langle f^{k-m}(\mathbf{x})A(\mathbf{x})\right\rangle\langle f^m(\mathbf{x})\rangle$, and thus it has the property of being inseparable or "**connected**". Define

$$\begin{aligned}
G(\lambda,\eta) &\equiv \left\langle e^{-\lambda f(\mathbf{x})-\eta A(\mathbf{x})}\right\rangle \\
H(\lambda,\eta) &\equiv \ln G(\lambda,\eta) = \ln\left\langle e^{-\lambda f(\mathbf{x})-\eta A(\mathbf{x})}\right\rangle
\end{aligned} \tag{21.13}$$

$$\begin{aligned}
\langle f^n(\mathbf{x})A(\mathbf{x})\rangle &= \left[(-1)^n\frac{d}{d\eta}(-1)^n\frac{d^n}{d\lambda^n}G\right]_{\lambda=0,\eta=0} = G^{(n,1)} \\
\langle f^n(\mathbf{x})A(\mathbf{x})\rangle_c &= \left[(-1)^n\frac{d}{d\eta}(-1)^n\frac{d^n}{d\lambda^n}H\right]_{\lambda=0,\eta=0} = H^{(n,1)}
\end{aligned} \tag{21.14}$$

$$
\begin{aligned}
G &= \sum_{k=0}^{n} G^{(k,0)} \frac{\lambda^k}{k!} + \sum_{k=0}^{n} G^{(k,1)} \frac{\lambda^k \eta}{k!} \\
H &= \sum_{k=0}^{n} H^{(k,0)} \frac{\lambda^k}{k!} + \sum_{k=0}^{n} H^{(k,1)} \frac{\lambda^k \eta}{k!}
\end{aligned}
\tag{21.15}
$$

$$
G = e^H
$$

$$
\sum_{k=0}^{n} G^{(k,0)} \frac{\lambda^k}{k!} + \sum_{k=0}^{n} G^{(k,1)} \frac{\lambda^k \eta}{k!} = \exp\left(\sum_{k=0}^{n} H^{(k,0)} \frac{\lambda^k}{k!} \right) \exp\left(\sum_{k=0}^{n} H^{(k,1)} \frac{\lambda^k \eta}{k!} \right) \tag{21.16}
$$

to zero order in η, we can obtain the relations between $G^{(k,0)}, H^{(k,0)}$.

$$
G^{(n,0)} = F_0 \left[\{ H^{(k,0)} | k \leq n \} \right] \tag{21.17}
$$

now to first order in η, we can obtain relations between $G^{(k,0)}$ and $H^{(k,0)}, H^{(k,1)}$:

$$
\begin{aligned}
G^{(n,1)} &= F_1 \left[\{ H^{(k,1)}, H^{(k,0)} | k \leq n \} \right] \\
&= F_1 \left[\{ H^{(k,1)}, F_0^{-1} \left[G^{(k,0)} \right] | k \leq n \} \right] \\
&\equiv F_1' \left[\{ H^{(k,1)}, G^{(k,0)} | k \leq n \} \right]
\end{aligned}
\tag{21.18}
$$

which is exactly a relation of the form $\langle f^n(\mathbf{x}) A(\mathbf{x}) \rangle = \sum_{k=0}^{n} \begin{pmatrix} n \\ k \end{pmatrix} \left\langle f^k(\mathbf{x}) A(\mathbf{x}) \right\rangle_c \left\langle f^{n-k}(\mathbf{x}) \right\rangle$. Since $H^{(k,1)}$ is independent of $H^{(m<k,0)}$, there should not exist any general expansion of the form

$$
H^{(k,1)} = F_3 \left[\{ H^{(m<k,0)}, G^{(k,0)} \} \right] \tag{21.19}
$$

and thus $H^{(k,1)} = \langle f^n(\mathbf{x}) A(\mathbf{x}) \rangle_c$ is "**connected**", and the function F_1' is of course unique.
The cancellation of Feynman diagrams can be easily seen as

$$
\begin{aligned}
\frac{\left\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \right\rangle}{\left\langle e^{-f(\mathbf{x})} \right\rangle} &= \frac{\sum_n \frac{1}{n!} \langle (-f)^n A \rangle}{\sum_n \frac{1}{n!} \langle (-f)^n \rangle} \\
&= \frac{\sum_n \frac{1}{n!} \sum_{l=0}^{\infty} \sum_{k=0}^{\infty} \delta_{n,l+k} \frac{n!}{k!l!} \left\langle (-f)^k A \right\rangle_c \left\langle (-f)^l \right\rangle}{\sum_n \frac{1}{n!} \langle (-f)^n \rangle} \\
&= \frac{\sum_{k=0}^{\infty} \frac{1}{k!} \left\langle f^k(\mathbf{x}) A(\mathbf{x}) \right\rangle_c \sum_{l=0}^{\infty} \frac{1}{l!} \left\langle f^l(\mathbf{x}) \right\rangle}{\sum_{n=0}^{\infty} \frac{1}{n!} \langle (-f)^n \rangle} \\
&= \sum_{k=0}^{\infty} \frac{1}{k!} \left\langle f^k(\mathbf{x}) A(\mathbf{x}) \right\rangle_c \\
&= \left\langle e^{-f(\mathbf{x})} A(\mathbf{x}) \right\rangle_c
\end{aligned}
\tag{21.20}
$$

Part V
The Coulomb Gas

The electron gas with long-range forces and a neutralizing background, also known as the jellium model, is probably the first challenge that was met by quantum many-body theory in the context of Solid State physics. It is extremely important conceptually since it is crucial to understand how, in a solid, the long-range Coulomb force becomes effectively short-range, or screened, at low energy. Other models, such as the Hubbard model that we will discussed later on, have their foundation rooted in the physics of screening. In fact, one of the most useful methods in modern electronic structure calculations uses perturbation theory to compute single-particle excitations, and the method they rely on, called the **GW approach**, is just an adaptation of what was developed for the Coulomb gas.

In this part, we assume that the **uniform neutralizing background** has infinite inertia. In a subsequent part of this book we will allow it to move, in other words to support sound waves, or phonons. We will consider electron-phonon interactions and see how these eventually lead to superconductivity.

The main physical phenomena to account for here are screening and plasma oscillations, at least as far as collective modes are concerned. The surprises come in when one tries to understand single-particle properties. Hartree-Fock theory is a disaster since it predicts that the effective mass of the electron at the Fermi level vanishes. The way out of this paradox will indicate to us how important it is to take screening into account.

We will start by describing the **source formalism** due to the **Schwinger-Martin school** and then start to do calculations. The advantage of this approach is that it allows more easily to devise non-perturbative approximations and to derive general theorems. It gives a systematic algebraic way to formulate perturbation theory when necessary, without explicit use of Wick's theorem. With this formalism, so-called **conserving approximations** can also be formulated naturally. The source, or **functional derivative formalism**, is however less appealing than Feynman rules for the Feynmann diagram approach to perturbation theory. When these two competing approaches were invented, it was forbidden to the practitioners of the source approach to draw Feynman diagrams, but nothing really forbids it. The students, anyway, drew the forbidden pictures hiding in the basement. The two formalisms are strictly equivalent.

After we introduce the formalism, we discuss first the density oscillations, where we will encounter screening and plasma oscillations. This will allow us to discuss the famous **Random Phase Approximation** (**RPA**). Then we move on to single particle properties and end with a general discussion of what would be needed to go beyond RPA. The electron gas is discussed in detail in a very large number of textbooks. The discussion here is brief and incomplete, its main purpose being to illustrate the physics involved.

22 The functional derivative approach

We basically want to compute imaginary time correlation functions. In the first section below, we show, in the very simple context of classical statistical mechanics, how introducing artificial external fields (source fields) allows one to compute correlation functions of arbitrary order for the problem without external fields. This is one more example where enlarging the space of parameters of interest actually simplifies matters in the end. In the other section, we show how to obtain Green's functions with source fields and then give an impressionist view of how we plan to use this idea for our problem.

22.1 External Fields to compute correlation functions

In elementary statistical mechanics, we can obtain the magnetization by differentiating the free energy with respect to the magnetic field

$$Z_h = \mathrm{Tr}\left[e^{-\beta(K-hM)}\right] \tag{22.1}$$

$$\langle M\rangle_h = \frac{1}{Z_h}\,\mathrm{Tr}\left[Me^{-\beta(K-hM)}\right] = \frac{\partial \ln Z_h}{\beta\partial h} \tag{22.2}$$

The indices h on $\langle M\rangle_h$ and Z_h reminds us that the magnetic field is non zero. We can obtain correlation functions of higher order by continuing the process

$$\begin{aligned}\frac{\partial^2 \ln Z_h}{\beta^2\partial h^2} &= \langle MM\rangle_h - \mathrm{Tr}\left[e^{-\beta(K-hM)}M\right]\frac{1}{Z_h^2}\frac{\partial\,\mathrm{Tr}\left[e^{-\beta(K-hM)}\right]}{\beta\partial h}\\ &= \langle MM\rangle_h - \langle M\rangle_h\langle M\rangle_h.\end{aligned} \tag{22.3}$$

Basically, if we know Z_h, we can keep differentiating to get all orders of correlation $\langle M^n\rangle_h$. To compute the zero-field susceptibility we simply set $h=0$ at the end.

Suppose that we now wish to compute not the total magnetization but the magnetization correlation between two spatial points $\mathbf{x}_1, \mathbf{x}_2$

$$\langle M(\mathbf{x}_1)\, M(\mathbf{x}_2)\rangle - \langle M(\mathbf{x}_1)\rangle\langle M(\mathbf{x}_2)\rangle \tag{22.4}$$

This can be achieved if we couple our system to a spatially varying field $h(\mathbf{x})$

$$Z[h] = \mathrm{Tr}\left[e^{-\beta\left(K-\int d^3\mathbf{x}h(\mathbf{x})M(\mathbf{x})\right)}\right] \tag{22.5}$$

now Z is a functional of $h(\mathbf{x})$.

To obtain the magnetization at a single point, we introduce the notion of functional derivative, which is just a simple generalization to the continuum of the idea of partial derivative

$$\begin{aligned}\frac{\delta}{\delta h(\mathbf{x}_1)}\int d^3\mathbf{x} h(\mathbf{x})M(\mathbf{x}) &= \int d^3\mathbf{x}\frac{\delta h(\mathbf{x})}{\delta h(\mathbf{x}_1)}M(\mathbf{x}) \\ &= \int d^3\mathbf{x}\delta(\mathbf{x}_1-\mathbf{x})M(\mathbf{x}) = M(\mathbf{x}_1)\end{aligned} \tag{22.6}$$

notice that the functional derivative $\frac{\delta}{\delta h(\mathbf{x}_1)}$ only acts on components of the function h, and the functional derivative is a generalization of the partial derivative of multivariable calculus

$$\frac{\partial y_1}{\partial y_2} = \delta_{1,2} \to \frac{\delta h(\mathbf{x})}{\delta h\left(\mathbf{x}_1\right)} = \delta\left(\mathbf{x}_1-\mathbf{x}\right) \tag{22.7}$$

With this, we have

$$\frac{\partial}{\beta\partial h(\mathbf{x})}\ln Z[h] = \langle M(\mathbf{x})\rangle_h \tag{22.8}$$

and the quantity we want is obtained from one more functional derivative

$$\begin{aligned}\frac{\partial}{\beta\partial h(\mathbf{x}_1)}\frac{\partial}{\beta\partial h(\mathbf{x}_2)}\ln Z[h] &= \frac{\partial}{\beta\partial h(\mathbf{x}_1)}\langle M(\mathbf{x}_2)\rangle_h \\ &= \langle M(\mathbf{x}_1)M(\mathbf{x}_2)\rangle_h - \langle M(\mathbf{x}_1)\rangle_h\langle M(\mathbf{x}_2)\rangle_h\end{aligned} \tag{22.9}$$

Correlation functions such as the one above are called **connected**. This means that the "trivial part", which would be the result if there were no correlations, is subtracted. In probability theory, these are **cumulants**.

22.2 Green's functions and higher order correlations from functional derivatives

In our case, we are interested in correlation functions that depend not only on space but also on real or imaginary time. In addition, we know that time-ordered products are relevant. Hence, we define the

$$Z[\phi] = \mathrm{Tr}\left[e^{-\beta K}T_\tau \exp\left(-\psi^\dagger(\overline{1})\phi(\overline{1},\overline{2})\psi(\overline{2})\right)\right] \tag{22.10}$$

where we used the short-hand $(1) = (\mathbf{x}_1, \tau_1; \sigma_1)$ with the overbar indicating integrals over space-time coordinates and spin sums:

$$\psi^\dagger(\overline{1})\phi(\overline{1},\overline{2})\psi(\overline{2}) = \sum_{\sigma_1,\sigma_2}\int d^3\mathbf{x}_1\int_0^\beta d\tau_1\int d^3\mathbf{x}_2\int_0^\beta d\tau_2\psi^\dagger_{\sigma_1}\left(\mathbf{x}_1,\tau_1\right)\phi_{\sigma_1,\sigma_2}\left(\mathbf{x}_1,\tau_1,\mathbf{x}_2,\tau_2\right)\psi_{\sigma_2}\left(\mathbf{x}_2,\tau_2\right) \tag{22.11}$$

We can think of $\psi^\dagger(\overline{1})\phi(\overline{1},\overline{2})\psi(\overline{2})$ as vector-matrix-vector multiplication. Some of the matrix or vector indices are continuous. All the operators above evolve in imaginary time with the same $\hat{K} = \hat{H} - \mu\hat{N}$ that enters the Boltzmann weight $e^{-\beta\hat{K}}$.

With the definition,

$$\mathcal{S}[\phi] = \exp\left(-\psi^\dagger(\overline{1})\phi(\overline{1},\overline{2})\psi(\overline{2})\right) \tag{22.12}$$

$$Z[\phi] = \mathrm{Tr}[e^{-\beta K}\mathcal{T}_\tau S[\phi]] \tag{22.13}$$

we can write the Matsubara Green's function as a functional derivative of the generating functions $\ln Z[\phi]$

$$\begin{aligned}\frac{\delta}{-\delta\phi(2,1)}\ln Z[\phi] &= \frac{\mathrm{Tr}[e^{-\beta K}\mathcal{T}_\tau\frac{\delta}{-\delta\phi(2,1)}S[\phi]]}{\mathrm{Tr}[e^{-\beta K}\mathcal{T}_\tau S[\phi]]} \\ &= \frac{\left\langle\mathcal{T}_\tau S[\phi]\psi^\dagger(2)\psi(1)\right\rangle}{\langle\mathcal{T}_\tau S[\phi]\rangle} \\ &= -\left\langle\mathcal{T}_\tau\psi(1)\psi^\dagger(2)\right\rangle_\phi \\ &= \mathcal{G}(1,2)_\phi\end{aligned} \tag{22.14}$$

where $\langle ... \rangle \equiv \mathrm{Tr}[e^{-\beta K}...]/\,\mathrm{Tr}[e^{-\beta K}]$ is the thermal average with respect to the system's Hamiltonian without any external coupling. The average with subscript ϕ

$$\langle ... \rangle_\phi \equiv \frac{\langle \mathcal{T}_\tau S[\phi]... \rangle}{\langle \mathcal{T}_\tau S[\phi] \rangle} = \frac{\mathrm{Tr}\left(e^{-\beta K}\mathcal{T}_\tau S[\phi]...\right)}{\mathrm{Tr}\left(e^{-\beta K}\mathcal{T}_\tau S[\phi]\right)} \tag{22.15}$$

includes the external coupling $\mathcal{T}_\tau S[\phi]$ in the density matrix. We also used the fact that differentiating $\frac{\delta}{-\delta\phi(2,1)}$ does not affect the time order. Finally

$$\frac{\delta\phi(\bar{1},\bar{2})}{\delta\phi(1,2)} = \delta(\bar{1}-1)\delta(\bar{2}-2) \tag{22.16}$$

$$\delta(\bar{1}-1) = \delta^3\left(\mathbf{x}_{\bar{1}} - \mathbf{x}_1\right)\delta\left(\tau_{\bar{1}} - \tau_1\right)\delta_{\sigma_{\bar{1}},\sigma_1}. \tag{22.17}$$

here $\bar{1},\bar{2}$ are merely another pair of indices different from $1,2$. Of course, calling them bars only means that they are dummy indices that will be summed over later.

Higher order correlation functions can be obtained by taking further functional derivatives

$$\begin{aligned}
\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} &= \frac{\delta}{-\delta\phi(3,4)}\frac{\left\langle \mathcal{T}_\tau S[\phi]\psi(1)\psi^\dagger(2)\right\rangle}{\langle \mathcal{T}_\tau S[\phi]\rangle} \\
&= \frac{\left\langle \mathcal{T}_\tau S[\phi]\psi(1)\psi^\dagger(2)\psi^\dagger(3)\psi(4)\right\rangle}{\langle \mathcal{T}_\tau S[\phi]\rangle} + \left\langle \mathcal{T}_\tau\psi(1)\psi^\dagger(2)\right\rangle_\phi \langle \mathcal{T}_\tau S[\phi]\rangle \frac{\delta}{-\delta\phi(3,4)}\frac{1}{\langle \mathcal{T}_\tau S[\phi]\rangle} \\
&= \frac{\left\langle \mathcal{T}_\tau S[\phi]\psi(1)\psi^\dagger(2)\psi^\dagger(3)\psi(4)\right\rangle}{\langle \mathcal{T}_\tau S[\phi]\rangle} - \left\langle \mathcal{T}_\tau\psi(1)\psi^\dagger(2)\right\rangle_\phi \frac{\left\langle \mathcal{T}_\tau S[\phi]\psi^\dagger(3)\psi(4)\right\rangle}{\langle \mathcal{T}_\tau S[\phi]\rangle} \\
&= \left\langle \mathcal{T}_\tau\psi(1)\psi^\dagger(2)\psi^\dagger(3)\psi(4)\right\rangle_\phi + \left\langle \mathcal{T}_\tau\psi(1)\psi^\dagger(2)\right\rangle_\phi \left\langle \mathcal{T}_\tau\psi(4)\psi^\dagger(3)\right\rangle_\phi \\
&= \left\langle \mathcal{T}_\tau\psi(1)\psi^\dagger(2)\psi^\dagger(3)\psi(4)\right\rangle_\phi + \mathcal{G}(1,2)_\phi\mathcal{G}(4,3)_\phi
\end{aligned} \tag{22.18}$$

The first term is called a four-point correlation function.

It is very important to understand that even when the system is translationally invariant, you should not assume that it is when using this formalism in the presence of the source term $\phi(1,2)$. This is because $\phi(1,2)$ has to break translational invariance to generate the correlation functions that are needed. Translational invariance is recovered at the end, when you have all the equations that you need. Only then can you set $\phi = 0$ and recover all the symmetries of the Hamiltonian.

22.3 Source fields for Green's functions, an impressionist view

Before we enter into even more indices and lengthy expressions, it is useful to have an impressionist view, a sort of road map that we will follow. We are addressing here the question of how can that formalism possibly be helpful. It is helpful because the **self-energy** will be expressed in terms of a four point correlation function which in turn can be found from a functional derivative of $\mathcal{G}_\sigma(\cdot,\cdot)_\phi$. It will be possible to find this functional derivative if we know $\mathcal{G}_\sigma(\cdot,\cdot)_\phi$. We do have an expression for that quantity so that, in a sense, it closes the loop. We will see things are not so simple in practice, but at least that is a start.

How do we find $\mathcal{G}_\sigma(,)_\phi$? It suffices to write the **equations of motion**. This is the first time in this Chapter that the explicit form of the Hamiltonian comes in. What is different from the non-interacting case is the presence of ϕ and of interactions.

$$\partial_{\tau_1}\mathcal{G}(1,2)_\phi = -\left\langle \mathcal{T}_\tau\left(\partial_{\tau_1}\psi(1)\right)\psi^\dagger(2)\right\rangle_\phi \tag{22.19}$$

When we compute the Heisenberg equation of motion for field operator $\psi(1)$

$$\begin{aligned}
\partial_{\tau_1}\psi(1) &= [K,\psi(1)] \\
&= [K_0,\psi(1)] + [V(\bar{2},\bar{3})\psi^\dagger(\bar{2})\psi^\dagger(\bar{3})\psi(\bar{3})\psi(\bar{2}),\psi(1)] \\
&= [K_0,\psi(1)] + V(\bar{2},\bar{3})[\psi^\dagger(\bar{2})\psi^\dagger(\bar{3})\psi(\bar{3})\psi(\bar{2}),\psi(1)]
\end{aligned} \tag{22.20}$$

$$\begin{aligned}
[\psi^\dagger(\bar{2})\psi^\dagger(\bar{3})\psi(\bar{3})\psi(\bar{2}),\psi(1)] &= \psi^\dagger(\bar{2})\psi(1)\psi(\bar{2}) - \psi^\dagger(\bar{3})\psi(\bar{3})\psi(1) \\
&= -2\psi^\dagger(\bar{2})\psi(\bar{2})\psi(1)
\end{aligned} \tag{22.21}$$

we will not go in details here, using this result in the definition of $\mathcal{G}$, the equation of motion for $\mathcal{G}$ will read something like

$$\left(\mathcal{G}_0^{-1} - \phi\right)\mathcal{G} = 1 - V\left\langle T_\tau\psi^\dagger\psi\psi\psi^\dagger\right\rangle \tag{22.22}$$

define

$$\begin{aligned}\Sigma\mathcal{G} &= -V\left\langle T_\tau \psi^\dagger \psi\psi\psi^\dagger\right\rangle \\ \Sigma &= -V\left\langle T_\tau \psi^\dagger \psi\psi\psi^\dagger\right\rangle \mathcal{G}^{-1}\end{aligned} \tag{22.23}$$

$$\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \phi - \Sigma \tag{22.24}$$

which is equivalent to Dyson's equation

$$\mathcal{G} = \mathcal{G}_{0\phi} + \mathcal{G}_{0\phi}\Sigma\mathcal{G} \tag{22.25}$$

with $\mathcal{G}_{0\phi} = \left(\mathcal{G}_0^{-1} - \phi\right)^{-1}$. The four-point correlation function is then obtained from a functional derivative of $\mathcal{G}$:

$$\left\langle T_\tau \psi^\dagger \psi\psi\psi^\dagger\right\rangle = \frac{\delta\mathcal{G}}{\delta\phi} - \mathcal{G}\mathcal{G} \tag{22.26}$$

To find the functional derivative,

$$\frac{\delta\left(\mathcal{G}^{-1}\mathcal{G}\right)}{\delta\phi} = \frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G} + \mathcal{G}^{-1}\frac{\delta\mathcal{G}}{\delta\phi} = 0 \tag{22.27}$$

$$\frac{\delta\mathcal{G}}{\delta\phi} = -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G} = -\mathcal{G}\frac{\delta}{\delta\phi}\left(\mathcal{G}_0^{-1} - \phi - \Sigma\right)\mathcal{G} = \mathcal{G}\frac{\delta}{\delta\phi}\left(\phi + \Sigma\right)\mathcal{G} \tag{22.28}$$

The last equation suggests that the functional dependence of Σ on ϕ comes only from the dependence of $\mathcal{G}$ on ϕ. The self-energy has no explicit dependence on ϕ. Hence, using the chain rule

$$\frac{\delta\Sigma}{\delta\phi} = \frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi} \tag{22.29}$$

we have the integral equation for $\frac{\delta\mathcal{G}}{\delta\phi}$

$$\frac{\delta\mathcal{G}}{\delta\phi} = \mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)\mathcal{G} \tag{22.30}$$

If we can solve this, we can find

$$\left(\mathcal{G}_0^{-1} - \phi\right)\mathcal{G} = 1 + \Sigma\mathcal{G} \tag{22.31}$$

with

$$\Sigma = -V\left(\frac{\delta\mathcal{G}}{\delta\phi} - \mathcal{G}\mathcal{G}\right)\mathcal{G}^{-1} \tag{22.32}$$

Since the integral equation for $\frac{\delta\mathcal{G}}{\delta\phi}$ requires that we know both $\mathcal{G}$ and $\frac{\delta\Sigma}{\delta\mathcal{G}}$ there will be some iteration process involved. The last three equations can be solved for $\phi = 0$, since ϕ has played its role and is no longer necessary at that point.

Equivalently, we can also write the integral equation into an equation for Σ:

$$\begin{aligned}\Sigma &= -V\left(\frac{\delta\mathcal{G}}{\delta\phi} - \mathcal{G}\mathcal{G}\right)\mathcal{G}^{-1} \\ &= -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)\mathcal{G} - \mathcal{G}\mathcal{G}\right)\mathcal{G}^{-1} \\ &= -V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi} + \mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right) - \mathcal{G}\right)\end{aligned} \tag{22.33}$$

If I had written an equation of motion for the four-point function, we would have seen that it depends on a six point function, and so on, so that is not the way to go. This would have been the analog of the so-called **BBGKY hierarchy** in classical transport theory. In the quantum context, it is called the **Martin-Schwinger hierarchy**.

23 Equations of Motion for $\mathcal{G}$ in the presence of source fields

Here we try to do everything more rigorously with all the bells and whistles. It is clear that the first step is to derive the equations of motion for the Green's function in the jellium model. That was one of the ways to find the Green's function in the non-interacting case, without source fields. That begins with the Hamiltonian and equations for motion for $\psi_\sigma(1)$ which will enter the equation of motion for $\mathcal{G}$.

23.1 Equations of motion for the field operator

The Hamiltonian we consider contains the kinetic energy and the electron-electron interaction. Note that we now introduce spin indices denoted by Greek indices:

$$\begin{aligned}
\hat{K} &= \hat{H} - \mu\hat{N} = \hat{H}_0 + \hat{V} + \hat{V}_n - \mu\hat{N} \\
\hat{H}_0 &= \frac{-1}{2m}\sum_{\sigma_1}\int d\mathbf{x}_1 \psi^\dagger_{\sigma_1}(\mathbf{x}_1)\nabla^2\psi_{\sigma_1}(\mathbf{x}_1) \\
\hat{V} &= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_1)\psi^\dagger_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1) \\
\hat{V}_n &= -\sum_{\sigma_1}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_2)n
\end{aligned} \tag{23.1}$$

The last piece, V_n represents the interaction between a "neutralizing background" of the same uniform density n as the electrons. The potential is the Coulomb potential

$$v(\mathbf{x}_1-\mathbf{x}_2) = \frac{e^2}{4\pi\varepsilon_0|\mathbf{x}_1-\mathbf{x}_2|} \tag{23.2}$$

Now define

$$V(1,2) = V_{\sigma_1,\sigma_2}(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2) \equiv \frac{e^2}{4\pi\varepsilon_0|\mathbf{x}_1-\mathbf{x}_2|}\delta(\tau_1-\tau_2) \tag{23.3}$$

In reality the potential is independent of spin and is instantaneous but introducing these dependencies simplifies the notation. Using the matrix notation and ignoring the V_n term (later it will be shown that we can compensate this by removing the $q=0$ term)

$$K = \psi^\dagger(\bar{1})(\frac{-\nabla^2_{\bar{1}}}{2m} - \mu)\psi(\bar{1}) + \frac{1}{2}V(\bar{1}-\bar{2})\psi^\dagger(\bar{1})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(\bar{1}) \tag{23.4}$$

The equation of motion

$$\begin{aligned}
\partial_{\tau_1}\psi(1) &= [K,\psi(1)] \\
&= (\frac{\nabla^2_1}{2m}+\mu)\psi(1) - \psi^\dagger(\bar{1})\psi(\bar{1})V(\bar{1}-1)\psi(1)
\end{aligned} \tag{23.5}$$

where we used

$$[\psi^\dagger(\bar{1})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(\bar{1}),\psi(1)] = \delta(1-\bar{2})\psi^\dagger(\bar{1})\psi(\bar{2})\psi(\bar{1}) - \delta(1-\bar{1})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(\bar{1}) \tag{23.6}$$

$$\begin{aligned}
&\frac{1}{2}V(\bar{1}-\bar{2})[\psi^\dagger(\bar{1})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(\bar{1}),\psi(1)] \\
=&\frac{1}{2}V(\bar{1}-\bar{2})\left(\delta(1-\bar{2})\psi^\dagger(\bar{1})\psi(\bar{2})\psi(\bar{1}) - \delta(1-\bar{1})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(\bar{1})\right) \\
=&\frac{1}{2}V(\bar{1}-1)\psi^\dagger(\bar{1})\psi(1)\psi(\bar{1}) - \frac{1}{2}V(1-\bar{2})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(1) \\
=&V(\bar{1}-1)\psi^\dagger(\bar{1})\psi(1)\psi(\bar{1})
\end{aligned} \tag{23.7}$$

In the full notation, the equation of motion looks like

$$\begin{aligned}
\frac{\partial\psi_\sigma(\mathbf{x},\tau)}{\partial\tau} &= \left[\hat{K},\psi_\sigma(\mathbf{x},\tau)\right] \\
&= (\frac{\nabla^2}{2m}+\mu)\psi_\sigma(\mathbf{x},\tau) - \sum_{\sigma_2}\int d\mathbf{x}_2 v(\mathbf{x}-\mathbf{x}_2)\psi^\dagger_{\sigma_2}(\mathbf{x}_2,\tau)\psi_{\sigma_2}(\mathbf{x}_2,\tau)\psi_\sigma(\mathbf{x},\tau)
\end{aligned} \tag{23.8}$$

We assume that the potential has no $q=0$ component because of the compensating effect of the positive background. The argument for the neutralizing background is as follows. If we had kept it, the above equation would have had an extra term

$$+n\left[\int d\mathbf{x}_2 v(\mathbf{x}-\mathbf{x}_2)\right]\psi_\sigma(\mathbf{x},\tau) \tag{23.9}$$

We will see that there is a contribution to the self-energy, the Hartree contribution that cancels this term. To an excellent degree of approximation we may say that the only effect of the neutralizing background is to remove the $q = 0$ component of the Coulomb potential. The result that we are about to derive would be different in other models, such as the Hubbard model, where the $q = 0$ component of the interaction potential is far from negligible.

23.2 Equations of motion for the Green's function

Starting with the definition

$$\mathcal{G}(1,2)_\phi = -\frac{\langle T_\tau \mathcal{S}[\phi]\psi(1)\psi^\dagger(2)\rangle}{\langle T_\tau \mathcal{S}[\phi]\rangle} \tag{23.10}$$

we now wish to act ∂_{τ_1} on $\mathcal{G}(1,2)_\phi$. The denomenator is not a function of τ_1.
The numerator has three contributions,

1. $\partial_{\tau_1}\psi(1)$

$$\begin{aligned} -\frac{\langle T_\tau \mathcal{S}[\phi]\partial_{\tau_1}\psi(1)\psi^\dagger(2)\rangle}{\langle T_\tau \mathcal{S}[\phi]\rangle} &= -\frac{\left\langle T_\tau \mathcal{S}[\phi]\left\{(\frac{\nabla_1^2}{2m}+\mu)\psi(1) - \psi^\dagger(\bar{2})\psi(\bar{2})V\left(1-\bar{2}\right)\psi(1)\right\}\psi^\dagger(2)\right\rangle}{\langle T_\tau \mathcal{S}[\phi]\rangle} \\ &= (\frac{\nabla_1^2}{2m}+\mu)\mathcal{G}(1,2)_\phi + \left\langle \mathcal{T}_\tau \psi^\dagger(\bar{2})V\left(1-\bar{2}\right)\psi(\bar{2})\psi(1)\psi^\dagger(2)\right\rangle_\phi \\ &\to (\frac{\nabla_1^2}{2m}+\mu)\mathcal{G}(1,2)_\phi + \left\langle \mathcal{T}_\tau \psi^\dagger(\bar{2^+})V\left(1-\bar{2}\right)\psi(\bar{2})\psi(1)\psi^\dagger(2)\right\rangle_\phi \end{aligned} \tag{23.11}$$

Note that we had to specify $\psi^\dagger(\bar{2^+})$ in the term with the potential energy. The superscript + specifies that the time in that field operator is later than the time in $\psi(\bar{2})$. In other words

$$2^+ \equiv \left(\mathbf{x}_2, \tau_2 + 0^+; \sigma_2\right) \tag{23.12}$$

Equal time does not mean anything in a time ordered product, we have to specify the order. The choice to take $\psi^\dagger\left(\overline{2^+}\right)$ keeps the field in the order it was in to begin with. Notice also that $T_\tau\left[e^{A+B}\right] = T_\tau\left[e^A e^B\right]$ even when $[A,B] \neq 0$.

2. $\mathcal{T}_\tau$ introduces $\theta(\tau_1 - \tau_2)$

$$\begin{aligned} &- \frac{\left\langle (T_\tau \mathcal{S}[\phi])\,\psi(1)\psi^\dagger(2)\right\rangle}{\langle (T_\tau \mathcal{S}[\phi])\rangle}\partial_{\tau_1}\theta(\tau_1-\tau_2) + \frac{\left\langle (T_\tau \mathcal{S}[\phi])\,\psi^\dagger(2)\psi(1)\right\rangle}{\langle (T_\tau \mathcal{S}[\phi])\rangle}\partial_{\tau_1}\theta(\tau_2-\tau_1) \\ =& -\frac{\left\langle (T_\tau \mathcal{S}[\phi])\,\{\psi(1),\psi^\dagger(2)\}\right\rangle}{\langle (T_\tau \mathcal{S}[\phi])\rangle}\delta(\tau_1-\tau_2) \\ =& -\delta(1-2) \end{aligned} \tag{23.13}$$

3. The boundary of the integrals coming from $S[\phi]$

The last one can be seen by moving the time-ordering operator

$$\begin{aligned} \left\langle T_\tau \mathcal{S}[\phi]\psi(1)\psi^\dagger(2)\right\rangle = \Bigg\langle & T_\tau \exp\left(-\int_{\tau_1}^{\beta} d\tau_{1'}\int d^3\mathbf{x}_{1'}\psi^\dagger\left(1'\right)\phi\left(1',\bar{2}\right)\psi(\bar{2})\right) \\ & \psi(1)\exp\left(-\int_0^{\tau_1} d\tau_{1'}\int d^3\mathbf{x}_{1'}\psi^\dagger\left(1'\right)\phi\left(1',\bar{2}\right)\psi(\bar{2})\right)\psi^\dagger(2)\Bigg\rangle \end{aligned} \tag{23.14}$$

where in the $\bar{2}$ we have hidden an integration $d\tau_2 d^3\mathbf{x}_2$. We thus have a contribution to the time derivative with

respect to τ_1 that comes from acting on the exponentials and reads

$$\begin{aligned}
&\left\langle T_\tau \exp\left(-\int_{\tau_1}^{\beta} d\tau_{1'} \int d^3\mathbf{x}_{1'} \psi^\dagger\left(1'\right) \phi\left(1', \overline{2}\right) \psi(\overline{2})\right)\right. \\
&\int d^3\mathbf{x}_{1'}\left[\psi^\dagger\left(\mathbf{x}_{1'}, \tau_1\right) \phi\left(\mathbf{x}_{1'}, \tau_1, \overline{2}\right) \psi(\overline{2}), \psi\left(\mathbf{x}_1, \tau_1\right)\right] \\
&\left.\exp\left(-\int_0^{\tau_1} d\tau_{1'} \int d^3\mathbf{x}_{1'} \psi^\dagger\left(1'\right) \phi\left(1', \overline{2}\right) \psi(\overline{2})\right) \psi^\dagger(2)\right\rangle \\
=& -\phi(1, \overline{2})\left\langle T_\tau \mathcal{S}[\phi] \psi(\overline{2}) \psi^\dagger(2)\right\rangle \\
=& -\phi(1, \overline{2})\left\langle T_\tau \mathcal{S}[\phi] \psi(\overline{2}) \psi^\dagger(2)\right\rangle
\end{aligned} \tag{23.15}$$

where we used the commutator

$$\int d^3\mathbf{x}_{1'} \phi\left(\mathbf{x}_{1'}, \tau_1, \overline{2}\right)\left[\psi^\dagger\left(\mathbf{x}_{1'}, \tau_1\right) \psi(\overline{2}), \psi\left(\mathbf{x}_1, \tau_1\right)\right] = -\phi\left(\mathbf{x}_1, \tau_1, \overline{2}\right) \psi(\overline{2}) \tag{23.16}$$

Collecting all the contributions, we can write

$$\left(\frac{\partial}{\partial \tau_1} - \frac{\nabla_1^2}{2m} - \mu\right) \mathcal{G}(1,2)_\phi = -\delta(1-2) + \left\langle T_\tau\left[\psi^\dagger(\overline{2^+}) V(1-\overline{2}) \psi(\overline{2}) \psi(1) \psi^\dagger(2)\right]\right\rangle_\phi - \phi(1, \overline{2}) \mathcal{G}(\overline{2}, 2)_\phi \tag{23.17}$$

if we define the non-interacting Green's function to be

$$\begin{aligned}
\left(\frac{\partial}{\partial \tau_1} - \frac{\nabla_1^2}{2m} - \mu\right) \mathcal{G}_0(1,2) &= -\delta(1-2) \\
\mathcal{G}_0^{-1}(1,2) &= -\left(\frac{\partial}{\partial \tau_1} - \frac{\nabla_1^2}{2m} - \mu\right) \delta(1-2)
\end{aligned} \tag{23.18}$$

check that

$$\begin{aligned}
\mathcal{G}_0^{-1}(1, \overline{2}) \mathcal{G}_0(\overline{2}, 2) &= \left(-\frac{\partial}{\partial \tau_1} + \frac{\nabla_1^2}{2m} + \mu\right) \delta(1-\overline{2}) \mathcal{G}_0(\overline{2}, 2) \\
&= \delta(1-\overline{2}) \left(-\frac{\partial}{\partial \tau_{\overline{2}}} + \frac{\nabla_{\overline{2}}^2}{2m} + \mu\right) \mathcal{G}_0(\overline{2}, 2) \\
&= \delta(1-\overline{2}) \delta(\overline{2}-2) \\
&= \delta(1-2)
\end{aligned} \tag{23.19}$$

notice that the integration by parts effectively results in the commutation

$$\left(-\frac{\partial}{\partial \tau_1} + \frac{\nabla_1^2}{2m} + \mu\right) \delta(1-\overline{2}) = \delta(1-\overline{2}) \left(-\frac{\partial}{\partial \tau_{\overline{2}}} + \frac{\nabla_{\overline{2}}^2}{2m} + \mu\right) \tag{23.20}$$

so we have

$$\begin{aligned}
\left(\frac{\partial}{\partial \tau_1} - \frac{\nabla_1^2}{2m} - \mu\right) \mathcal{G}(1,2)_\phi &= \delta(1-\overline{2}) \left(\frac{\partial}{\partial \tau_{\overline{2}}} - \frac{\nabla_{\overline{2}}^2}{2m} - \mu\right) \mathcal{G}(\overline{2}, 2)_\phi \\
&= \left(\frac{\partial}{\partial \tau_1} - \frac{\nabla_1^2}{2m} - \mu\right) \delta(1-\overline{2}) \mathcal{G}(\overline{2}, 2)_\phi \\
&= -\mathcal{G}_0^{-1}(1, \overline{2}) \mathcal{G}(\overline{2}, 2)_\phi
\end{aligned} \tag{23.21}$$

so we can rewrite the relation as

$$\left(\mathcal{G}_0^{-1}(1, \overline{2}) - \phi(1, \overline{2})\right) \mathcal{G}(\overline{2}, 2)_\phi = \delta(1-2) - V(1-\overline{2}) \left\langle T_\tau\left[\psi^\dagger(\overline{2^+}) \psi(\overline{2}) \psi(1) \psi^\dagger(2)\right]\right\rangle_\phi \tag{23.22}$$

comparing with Dyson's equation

$$\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \phi - \Sigma \tag{23.23}$$

we can identify the explicit form of self-energy

$$\Sigma(1, \overline{2})_\phi \mathcal{G}(\overline{2}, 2)_\phi = -V(1-\overline{2}) \left\langle T_\tau\left[\psi^\dagger(\overline{2^+}) \psi(\overline{2}) \psi(1) \psi^\dagger(2)\right]\right\rangle_\phi \tag{23.24}$$

The equation of motion can then also be written as

$$\left(\mathcal{G}_0^{-1}(1,\bar{2}) - \phi(1,\bar{2}) - \Sigma(1,\bar{2})\right)\mathcal{G}(\bar{2},2)_\phi = \delta(1-2) \tag{23.25}$$

which also reads

$$\mathcal{G}^{-1}(1,2)_\phi = \mathcal{G}_0^{-1}(1,2) - \phi(1,2) - \Sigma(1,2)_\phi \tag{23.26}$$

The self-energy is related to a four-point function which is directly related to the Coulomb potential.

23.3 Four-point function from functional derivative

Since we need a four-point function to compute the self-energy and we know $\mathcal{G}_\phi$ if we know the self-energy, let us find an equation for the four-point function in terms of functional derivatives

$$\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} = \left\langle T_\tau\psi(1)\psi^\dagger(2)\psi^\dagger(3)\psi(4)\right\rangle_\phi + \mathcal{G}(1,2)_\phi\mathcal{G}(4,3)_\phi \tag{23.27}$$

Using the relation in abstract matrix notation and indices

$$\begin{aligned}\frac{\delta\mathcal{G}}{\delta\phi} &= -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G}\\ \frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} &= -\mathcal{G}(1,\bar{1})_\phi\frac{\delta\mathcal{G}^{-1}(\bar{1},\bar{2})_\phi}{\delta\phi(3,4)}\mathcal{G}(\bar{2},2)_\phi\end{aligned} \tag{23.28}$$

and Dyson's relation

$$\begin{aligned}\mathcal{G}_\phi^{-1} &= \mathcal{G}_0^{-1} - \phi - \Sigma_\phi\\ \mathcal{G}^{-1}(1,2)_\phi &= \mathcal{G}_0^{-1}(1,2) - \phi(1,2) - \Sigma(1,2)_\phi\end{aligned} \tag{23.29}$$

we have

$$\begin{aligned}\frac{\delta\mathcal{G}}{\delta\phi} &= \mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\frac{\delta\Sigma}{\delta\phi}\mathcal{G}\\ \frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} &= \mathcal{G}(1,\bar{1})_\phi\frac{\delta\phi(\bar{1},\bar{2})}{\delta\phi(3,4)}\mathcal{G}(\bar{2},2)_\phi + \mathcal{G}(1,\bar{5})_\phi\frac{\delta\Sigma(\bar{5},\bar{6})_\phi}{\delta\phi(3,4)}\mathcal{G}(\bar{6},2)_\phi\\ &= \mathcal{G}(1,3)_\phi\mathcal{G}(4,2)_\phi + \mathcal{G}(1,\bar{5})_\phi\frac{\delta\Sigma(\bar{5},\bar{6})_\phi}{\delta\phi(3,4)}\mathcal{G}(\bar{6},2)_\phi\end{aligned} \tag{23.30}$$

If we take the convention that $\mathcal{G}(1,2)$ is represented by an arrow going from 1 to 2, then $\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)}$ is $\mathcal{G}(1,2)$ being "pinched" by $\phi(3,4)$, i.e. having an arrow starting at 1 and ending at 2 with 3; 4 at the bottom. (See diagram Ref. 36-1 LHS)

This last equation shows that Σ has no explicit dependence on ϕ. It depends on ϕ only through its dependence on $\mathcal{G}$. We will see this is a **self-consistent assumption**. Taking that into account, and using the chain rule, this last equation can also be written in the form

$$\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} = \mathcal{G}(1,3)_\phi\mathcal{G}(4,2)_\phi + \mathcal{G}(1,\bar{5})_\phi\left(\frac{\delta\Sigma(\bar{5},\bar{6})_\phi}{\delta\mathcal{G}(\bar{7},\bar{8})}\frac{\delta\mathcal{G}(\bar{7},\bar{8})_\phi}{\delta\phi(3,4)}\right)\mathcal{G}(\bar{6},2)_\phi \tag{23.31}$$

This general equation can also be written in short-hand notation

$$\frac{\delta\mathcal{G}}{\delta\phi} = \mathcal{G}\wedge\mathcal{G} + \mathcal{G}\ \begin{matrix}\frac{\delta\Sigma}{\delta\mathcal{G}}\\ \frac{\delta\mathcal{G}}{\delta\phi}\end{matrix}\ \mathcal{G} \tag{23.32}$$

where the wedge $\wedge$ reminds us that the indices adjacent to it are the same as those of ϕ and where the two terms on top of one another are matrix multiplied top down as well. In the top down multiplication, it is pairs of indices of $\mathcal{G}$ that are considered as a single matrix index. (Ref. Fig. 36-1) illustrates the equation with the indices. The diagrams go from top to bottom to remind ourselves of where the indices are in the algebraic equation, but we may rotate the diagrams in any direction we want.

$\frac{\delta\Sigma}{\delta\mathcal{G}}$ is the **vertex function** which is irreducible in a particle-hole channel. (There are two particle-hole channels). This means that if we iterate the equation for $\frac{\delta\mathcal{G}}{\delta\phi}$, we generate all the diagrams that have Green's function lines

going in opposite direction. Those diagrams for $\frac{\delta\mathcal{G}}{\delta\phi}$ can thus be cut in two by cutting these two lines. They are reducible. $\frac{\delta\Sigma}{\delta\mathcal{G}}$ contains the diagrams that cannot be cut in two in this way. It sort of plays the role of a **self-energy for response functions**.

Notice also that when we take infinitesimally close points in $\mathcal{G}$ and ϕ, and without interaction, we can use Wick's theorem

$$\begin{aligned}\frac{\delta\mathcal{G}\left(1,1^{+}\right)_{0}}{\delta\phi\left(2^{+},2\right)} &= \left\langle T_{\tau}\psi(1)\psi^{\dagger}(1^{+})\psi^{\dagger}(2^{+})\psi(2)\right\rangle_{0}+\left\langle \mathcal{T}_{\tau}\psi(1)\psi^{\dagger}(1^{+})\right\rangle_{0}\left\langle \mathcal{T}_{\tau}\psi(2)\psi^{\dagger}(2^{+})\right\rangle_{0}\\ &= -\left\langle \mathcal{T}_{\tau}\psi(1)\psi^{\dagger}(2^{+})\right\rangle_{0}\left\langle \mathcal{T}_{\tau}\psi^{\dagger}(1^{+})\psi(2)\right\rangle_{0}\\ &= \mathcal{G}(1,2)_{0}\mathcal{G}(2,1)_{0}\end{aligned} \tag{23.33}$$

this is called the exchange term. It makes sure that two electrons with the same spin are not on top of each other. This comes from the Pauli exclusion principle.

23.4 Self-energy from functional derivatives

To compute the self-energy

$$\Sigma(1,3)_{\phi}=-V(1-\overline{2})\left\langle T_{\tau}\left[\psi^{\dagger}(\overline{2}^{+})\psi(\overline{2})\psi(1)\psi^{\dagger}(\overline{4})\right]\right\rangle_{\phi}\mathcal{G}^{-1}(\overline{4},3)_{\phi} \tag{23.34}$$

replacing the four-point correlation function by the functional derivative term,

$$\Sigma(1,3)_{\phi}=-V(1-\overline{2})\left[\frac{\delta\mathcal{G}(1,\overline{4})_{\phi}}{\delta\phi(\overline{2}^{+},\overline{2})}-\mathcal{G}(\overline{2},\overline{2}^{+})_{\phi}\mathcal{G}(1,\overline{4})_{\phi}\right]\mathcal{G}^{-1}(\overline{4},3)_{\phi} \tag{23.35}$$

Historically, the expressions self-energy is inspired by the fact that it is the electromagnetic field of the electron itself that leads to modifications of the properties of the electron even when it is moving in a vacuum. In the latter case, the electromagnetic field of the electron contains virtual photons that can in turn create virtual electron-positron pairs, the analog of electron-hole excitations.

Now write

$$\frac{\delta\mathcal{G}(1,\overline{4})_{\phi}}{\delta\phi(\overline{2}^{+},\overline{2})}=\mathcal{G}(1,\overline{2}^{+})_{\phi}\mathcal{G}(\overline{2},\overline{4})_{\phi}+\mathcal{G}(1,\overline{7})_{\phi}\left(\frac{\delta\Sigma(\overline{7},\overline{8})_{\phi}}{\delta\mathcal{G}(\overline{5},\overline{6})_{\phi}}\frac{\delta\mathcal{G}(\overline{5},\overline{6})_{\phi}}{\delta\phi(\overline{2}^{+},\overline{2})}\right)\mathcal{G}(\overline{8},\overline{4})_{\phi} \tag{23.36}$$

substitute this into the self-energy expression,

$$\begin{aligned}\Sigma(1,3)_{\phi} &= -V(1-\overline{2})\mathcal{G}(1,\overline{2}^{+})_{\phi}\mathcal{G}(\overline{2},\overline{4})_{\phi}\mathcal{G}^{-1}(\overline{4},3)_{\phi}\\ &\quad+V(1-\overline{2})\mathcal{G}(\overline{2},\overline{2}^{+})_{\phi}\mathcal{G}(1,\overline{4})_{\phi}\mathcal{G}^{-1}(\overline{4},3)_{\phi}\\ &\quad-V(1-\overline{2})\mathcal{G}(1,\overline{7})_{\phi}\left(\frac{\delta\Sigma(\overline{7},\overline{8})_{\phi}}{\delta\mathcal{G}(\overline{5},\overline{6})_{\phi}}\frac{\delta\mathcal{G}(\overline{5},\overline{6})_{\phi}}{\delta\phi(\overline{2}^{+},\overline{2})}\right)\mathcal{G}(\overline{8},\overline{4})_{\phi}\mathcal{G}^{-1}(\overline{4},3)_{\phi}\end{aligned} \tag{23.37}$$

the final expression is

$$\begin{aligned}\Sigma(1,3)_{\phi} &= -V(1-3)\mathcal{G}(1,3^{+})_{\phi}+V(1-\overline{2})\mathcal{G}(\overline{2},\overline{2}^{+})_{\phi}\delta(1-3)\\ &\quad-V(1-\overline{2})\mathcal{G}(1,\overline{4})_{\phi}\left(\frac{\delta\Sigma(\overline{4},3)_{\phi}}{\delta\mathcal{G}(\overline{5},\overline{6})_{\phi}}\frac{\delta\mathcal{G}(\overline{5},\overline{6})_{\phi}}{\delta\phi(\overline{2}^{+},\overline{2})}\right)\end{aligned} \tag{23.38}$$

$$\Sigma=-V\left(\mathcal{G}\frac{\delta\phi}{\delta\phi}+\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)-\mathcal{G}\right) \tag{23.39}$$

in the first two terms $V(1-3)$ and $\delta(1-3)$ both contain $\delta(\tau_1-\tau_3)$, so their Fourier Transform will be constant in ω. The last term is the only one that will have a frequency dependence, and hence an imaginary part, to the self-energy. The other two terms in the above equation are the Hartree-Fock contribution that we will discuss at length later on. The equation for the self-energy is represented schematically in Ref. Fig. 36-2. Note that the diagrams are one-particle irreducible, i.e. they cannot be cut in two separate pieces by cutting a single propagator.

It is clear from the diagrammatic illustration of the self-energy in Fig. 36-2 that all internal indices are integrated over, as the Feynman rules would specify. In addition, the diagrams are connected and none of them can be cut into two distinct pieces by cutting one Green's function line. We say that the self-energy contains all the diagrams that are one-particle irreducible. The Feynman rules tell us that the self-energy contains all the topologically distinct connected diagrams that end and begin with an interaction and a Green's function at the same point. There are rules for their sign as well: One minus sign for each order in perturbation theory and one minus sign for every closed loop. The Feynman rules are generally formulated in terms of bare Green's functions. Here, the dressed Green's functions appear but, it is also possible to recover the perturbation theory in terms of bare Green's functions.

23.5 Diagrammatic Representation for Schwinger's formalism

In position space, we have $\mathcal{G}(1,2)$, $\Sigma(1,2)$, $V(1,2)$, $\mathcal{G}_0(1,2)$, $\frac{\delta\mathcal{G}(1,2)}{\delta\phi(3,4)}$, $\frac{\delta\Sigma(1,2)}{\delta\mathcal{G}(3,4)}$,

24 Hartree-Fock and RPA

These are the two most famous approximations: **Hartree-Fock** for the **self-energy** and **RPA** for the **density-density correlation** function. We will see later on why these come out naturally from simple considerations, including the variational principle.

24.1 Functional derivatives can be used to generate perturbation theory

The Schwinger formalism generates very naturally an expansion in powers of the dressed Green's function. The diagrams that are found for the self-energy then do not include self-energy insertions. This is called the **skeleton expansion**. This is formally very nice and this expansion can be used to derive a number of exact results, such as the **Luttinger theorem**. However, it has some drawbacks on the limitations of conserving approximations. The expansion in terms of the bare Green's function is often much better behaved, but it is a bit more awkward to generate with the Schwinger formalism. This is discussed in the following two subsections.

24.1.1 Skeleton expansion

The relations we have obtained

$$\begin{aligned}\Sigma &= \left(V\mathcal{G} - V\mathcal{G}\frac{\delta\phi}{\delta\phi}\right) - V\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)\\ \frac{\delta\mathcal{G}}{\delta\phi} &= \mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} + \mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)\mathcal{G}\end{aligned} \tag{24.1}$$

can be used iteratively to generate perturbation theory for the self-energy in powers of V. The second equation already includes Dyson's equation. In the non-interacting case $V = 0$ we have $\Sigma = 0$. The first order term is given by substituting $\mathcal{G} \to \mathcal{G}_0$ in the expression for Σ, the two terms $V\mathcal{G}_0 - V\mathcal{G}_0\frac{\delta\phi}{\delta\phi}$ are $\mathcal{O}(V)$, while the third term involves $V\frac{\delta\Sigma}{\delta\mathcal{G}}$ which is $\mathcal{O}(V^2)$ since Σ already have $\mathcal{O}(V)$ terms. Therefore, the lowest order term in Σ is

$$\Sigma^{(1)}(1,3)_\phi = V(1-\overline{2})\mathcal{G}(\overline{2},\overline{2}^+)_\phi\delta(1-3) - V(1-3)\mathcal{G}(1,3^+)_\phi \tag{24.2}$$

This is the **Hartree-Fock approximation**. We shall expand on it later.
To obtain the second order, we recover

$$\Sigma^{(2)}(1,3)_\phi = -V(1-\overline{2})\mathcal{G}(1,\overline{4})_\phi\left(\frac{\delta\Sigma(\overline{4},3)_\phi}{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}\frac{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}{\delta\phi(\overline{2}^+,\overline{2})}\right) \tag{24.3}$$

we need $\delta\Sigma/\delta\mathcal{G}$ to first order in V and $\delta\mathcal{G}/\delta\phi$ to zeroth order in V. The former can be obtained by differentiating $\Sigma^{(1)}(\overline{4},3)_\phi$

$$\begin{aligned}\frac{\delta\Sigma(\overline{4},3)_\phi}{\delta\mathcal{G}(\overline{5},\overline{6})_\phi} &= \frac{\delta}{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}\left[V(\overline{4}-\overline{2})\mathcal{G}\left(\overline{2},\overline{2^+}\right)_\phi\delta(\overline{4}-3) - V(\overline{4}-3)\mathcal{G}\left(\overline{4},3^+\right)_\phi\right]\\ &= V(\overline{4}-\overline{2})\delta(\overline{2}-\overline{5})\delta(\overline{2}^+-\overline{6})\delta(\overline{4}-3) - V(\overline{4}-3)\delta(\overline{4}-\overline{5})\delta(\overline{3}^+-\overline{6})\end{aligned} \tag{24.4}$$

while

$$\frac{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}{\delta\phi(\overline{2}^+,\overline{2})} = \mathcal{G}(\overline{5},\overline{2}^+)_\phi\mathcal{G}(\overline{2},\overline{6})_\phi \tag{24.5}$$

Therefore,

$$\begin{aligned}\Sigma^{(2)}(1,3)_\phi &= -V(1-\overline{2})\mathcal{G}(1,\overline{4})_\phi\left(\frac{\delta\Sigma(\overline{4},3)_\phi}{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}\frac{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}{\delta\phi(\overline{2}^+,\overline{2})}\right)\\ &= -V(1-\overline{2})\mathcal{G}(1,\overline{4})_\phi\mathcal{G}(\overline{5},\overline{2}^+)_\phi\mathcal{G}(\overline{2},\overline{6})_\phi V(\overline{4}-\overline{2})\delta(\overline{2}-\overline{5})\delta(\overline{2}^+-\overline{6})\delta(\overline{4}-3)\\ &\quad + V(1-\overline{2})\mathcal{G}(1,\overline{4})_\phi\mathcal{G}(\overline{5},\overline{2}^+)_\phi\mathcal{G}(\overline{2},\overline{6})_\phi V(\overline{4}-3)\delta(\overline{4}-\overline{5})\delta(\overline{3}^+-\overline{6})\\ &= -V(1-\overline{2})V(\overline{4}-\overline{2})\mathcal{G}(1,\overline{3})_\phi\mathcal{G}(\overline{2},\overline{2}^+)_\phi\mathcal{G}(\overline{2},\overline{2}^+)_\phi\\ &\quad + V(1-\overline{2})V(\overline{4}-3)\mathcal{G}(1,\overline{4})_\phi\mathcal{G}(\overline{4},\overline{2}^+)_\phi\mathcal{G}(\overline{2},\overline{3}^+)_\phi\end{aligned} \tag{24.6}$$

The second order diagrams thus looks as illustrated on Fig. (37-1). The iterative process becomes more and more complicated as the order of perturbation increases, but it is clear that it can be done.

$$\begin{aligned}\Sigma &= \left(V\mathcal{G} - V\mathcal{G}\frac{\delta\phi}{\delta\phi}\right) - V\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right) \\ &= \left(V\mathcal{G} - V\mathcal{G}\frac{\delta\phi}{\delta\phi}\right) - V\mathcal{G}\frac{\delta\Sigma}{\delta\mathcal{G}}\mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} - V\mathcal{G}\frac{\delta\Sigma}{\delta\mathcal{G}}\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)\mathcal{G} \\ &= \left(V\mathcal{G} - V\mathcal{G}\frac{\delta\phi}{\delta\phi}\right) - V\mathcal{G}\frac{\delta\Sigma}{\delta\mathcal{G}}\mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G} - V\mathcal{G}\frac{\delta\Sigma}{\delta\mathcal{G}}\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\mathcal{G}\frac{\delta\phi}{\delta\phi}\mathcal{G}\right)\mathcal{G} - V\mathcal{G}\frac{\delta\Sigma}{\delta\mathcal{G}}\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\mathcal{G}\left(\frac{\delta\Sigma}{\delta\mathcal{G}}\frac{\delta\mathcal{G}}{\delta\phi}\right)\mathcal{G}\right)\mathcal{G} \\ &= ...\end{aligned} \tag{24.7}$$

In general, we can let

$$\Sigma = \Sigma^{(1)}V + \Sigma^{(2)}V^2 + \Sigma^{(3)}V^3 + ... \tag{24.8}$$

and plug into the above equation. To each order of V we can then generate an equation. Solving these equations iteratively then gives the final result.

The perturbation theory that we have just found is in powers of the interaction with dressed propagators. This is the so-called skeleton expansion where self-energies never appear on a Green's function. The jargon is that there are non self-energy insertions. For example, a term such as the one illustrated in Fig. (37-2) does not appear. The following section shows that such diagrams appear when we expand in powers of the bare Green's function.

24.1.2 Expansion in terms of the bare Green's function

The Feynman rules in Chapter (38) give a way to generate all self-energy diagrams, but it is easy to miss some terms. With the Schwinger formalism, one way is to start from the skeleton expansion, that can be found analytically, as I have show above. The first-order diagrams for the self-energy in powers of the potential using $\mathcal{G}_0$ is obtained simply by replacing $\mathcal{G}$ by $\mathcal{G}_0$ in the skeleton expansion.

Say we want the third order diagrams for the self-energy. The idea is to keep using the skeleton expansion and then recursively use Dyson's equation

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G} \tag{24.9}$$

that can be iterated to give

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0 + \cdots \tag{24.10}$$

Assume that, as above, we have found the self-energy expansion to second order in the external potential with $\mathcal{G}_0$ propagators. To third order, we must add all the contributions below:

1. Replace all $\mathcal{G}$ by $\mathcal{G}_0$ in the third order skeleton diagram.
2. In the second-order skeleton diagram, replace in turn successively all but one of the $\mathcal{G}$ by $\mathcal{G}_0$ and the left-over $\mathcal{G}$ by $\mathcal{G}_0\Sigma\mathcal{G}_0$ with Σ calculated to first order with $\mathcal{G}_0$ propagators.
3. In the first-order skeleton diagram
   (a) replace successively all $\mathcal{G}$ except one by $\mathcal{G}_0$ and the left-over $\mathcal{G}$ by $\mathcal{G}_0\Sigma\mathcal{G}_0$ with Σ calculated to second order in the external potential with $\mathcal{G}_0$ propagators.
   (b) replace successively all $\mathcal{G}$ except one by $\mathcal{G}_0$ and the left-over $\mathcal{G}$ by $\mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0$ with Σ calculated to first order in the external potential with $\mathcal{G}_0$ propagators.
   (c) replace simultaneously the two $\mathcal{G}$ of the first-order skeleton expansion by $\mathcal{G}_0\Sigma\mathcal{G}_0$ with Σ to first order in the external potential with $\mathcal{G}_0$ propagators.

The procedure is clear but tedious. It suffices to keep track of perturbation order recursively, going back in the order of the skeleton expansion and using Dyson's equation to replace $\mathcal{G}$.

24.2 Hartree-Fock and RPA in space-time

We have already derived the Hartree-Fock contribution to self-energy

$$\Sigma^{(1)}(1,3)_\phi = V(1-\overline{2})\mathcal{G}(\overline{2},\overline{2}^+)_\phi\delta(1-3) - V(1-3)\mathcal{G}(1,3^+)_\phi \tag{24.11}$$

to obtain RPA, use $\delta\Sigma/\delta\mathcal{G}$ in Hartree-Fock approximation:

$$\frac{\delta\Sigma(5,6)_\phi}{\delta\mathcal{G}(7,8)_\phi} = V(5-7)\delta(7-8)\delta(5-6) - V(5-6)\delta(7-5)\delta(8-6) \tag{24.12}$$

It is easier to imagine the result by looking back at the illustration of the Hartree-Fock term in Ref. Fig. 36-1. The result of the functional derivative is illustrated in Ref. Fig. 37-3. When two coordinates are written at the same point, it is because there is a delta function.

Substituting back in the equation for the exact four-point function, we find

$$\begin{aligned}\frac{\delta\mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} =& \mathcal{G}(1,3)_\phi\mathcal{G}(4,2)_\phi \\ &+ \mathcal{G}(1,\overline{5})_\phi\left(V(\overline{5}-\overline{7})\frac{\delta\mathcal{G}(\overline{7},\overline{7})_\phi}{\delta\phi(3,4)}\right)\mathcal{G}(\overline{5},2)_\phi \\ &- \mathcal{G}(1,\overline{5})_\phi\left(V(\overline{5}-\overline{6})\frac{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}{\delta\phi(3,4)}\right)\mathcal{G}(\overline{6},2)_\phi.\end{aligned} \tag{24.13}$$

This expression is easy to deduce from the general diagrammatic representation of the general integral equation Ref. Fig. 36-1 by replacing the irreducible vertex by that in Ref. Fig. 37-3 that follows from the Hartree-Fock approximation. This is illustrated in Ref. Fig. 37-4.

To obtain a better approximation for Σ, we should include the second order term

$$\Sigma^{(2)}(1,3)_\phi = -V(1-\overline{2})\mathcal{G}(1,\overline{4})_\phi\frac{\delta\Sigma(\overline{4},3)_\phi}{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}\frac{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}{\delta\phi(\overline{2}^+,\overline{2})} \tag{24.14}$$

which requires $\frac{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}{\delta\phi(\overline{2}^+,\overline{2})}$. In fact, it turns out that we need only $\frac{\delta\mathcal{G}(1,1^+)_\phi}{\delta\phi(2^+,2)}$ which is

$$\begin{aligned}\frac{\delta\mathcal{G}(1,1^+)_\phi}{\delta\phi(2^+,2)} =& \mathcal{G}(1,2)_\phi\mathcal{G}(2,1)_\phi \\ &+ \mathcal{G}(1,\overline{5})_\phi\left(V(\overline{5}-\overline{7})\frac{\delta\mathcal{G}(\overline{7},\overline{7})_\phi}{\delta\phi\,(2^+,2)}\right)\mathcal{G}(\overline{5},1)_\phi \\ &- \mathcal{G}(1,\overline{5})_\phi\left(V(\overline{5}-\overline{6})\frac{\delta\mathcal{G}(\overline{5},\overline{6})_\phi}{\delta\phi\,(2^+,2)}\right)\mathcal{G}(\overline{6},1)_\phi.\end{aligned} \tag{24.15}$$

This equation is referred to as the **generalized RPA**. When the last term is negelected, this is the **RPA**. We will discuss this in more details later.

24.3 Hartree-Fock and RPA in momentum-frequency space with $\phi = 0$

We are ready to set $\phi = 0$. Once this is done, we can use translational invariance so that $\Sigma(1,2) = \Sigma(1-2)$ and $\mathcal{G}(1,2) = \mathcal{G}(1-2)$. In addition, **spin rotational invariance** implies that these objects are diagonal in spin space. We can now define the Fourier Transform

$$\begin{aligned}\mathcal{G}_\sigma(k) &= \int d\,(\mathbf{x}_1-\mathbf{x}_2)\int_0^\beta d\,(\tau_1-\tau_2)\,e^{-i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{ik_n(\tau_1-\tau_2)}\mathcal{G}_\sigma(1-2) \\ \mathcal{G}_\sigma(1-2) &= \int\frac{d^3\mathbf{k}}{(2\pi)^3}T\sum_{n=-\infty}^{\infty}e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{-ik_n(\tau_1-\tau_2)}\mathcal{G}_\sigma(k) \\ \mathcal{G}_\sigma(1-2) &= \frac{1}{V}\sum_{\mathbf{k}}T\sum_{n=-\infty}^{\infty}e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{-ik_n(\tau_1-\tau_2)}\mathcal{G}_\sigma(k)\end{aligned} \tag{24.16}$$

In this expression, k_n is a fermionic Matsubara frequency and the Green's function is diagonal in spin indices σ_1 and σ_2. We can collectively represent $k = (\mathbf{k}, ik_n)$. For clarity then, we have explicitly written a single spin label

so that now $1 = (\mathbf{x}_1, \tau_1)$. The inverse Fourier Transform has been written in two different forms, one in discrete momentum and one in continuous momentum. We have used the replacement

$$\frac{1}{V}\sum_{\mathbf{k}} \to \int \frac{d^3\mathbf{k}}{(2\pi)^3} \tag{24.17}$$

Similarly, for the potential we define

$$\begin{aligned} V_{\sigma,\sigma'}(q) &= \int d\left(\mathbf{x}_1 - \mathbf{x}_2\right) \int_0^\beta d\left(\tau_1 - \tau_2\right) e^{-i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{iq_n(\tau_1-\tau_2)} V_{\sigma,\sigma'}(1-2) \\ V_{\sigma,\sigma'}(1-2) &= \int \frac{d^3\mathbf{q}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-iq_n(\tau_1-\tau_2)} V_{\sigma,\sigma'}(q) \\ V_{\sigma,\sigma'}(1-2) &= \frac{1}{V}\sum_{\mathbf{q}} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)} e^{-iq_n(\tau_1-\tau_2)} V_{\sigma,\sigma'}(q) \end{aligned} \tag{24.18}$$

where q_n is a bosonic Matsubara frequency. Again we have explicitly written the spin indices even if $V_{\sigma\sigma'}$ is independent of spin.

We thus make the following rule:

- When in position space there is an arrow pointing from 1 to 2 representing $\mathcal{G}(1-2)$, in the translationally invariant case, in momentum space, we think of this arrow as carrying momentum k.
- An interaction $V(1-2)$ in a diagram is represented by a dotted line. In momentum space, this line carries momentum q. Notice that $V(1-2) = V(2-1)$ so we can choose any direction, as long as we stick with it.

Consider an internal vertex (say $\bar{2}$), as illustrated in Fig.(37-5), since we have performed a Fourier Transform for all lines in the diagram, there is a factor associated with vertex 2: $e^{-i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q})\cdot\mathbf{x}_2} e^{i(k_{1,n}-k_{2,n}+q_n)\tau_2}$. Since all internal vertices are integrated over ($\bar{2}$ hides integration), this gives (leaving aside the spin coordinates)

$$\begin{aligned} &\int d\mathbf{x}_2 \int_0^\beta d\tau_2 e^{-i(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q})\cdot\mathbf{x}_2} e^{i(k_{1,n}-k_{2,n}+q_n)\tau_2} \\ =&(2\pi)^3 \delta\left(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{q}\right) \beta \delta_{(k_{2,n}-k_{1,n}),q_n} \\ =&V\delta_{\mathbf{k}_1-\mathbf{k}_2,\mathbf{q}} \beta \delta_{(k_{2,n}-k_{1,n}),q_n} \end{aligned} \tag{24.19}$$

a delta function in continuous or discrete momentum form. Note that the sum of two fermionic Matsubara frequencies is a bosonic Matsubara frequency, so $k_{1,n} - k_{2,n} + q_n$ is bosonic and thus periodic in β. The conclusion of this is that momentum and Matsubara frequencies are conserved at each interaction vertex. In other words, we obtain the following rule:

- The sum of all wave vectors entering an interaction vertex vanishes.
- One must integrate over the momentum that are not determined by momentum conservation. In general, there are as many integrals to perform as there are closed loops in a diagram.
- We must also sum over spins that appear in internal indices, conserving spin at each interaction vertex when the interaction has this property. The propagator $\mathcal{G}$ will then be diagonal in spin index.

As and example, for the Hartree-Fock approximation (now with $\phi = 0$)

$$\Sigma^{(1)}(1-3) = V(1-\overline{2})\mathcal{G}(\overline{2}-\overline{2}^+)\delta(1-3) - V(1-3)\mathcal{G}(1-3^+) \tag{24.20}$$

Define

$$\begin{aligned} \frac{1}{\mathcal{V}}\sum_k e^{ikx} &\equiv \frac{1}{\mathcal{V}}\sum_{\mathbf{k}} T \sum_{n=-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_3)} e^{-ik_n(\tau_1-\tau_3)} \\ \int dx e^{-ikx} &\equiv \frac{1}{V}\sum_{\mathbf{k}} T \sum_{n=-\infty}^{\infty} \int d\mathbf{x} \int_0^\beta d\tau e^{-i\mathbf{k}\cdot\mathbf{x}} e^{ik_n\tau} \end{aligned} \tag{24.21}$$

we can perform a Fourier Transform

$$\begin{aligned}
\Sigma(k) &= \int dx e^{-ik(x_1-x_3)}\Sigma^{(1)}(1-3) \\
&= \int dx e^{-ik(x_1-x_3)}\left[V(1-\bar{2})\mathcal{G}(\bar{2}-\bar{2}^+)\delta(1-3) - V(1-3)\mathcal{G}(1-3^+)\right] \\
&= \int dx e^{-ik(x_1-x_3)}\delta(1-3)\mathcal{G}(\bar{2}-\bar{2}^+)\int dx_{\bar{2}} V(1-\bar{2}) - \int dx e^{-ik(x_1-x_3)}V(1-3)\mathcal{G}(1-3^+) \\
&= V(q=0)\mathcal{G}(\bar{2}-\bar{2}^+) - \frac{1}{\mathcal{V}^2}\sum_{q_1 k_1} V(q_1)\mathcal{G}(k_1)\int dx e^{-ik(x_1-x_3)}e^{iq_1(x_1-x_3)}e^{ik_1(x_1-x_3^+)} \\
&= V(q=0)\mathcal{G}(\bar{2}-\bar{2}^+) - \frac{1}{\mathcal{V}}\sum_{q_1 k_1} V(q_1)\mathcal{G}(k_1)e^{-ik_1 0^+}\delta_{-k+q_1+k_1} \\
&= V(q=0)\mathcal{G}(\bar{2}-\bar{2}^+) - e^{ik_n 0^+}\frac{1}{\mathcal{V}}\sum_q e^{iq_n 0^+}V(q)\mathcal{G}(k+q)
\end{aligned} \tag{24.22}$$

$$\Sigma(k) = V(q=0)n - e^{ik_n 0^+}\frac{1}{\mathcal{V}}\sum_q V(q)\mathcal{G}(k+q) \tag{24.23}$$

Notice that we have dropped $e^{iq_n 0^+}$ in the bosonic summation $\sum_{iq_n}$ (why?).

The sign of the wave vector q, or direction of the arrow in the diagram, must be decided once for each diagram but this choice is arbitrary since the potential is invariant under the interchange of coordinates, as mentioned above. This is illustrated in Ref. Fig. 37-6. Note that here the $q=0$ contribution in the Hartree (socalled tadpole diagram) is cancelled by the positive ion background since $\mathcal{G}(\bar{2}-\bar{2}^+)$ is just the electron density,

$$\begin{aligned}
\mathcal{G}(\bar{2}-\bar{2}^+) &= \frac{1}{V}\sum_{\mathbf{k}} T\sum_{n=-\infty}^{\infty} e^{-ik_n 0^-}\mathcal{G}_\sigma(k) \\
&= \frac{1}{V}\sum_{\mathbf{k}} \mathcal{G}_\sigma(\mathbf{k};\tau=0^-) \\
&= \frac{1}{V}\sum_{\mathbf{k}} f\left(\zeta_{\mathbf{k}}\right) \\
&= \frac{N}{V} = n
\end{aligned} \tag{24.24}$$

25 Feynman Rules for two-body interactions

Perturbation theory can also be obtained simply by using Wick's theorem. This generates an infinite set of terms. Diagrams are a simple way to represent and remember the various terms that are generated. Furthermore, associating specific algebraic quantities and integration rules with the various pieces of the diagrams, allows one to write the explicit expression for a given term without returning to Wick's theorem. In case of doubt though, Wick's theorem is what should be used. The specific rules will depend on the type of interaction considered.

25.1 Hamiltonian and notation

The Hamiltonian we considered is the same as before, the

$$\begin{aligned}
K &= H - \mu N = H_0 + V + V_n - \mu N \\
H_0 &= \frac{1}{2m}\sum_{\sigma_1}\int d\mathbf{x}_1 \boldsymbol{\nabla}\psi^\dagger_{\sigma_1}(\mathbf{x}_1)\cdot\boldsymbol{\nabla}\psi_{\sigma_1}(\mathbf{x}_1) \\
V &= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_1)\psi^\dagger_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1) \\
V_n &= -\sum_{\sigma_1}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_2)n
\end{aligned} \tag{25.1}$$

with Coulomb potential

$$v\left(\mathbf{x}_1-\mathbf{x}_2\right)=\frac{e^2}{\left|\mathbf{x}_1-\mathbf{x}_2\right|} \tag{25.2}$$

we will use the following notations

$$V(1,2)=V_{\sigma_1,\sigma_2}\left(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2\right)=\frac{e^2}{\left|\mathbf{x}_1-\mathbf{x}_2\right|}\delta\left(\tau_1-\tau_2\right) \tag{25.3}$$

$$\begin{gathered}\int_1=\int_0^\beta d\tau_1\int d\mathbf{x}_1\sum_{\sigma_1=\pm1}\\ \psi(1)=\psi_{I\sigma_1}\left(\mathbf{x}_1,\tau_1\right)\end{gathered} \tag{25.4}$$

Let us say we want to compute the one-body Green's function in the interaction representation

$$\begin{aligned}\mathcal{G}_{\sigma_1\sigma_2}\left(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2\right)&=-\left\langle T_\tau\psi_H(\mathbf{x}_1,\tau_1)\psi_H^\dagger(\mathbf{x}_2,\tau_2)\right\rangle\\&=-\frac{\left\langle\mathcal{T}_\tau\left[U_I(\beta,0)\psi_H(\mathbf{x}_1,\tau_1)\psi_H^\dagger(\mathbf{x}_2,\tau_2)\right]\right\rangle_0}{\left\langle U_I(\beta,0)\right\rangle_0}\\&=-\left\langle\mathcal{T}_\tau\left[U_I(\beta,0)\psi_H(\mathbf{x}_1,\tau_1)\psi_H^\dagger(\mathbf{x}_2,\tau_2)\right]\right\rangle_{0c}\end{aligned} \tag{25.5}$$

where in the last step we used linked cluster theorem, and $\langle...\rangle_{0c}$ means we are only summing over connected terms. The evolution operator is

$$\begin{aligned}U_I(\beta,0)&=\mathcal{T}_\tau\exp\left\{-\int_0^\beta d\tau_1V_I\left(\tau_1\right)\right\}\\&=\mathcal{T}_\tau\exp\left\{-\frac{1}{2}\sum_{\sigma_1,\sigma_2}\int_0^\beta d\tau_1\int d\mathbf{x}_1\int d\mathbf{x}_2v\left(\mathbf{x}_1-\mathbf{x}_2\right)\psi_{\sigma_1}^\dagger\left(\mathbf{x}_1\right)\psi_{\sigma_2}^\dagger\left(\mathbf{x}_2\right)\psi_{\sigma_2}\left(\mathbf{x}_2\right)\psi_{\sigma_1}\left(\mathbf{x}_1\right)\right\}\\&=\mathcal{T}_\tau\exp\left\{-\frac{1}{2}\int_1\int_2V(1,2)\psi^\dagger(1)\psi^\dagger(2)\psi(2)\psi(1)\right\}\end{aligned} \tag{25.6}$$

25.2 Position space Feynman Rules

We start with a Taylor expansion of U_I

$$\begin{aligned}\mathcal{G}(1,2)&=-\left\langle\mathcal{T}_\tau\left[U_I(\beta,0)\psi(1)\psi^\dagger(2)\right]\right\rangle_{0c}\\&=-\sum_{n=0}^\infty\frac{1}{n!}\left\langle\mathcal{T}_\tau\left[\left(-\frac{1}{2}\int_1\int_2V(1,2)\psi^\dagger(1)\psi^\dagger(2)\psi(2)\psi(1)\right)^n\psi(1)\psi^\dagger(2)\right]\right\rangle_{0c}\end{aligned} \tag{25.7}$$

it suffices to apply Wick's theorem to evaluate this to an order n. We will do so systematically, which will be summarized by Feynman Rules. We will first state the rules and then justify it by Wick's theorem.

The Rules are

1. Draw two "external" points, labeled 1 and 2 and n dotted lines with two ends (vertices). Join all external points and vertices with lines, so that each internal vertex has a line that comes in and a line that comes out while one line comes in external point 2 and one line comes out of point 1. The resulting diagrams must be
   (a) Connected
   (b) Topologically distinct
2. Label all the vertices of interaction lines with dummy variables representing space, imaginary time and spin.
3. Associate a factor $\mathcal{G}(1,2)$ to every line going from a vertex or external point labeled 1 to a vertex or external point labeled 2.
4. Associate a factor $V(1',2')$ to every dotted line between a vertex labeled $1'$ and a vertex labeled $2'$.

5. Integrate on all internal space, imaginary time and spin indices associated with interaction vertices. Notice that spin is conserved at each interaction vertex.

6. Associate a factor $(-1)^n(-1)^F$ to every diagram. The parameter n is the order of the diagram while F is the number of closed fermion loops.

7. Associate to every fermion line joining two of the vertices of the same interaction line the factor

$$\begin{aligned} V(1,2)\mathcal{G}(1,2) &\equiv V(1,2)\mathcal{G}\left(1,2^+\right) \\ &\equiv V(1,2)\mathcal{G}_{\sigma_1,\sigma_2}\left(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_1^+\right) \end{aligned} \tag{25.8}$$

This last rule must be added because otherwise the rules given before are ambiguous since the Coulomb potential is instantaneous (at equal time) and Green's functions have two possible values at equal time. So it is necessary to specify which of these values it takes. The chosen order is discussed further in the following subsection.

Now we justify the Feynman rules. First write

$$\begin{aligned} \mathcal{G}(1,2) &= \sum_{n=0}^{\infty}\mathcal{G}^{(n)}(1,2) \\ \mathcal{G}^{(n)}(1,2) &= -\frac{(-1)^n}{n!2^n}\left\langle\mathcal{T}_\tau\left[U^n\psi(1)\psi^\dagger(2)\right]\right\rangle_{0c} \\ U &\equiv V(\bar{1},\bar{2})\psi^\dagger(\bar{1})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(\bar{1}) \\ &= \int_1\int_2 V(1,2)\psi^\dagger(1)\psi^\dagger(2)\psi(2)\psi(1) \end{aligned} \tag{25.9}$$

For a given order n, to evaluate $\mathcal{G}^{(n)}$, we use Wick's theorem to break down the time-ordered product $\left\langle\mathcal{T}_\tau\left[U^n\psi(1)\psi^\dagger(2)\right]\right\rangle_{0c}$. This is of the form $\left\langle\mathcal{T}\left(V\psi^\dagger\psi^\dagger\psi\psi\right)^n\psi\psi^\dagger\right\rangle_{0c}$. We now associate each annilation/creation field with an open/closed dot and draw them on a diagram. Index every dot by its coordinates (internal vertices have dummy coordinates $\bar{1},\bar{2}$... to be integrated over later). Notice that each U brings out $V(\bar{1},\bar{2})\psi^\dagger(\bar{1})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(\bar{1})$: open circle at 1,2 + a closed circle at 1,2 + interaction between (1,2). The interaction $V(\bar{1},\bar{2})$ is represented by a dotted line joining $1,2$ and is not directed since $V(\bar{1},\bar{2}) = V(\bar{2},\bar{1})$[5]. Wick's theorem states that we should sum over all fully connected pairs where each ψ is joined with another $\psi^\dagger$ to form a Green's function. Translating into the diagrammatic language, each open dot should be joined with a closed dot, and since the order matters, the line joining them will be directed from $\psi(1)$ to $\psi^\dagger(2)$, this will be associated with $\left\langle\mathcal{T}\psi(1)\psi^\dagger(2)\right\rangle_{0c}$. The diagrams also need to be connected, as required by the index c. Each combination then is an indexed Feynman diagram with two external dots and of order n. We have $F_{i,2,n} = \{F^1_{i,2,n}, F^2_{i,2,n}, ..., F^r_{i,2,n}\}$.

$$\begin{aligned} \mathcal{G}^{(n)}(1,2) &= \sum_r F^r_{i,2,n} \\ F^r_{i,2,n} &= -\frac{(-1)^n(-1)^F}{n!2^n}\left\langle\mathcal{T}_\tau\psi(.)\psi^\dagger(.)\right\rangle_0 ... \left\langle\mathcal{T}_\tau\psi(.)\psi^\dagger(.)\right\rangle_0 \\ &= \frac{(-1)^n(-1)^F}{n!2^n}V...V\mathcal{G}_0(\cdot,\cdot)...\mathcal{G}_0(\cdot,\cdot) \end{aligned} \tag{25.10}$$

with some particular order of indices prescribed by r. The sign is correct since there are always an odd number of Green's functions. The sign $(-1)^F$ comes from permuting the fields to a the order given above. We will show later that F is equal to the number of fermionic loops.

A further simplification comes from the fact that there is a huge number of degeneracies among the diagrams, since $\left\langle\mathcal{T}_\tau\left[U^n\psi(1)\psi^\dagger(2)\right]\right\rangle_{0c}$ is unchanged when we exchange two indices $\bar{1}\leftrightarrow\bar{2}$ in $V(\bar{1},\bar{2})\psi^\dagger(\bar{1})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(\bar{1})$ or when we exchange two pairs of indices from two different U: $\bar{1},\bar{2}\leftrightarrow\bar{3},\bar{4}$ in $V(\bar{1},\bar{2})\psi^\dagger(\bar{1})\psi^\dagger(\bar{2})\psi(\bar{2})\psi(\bar{1})V(\bar{3},\bar{4})\psi^\dagger(\bar{3})\psi^\dagger(\bar{4})\psi(\bar{4})\psi(\bar{3})$. This means that we can use the same diagram to represent cases whose only difference come from permutations between a pair of two internal vertices or among different pairs of vertices. Each diagram now have degeneracy $2^n n!$. We define $F^r_{2,n} \equiv 2^n n! F^r_{i,2,n}$, so that

$$\begin{aligned} \mathcal{G}^{(n)}(1,2) &= \sum_r F^r_{2,n} \\ F^r_{2,n} &= (-1)^n(-1)^F V..V\mathcal{G}_0(\cdot,\cdot)...\mathcal{G}_0(\cdot,\cdot) \end{aligned} \tag{25.11}$$

[5]When discussing the rules, I assume $\bar{1},\bar{2},...$ to be summed over at the very end. So far all the relations are not summed over.

To find out what F is, start with the origional order $\left\langle \mathcal{T}\left(V\psi^\dagger\psi^\dagger\psi\psi\right)^n\psi\psi^\dagger\right\rangle_{0c}$, to simplify the notation, I write the indices only and focus on the signs

$$\left(\bar{1}^\dagger\bar{2}^\dagger\bar{2}\bar{1}\right)\left(\bar{3}^\dagger\bar{4}^\dagger\bar{4}\bar{3}\right)...12^\dagger=\left(\bar{1}^\dagger\bar{1}\right)\left(\bar{2}^\dagger\bar{2}\right)\left(\bar{3}^\dagger\bar{3}\right)\left(\bar{4}^\dagger\bar{4}\right)...(2\bar{n}^\dagger 2\bar{n})\left(12^\dagger\right) \tag{25.12}$$

So if the indices are joined like RHS in pairs, we will have no sign change[6]. Each fermionic line is either in the main branch[7] joining 1 and $2^\dagger$ or in a fermionic loop. Starting from $\left(12^\dagger\right)$, we can add an arbitrary number of points in to form the main branch without introducing any sign

$$\begin{aligned}\left(\bar{1}^\dagger\bar{1}\right)\left(12^\dagger\right)&=\left(1\bar{1}^\dagger\bar{1}2^\dagger\right)\\ \left(\bar{1}^\dagger\bar{1}\right)\left(\bar{2}^\dagger\bar{2}\right)\left(12^\dagger\right)&=\left(1\bar{1}^\dagger\bar{1}\bar{2}^\dagger\bar{2}2^\dagger\right)\end{aligned} \tag{25.13}$$

to form fermionic loops, just move the last operator to the forefront, passing through an odd number of fields

$$\begin{aligned}\left(\bar{1}^\dagger\bar{1}\right)&=-\left(\bar{1}\bar{1}^\dagger\right)\\ \left(\bar{1}^\dagger\bar{1}\right)\left(\bar{2}^\dagger\bar{2}\right)&=-\left(\bar{2}\bar{1}^\dagger\bar{1}\bar{2}^\dagger\right)\\ \left(\bar{1}^\dagger\bar{1}\right)\left(\bar{2}^\dagger\bar{2}\right)\left(\bar{3}^\dagger\bar{3}\right)&=-\left(\bar{3}\bar{1}^\dagger\bar{1}\bar{2}^\dagger\bar{2}\bar{3}^\dagger\right)\end{aligned} \tag{25.14}$$

so each fermionic loop introduces a sign change. The overall sign coming from the permutation of fields will be given by the total number of fermionic loops F in a given diagram.

A remark is in order concerning spin. In a diagram without loops, as in Ref. Fig.(38- 6), there is a single spin label running from one end of the diagram to the other. Every time we introduce a loop, there is now a sum over the spin of the fermion in the loop. In the special case where $V(1,2)$ is independent of the spins at the vertices 1 and 2, as is the case for Coulomb interactions, then it is possible to simply disregard spin and add the rule that there is a factor of 2 associated with every fermion loop.

25.2.1 Example: $n=1$ in position space

Take the first order terms

$$\begin{aligned}\mathcal{G}^{(1)}(1,2)&=\sum_r F^r_{2,1}\\ F^r_{2,1}&=(-1)^1(-1)^F V..V\mathcal{G}_0(\cdot,\cdot)...\mathcal{G}_0(\cdot,\cdot)\end{aligned} \tag{25.15}$$

we have one interaction and two external points. There are two Feynman diagrams, listed as C,E in ,Ref. Fig.38-3. Following all the rules, we have

$$\begin{aligned}F^C_{2,1}&=(-1)^1(-1)^1V(\bar{1},\bar{2})\mathcal{G}_0(1,\bar{1})\mathcal{G}_0(\bar{1},2)\mathcal{G}_0(\bar{2},\bar{2}^+)\\ &=\int_{1'}\int_{2'}V(1',2')\mathcal{G}_0(1,1')\mathcal{G}_0(1',2)\mathcal{G}_0(2',2'^+)\end{aligned} \tag{25.16}$$

$$\begin{aligned}F^E_{2,1}&=(-1)^1(-1)^0V(\bar{1},\bar{2})\mathcal{G}_0(1,\bar{1})\mathcal{G}_0(\bar{1},\bar{2}^+)\mathcal{G}_0(\bar{2},2)\\ &=-\int_{1'}\int_{2'}V(1',2')\mathcal{G}_0(1,1')\mathcal{G}_0(1',2'^+)\mathcal{G}_0(2',2)\end{aligned} \tag{25.17}$$

25.3 Momentum Space Feynman Rules

Feynman's rule in position space are written as spatial integrals and V, $\mathcal{G}$ in position space. If the system is translationally invariant and spin-rotationally invariant, we can then write $\mathcal{G}_0(1,2)=\mathcal{G}_0(1-2)$. Together with the fact that $V(1,2)=V(1-2)$, the diagrams now look like (as an simple example)[8]

$$\begin{aligned}F^C_{2,1}&=\sum_{\sigma_{1'}\sigma_{2'}}\int_{1'}\int_{2'}V_{\sigma_{1'}\sigma_{2'}}(1'-2')\mathcal{G}_{\sigma_1\sigma_{1'}}(1-1')\mathcal{G}_{\sigma_{1'}\sigma_2}(1'-2)\mathcal{G}_{\sigma_{2'}\sigma_{2'}}(2'-2'^+)\\ F^E_{2,1}&=-\sum_{\sigma_{1'}\sigma_{2'}}\int_{1'}\int_{2'}V_{\sigma_{1'}\sigma_{2'}}(1'-2')\mathcal{G}_{\sigma_1\sigma_{1'}}(1-1')\mathcal{G}_{\sigma_{1'}\sigma_{2'}}(1'-2'^+)\mathcal{G}_{\sigma_{2'}\sigma_2}(2'-2)\end{aligned} \tag{25.18}$$

[6]Actually, this diagram would be disconnected so it should not be counted. Nevertheless, it helps us find out the sign

[7]The fermionic line between external points

[8]Here $\mathcal{G}=\mathcal{G}_0$, we dropped the lower index because we will add back the spin index σ below. This should not result in any confusion for now.

It is advantageous to write these spatial integrals into momentum-integrals, to do so we introduce the Fourier Transform

$$\begin{aligned}
\mathcal{G}_\sigma(k) &= \int_1 e^{-ik(x_1-x_2)}\mathcal{G}_\sigma(1-2) \\
\mathcal{G}_\sigma(1-2) &= \sum_k e^{+ik(x_1-x_2)}\mathcal{G}_\sigma(k) \\
V_{\sigma,\sigma'}(q) &= \int_1 e^{-iq(x_1-x_2)}V_{\sigma,\sigma'}(1-2) \\
V_{\sigma,\sigma'}(1-2) &= \sum_q e^{+iq(x_1-x_2)}V_{\sigma,\sigma'}(q)
\end{aligned} \tag{25.19}$$

where $\mathcal{G}_\sigma$ now contain a single spin index, this is possible due to spin-rotational invariance $\mathcal{G}_{\sigma_1\sigma_2} = \delta_{\sigma_1,\sigma_2}\mathcal{G}$. We have used short-hand notation[9]

$$\begin{aligned}
\int_1 &\equiv \int d\mathbf{x}_1 \int_0^\beta d\tau_1 \\
\sum_k &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} T\sum_{ik_n} \\
k &= (\mathbf{k}, -ik_n)\,, \quad \text{fermionic} \\
q &= (\mathbf{q}, -iq_n)\,, \quad \text{bosonic} \\
x &= (\mathbf{x}, \tau) \\
\delta(q) &= (2\pi)^3\delta(\mathbf{q})\beta\delta_{q_n} \\
\delta(x) &= \delta(\mathbf{x})\delta(\tau) \\
\frac{1}{V}\sum_{\mathbf{k}} &\leftrightarrow \int \frac{d^3\mathbf{k}}{(2\pi)^3}, \quad \text{discrete-to-continuous} \\
e^{-ikx} &= e^{-i\mathbf{k}\cdot\mathbf{x}}e^{ik_n\tau} \\
\mathcal{F} &= \int_x e^{-ikx} \\
\mathcal{F}^{-1} &= \sum_k e^{ikx}
\end{aligned} \tag{25.20}$$

in full-form

$$\begin{aligned}
\mathcal{G}_\sigma(k) &= \int d\left(\mathbf{x}_1-\mathbf{x}_2\right)\int_0^\beta d\left(\tau_1-\tau_2\right)e^{-i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{ik_n(\tau_1-\tau_2)}\mathcal{G}_\sigma(1-2) \\
\mathcal{G}_\sigma(1-2) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3}T\sum_{n=-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{-ik_n(\tau_1-\tau_2)}\mathcal{G}_\sigma(k) \\
V_{\sigma,\sigma'}(q) &= \int d\left(\mathbf{x}_1-\mathbf{x}_2\right)\int_0^\beta d\left(\tau_1-\tau_2\right)e^{-i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{iq_n(\tau_1-\tau_2)}V_{\sigma,\sigma'}(1-2) \\
V_{\sigma,\sigma'}(1-2) &= \int \frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{n=-\infty}^{\infty} e^{i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)}e^{-iq_n(\tau_1-\tau_2)}V_{\sigma,\sigma'}(q)
\end{aligned} \tag{25.21}$$

[9]Notice that $\int_1$ does not include the spin summation $\sum_{\sigma_1=\pm1}$.

We can in fact evaluate $V(q)$ explicitly for Coulomb interaction

$$\begin{aligned} V(q) &= \int d\mathbf{x} \int_0^\beta d\tau e^{-i\mathbf{q}\cdot\mathbf{x}} e^{iq_n\tau} V(\mathbf{x},\tau) \\ &= \int d\mathbf{x} \int_0^\beta d\tau e^{-i\mathbf{q}\cdot\mathbf{x}} e^{iq_n\tau} \frac{e^2}{|\mathbf{x}|}\delta(\tau) \\ &= e^2 \int d\mathbf{x} \frac{e^{-i\mathbf{q}\cdot\mathbf{x}}}{|\mathbf{x}|} \\ &= \frac{4\pi e^2}{q^2} \end{aligned} \tag{25.22}$$

Again we have explicitly written the spin indices even if $V_{\sigma,\sigma'}(1-2)$ is independent of spin. The spin σ is the same as the spin of the two propagators attaching to the vertex 1 while σ' is the same as the spin of the two propagators attaching to the vertex 2.

Now we rewrite $F^C_{2,1}$:

$$\begin{aligned} F^C_{2,1} &= \sum_{\sigma_{1'}\sigma_{2'}} \int_{1'}\int_{2'} V_{\sigma_{1'}\sigma_{2'}}(1'-2')\mathcal{G}_{\sigma_1\sigma_{1'}}(1-1')\mathcal{G}_{\sigma_{1'}\sigma_2}(1'-2)\mathcal{G}_{\sigma_{2'}\sigma_{2'}}(2'-2'^+) \\ &= \left(\delta_{\sigma_1\sigma_2} 2\mathcal{G}(0^-)\right) \int_{1'}\int_{2'} V_{\sigma_1\sigma_{2'}}(1'-2')\mathcal{G}_{\sigma_1}(1-1')\mathcal{G}_{\sigma_1}(1'-2) \\ &= \left(\delta_{\sigma_1\sigma_2} 2\mathcal{G}(0^-)\right) \int_{1'}\int_{2'} \times \\ &\quad \left(\sum_q V_{\sigma_1\sigma_{2'}}(q) e^{+iq(x_{1'}-x_{2'})}\right)\left(\sum_{k_1} \mathcal{G}_{\sigma_1}(k_1) e^{+ik_1(x_1-x_{1'})}\right)\left(\sum_{k_2} \mathcal{G}_{\sigma_1}(k_2) e^{+ik_2(x_{1'}-x_2)}\right) \\ &= \left(\delta_{\sigma_1\sigma_2} 2\mathcal{G}(0^-)\right) \sum_{q,k_1,k_2} V_{\sigma_1\sigma_{2'}}(q)\mathcal{G}_{\sigma_1}(k_1)\mathcal{G}_{\sigma_1}(k_2)\times \\ &\quad \int_{1'}\int_{2'} e^{+iq(x_{1'}-x_{2'})} e^{+ik_1(x_1-x_{1'})} e^{+ik_2(x_{1'}-x_2)} \end{aligned} \tag{25.23}$$

the last integral can be separated by vertices

$$\begin{aligned} \int_{1'}\int_{2'} e^{+iq(x_{1'}-x_{2'})} e^{+ik_1(x_1-x_{1'})} e^{+ik_2(x_{1'}-x_2)} &= e^{ik_1(x_1-x_2)} \int_{1'} e^{ix_{1'}(q-k_1+k_2)} \int_{2'} e^{ix_{2'}q} \\ &= e^{ik_1(x_1-x_2)}\delta(q-k_1+k_2)\delta(q) \end{aligned} \tag{25.24}$$

this gives

$$F^C_{2,1}(1-2) = \sum_{k_1} e^{ik_1(x_1-x_2)} \left(\delta_{\sigma_1\sigma_2} 2\mathcal{G}(2'-2'^+)\right) V(q=0)\mathcal{G}_{\sigma_1}(k_1)\mathcal{G}_{\sigma_1}(k_1) \tag{25.25}$$

this automatically give the Fourier Transform

$$F^C_{2,1}(k) = \left(\delta_{\sigma_1\sigma_2} 2\mathcal{G}(0^-)\right) V(q=0)\mathcal{G}_{\sigma_1}(k)\mathcal{G}_{\sigma_1}(k) \tag{25.26}$$

For a more general Feynman diagram in position space, we will do the Fourier Transform for each Green's and interaction, each of which will have some momentum k or q. At each vertex we have two fermionic lines and one interaction line connected to it, and correspondingly

$$\int_{1'} e^{ix_{1'}(q-k_1+k_2)} = \delta(q-k_1+k_2) \tag{25.27}$$

so the three lines connected at each vertex must conserve momentum. Using all the momentum conservation, we should have an additional factor $e^{ik(x_1-x_2)}$, which will give the Fourier Transform of the $F(1-2) \to F(k)$, so we always have an overall momentum k. All factors e^{ikx} will be integrated over, either as momentum conservation or as the final Fourier Transform. There may be some undetermined momentum, correspondingly there will be a summation $\sum_k$ or $\sum_q$.

The Feynman rules for Green's function in momentum space thus read as follows.

1. For a term of order n, draw all connected, topologically distinct diagrams with n interaction lines and $2n+1$ oriented propagator lines, taking into account that at every interaction vertex one line comes in and one line comes out.

2. Assign a direction to the interaction lines. Assign also a wave number and a discrete frequency to each propagator and interaction line, conserving momentum and Matsubara frequency at each vertex.

3. To each propagator line, assign
$$\mathcal{G}^0_\sigma(k) = \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{25.28}$$
(We have to remember that the propagator is independent of spin but still carries a spin label that is summed over.)

4. To each interaction line, associate a factor $V_{\sigma,\sigma'}(q)$, with iq_n a bosonic Matsubara frequency. Note that each of the spin labels is associated with one of the vertices and that it is the same as the spin of the fermion lines attached to it.

5. Perform an integral over wave vector and a sum over Matsubara frequency, namely $\sum_k \equiv \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{n=-\infty}^{\infty}$ for each momentum and frequency that is not fixed by conservation at the vertex.

6. Sum over all spin indices that are not fixed by conservation of spin.

7. Associate a factor $(-1)^n(-1)^F$ where F is the number of closed Fermion loops to every diagram of order n.

8. For Green's functions whose two ends are on the same interaction line, associate a convergence factor $e^{ik_n 0^+}$ before doing the sum over Matsubara frequency k_n. (This corresponds to the choice $\mathcal{G}(1, 2^+)$ in the position-space rules above).

25.3.1 Example: $n = 1$ in momentum space

We now directly write down the Feynman diagrams in momentum space for $F^C_{2,1}, F^E_{2,1}$:

$$\begin{aligned} F^C_{2,1}(k) &= (-1)^1(-1)^1 \sum_{\sigma'} \mathcal{G}_{0\sigma}(k)\mathcal{G}_{0\sigma}(k)V_{\sigma\sigma'}(q=0)\mathcal{G}_{0\sigma'}(0^-) \\ &= \mathcal{G}_{0\sigma}(k)\mathcal{G}_{0\sigma}(k)V(q=0)\left(2\mathcal{G}_0(0^-)\right) \end{aligned} \tag{25.29}$$

$$\begin{aligned} F^E_{2,1}(k) &= (-1)^1(-1)^0 \sum_{q} \mathcal{G}_{0\sigma}(k)\mathcal{G}_{0\sigma}(k)\mathcal{G}_{0\sigma}(k-q)V_{\sigma\sigma}(q) \\ &= -\int \frac{d^3\mathbf{q}}{(2\pi)^3} T \sum_{q_n} \mathcal{G}_{0\sigma}(k)\mathcal{G}_{0\sigma}(k)\mathcal{G}_{0\sigma}(k-q)V_{\sigma\sigma}(q) \end{aligned} \tag{25.30}$$

25.4 Feynman rules for the irreducible self-energy

Start with Dyson's equation
$$\mathcal{G}_\sigma(k) = \mathcal{G}^0_\sigma(k) + \mathcal{G}^0_\sigma(k)\Sigma_\sigma(k)\mathcal{G}_\sigma(k) \tag{25.31}$$
or, since every quantity is now spin-independent, we can treat them as scalars and write
$$\mathcal{G}_\sigma(k) = \frac{1}{[\mathcal{G}^0_\sigma(k)]^{-1} - \Sigma_\sigma(k)} \tag{25.32}$$
This is the so-called Dyson equation. The iterative solution of this equation
$$\mathcal{G}_\sigma(k) = \mathcal{G}^0_\sigma(k) + \mathcal{G}^0_\sigma(k)\Sigma_\sigma(k)\mathcal{G}^0_\sigma(k) + \mathcal{G}^0_\sigma(k)\Sigma_\sigma(k)\mathcal{G}^0_\sigma(k)\Sigma_\sigma(k)\mathcal{G}^0_\sigma(k) + \dots \tag{25.33}$$
clearly shows that all diagrams that can be cut in two pieces by cutting one fermion line $\mathcal{G}^0_\sigma(k)$ will automatically be generated by Dyson's equation. In other words, we define the one-particle irreducible self-energy by the set of diagrams that are generated by Feynman's rules for the propagator but that, after truncating the two external fermion lines, cannot be cut in two disjoint pieces by cutting a $\mathcal{G}^0_\sigma(k)$ line. As an example, the diagram on the left of

Ref. Fig.(38-10) is **one-particle reducible** and hence does not belong to the one-particle irreducible self-energy, but the two diagrams on the right of this figure do.

Terminology: To be shorter, one sometimes refers to the one-particle irreducible self-energy using the term proper self-energy. In almost everything that follows, we will be even more concise and refer simply to the self-energy. We will mean one-particle irreducible self-energy. The other definitions that one can give for the self-energy do not have much interest in practice.

25.4.1 Is self-energy function retarded (?)

It should be noticed that when we analytically continue $ik_n \to z$ in Dyson's equation

$$\begin{aligned} \mathcal{G}_\sigma(\mathbf{k}, ik_n) &= \mathcal{G}^0_\sigma(\mathbf{k}, ik_n) + \mathcal{G}^0_\sigma(\mathbf{k}, ik_n)\Sigma_\sigma(\mathbf{k}, ik_n)\mathcal{G}_\sigma(\mathbf{k}, ik_n) \\ G(\mathbf{k}, z) &= G_0(\mathbf{k}, z) + G_0(\mathbf{k}, z)\Sigma(\mathbf{k}, z)G(\mathbf{k}, z) \end{aligned} \tag{25.34}$$

to go to retarded representation, we need to show that $\Sigma(\mathbf{k}, z)$ is analytic in the upper-half plane. Which would lead to the retarded self-energy

$$\Sigma^R(\mathbf{k}, \omega) \equiv \Sigma(\mathbf{k}, ik_n = \omega + i\eta) \tag{25.35}$$

to show the analyticity of $\Sigma(\mathbf{k}, z)$, we use the RPA order self energy as an example (this will be calculated later)

$$\begin{aligned} \Sigma^{(2)}(\mathbf{k}, ik_n) &= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} T \sum_{ik'_n} \frac{V_{\mathbf{k}'-\mathbf{k}}}{\varepsilon_L\left(\mathbf{k}'-\mathbf{k}, ik'_n - ik_n\right)/\varepsilon_0} \mathcal{G}\left(\mathbf{k}', ik'_n\right) e^{ik'_n\eta} \\ \Sigma^{(2)}(\mathbf{k}, z) &= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} T \sum_{ik'_n} \frac{V_{\mathbf{k}'-\mathbf{k}}}{\varepsilon_L\left(\mathbf{k}'-\mathbf{k}, ik'_n - z\right)/\varepsilon_0} \mathcal{G}\left(\mathbf{k}', ik'_n\right) e^{ik'_n\eta} \end{aligned} \tag{25.36}$$

when $z'' > 0$, the factor

25.5 Feynman diagrams and the Pauli exclusion principle

Since operators can be anticommuted at will in a time-ordered product at the price of a simple sign change, it is clear that whenever there are two destruction operators or two creation operators for the same state, the contraction should vanish. This is just the Pauli exclusion principle.

On the other hand, if we look at a self-energy diagram like the middle one in Ref. Fig.(38-10) there are contributions that violate the Pauli exclusion principle. The diagram has value

$$\sum_{\sigma'} \sum_{k',q} \mathcal{G}_\sigma(k-q)\mathcal{G}_{\sigma'}(k')\mathcal{G}_{\sigma'}(k'+q)V_{\sigma\sigma'}(q)V_{\sigma\sigma'}(q) \tag{25.37}$$

When we perform the sum over wave vectors and over spins in the closed loop, the right-going line $\mathcal{G}_{\sigma'}(k'+q)$ will eventually be identical as $\mathcal{G}_\sigma(k-q)$ when $\mathbf{k}'+\mathbf{q} = \mathbf{k}-\mathbf{q}$ and $\sigma' = \sigma$. We then have two fermion lines in the same state attached to the same interaction line.

If we transform $\mathcal{G}(\mathbf{k}, ik_n) \to \mathcal{G}(\mathbf{k}, \tau)$ back to imaginary time but stay in momentum space, each interaction $V(1,2) \propto \delta(\tau_1 - \tau_2)$, so the two identical fermionic lines now start at the same time. This means we have two identical creation operators $\psi^\dagger(\mathbf{k}, \tau_1)\psi^\dagger(\mathbf{k}, \tau_1)$ and similarly $\psi(\mathbf{k}, \tau_2)\psi(\mathbf{k}, \tau_2)$ at the other end. This contribution should be absent if the Pauli exclusion principle is satisfied.

What happens in diagrams is that this contribution is exactly canceled by the diagram where we have exchanged the two right-going lines, in other words the last diagram on this figure. Indeed, this diagram has opposite sign, since it has one less fermion loop, and the special case $\mathbf{q} = \mathbf{q}'$ precisely cancels the unwanted contribution from the middle graph in Ref. Fig.(38-10).

The important lesson of this is that unless we include all the exchange graphs, there is no guarantee in diagrammatic techniques that the Pauli exclusion principle will be satisfied. We are tempted to say that this does not matter so much because it is a set of **measure zero** but in fact we will see practical cases in short-range models where certain approximate methods do **unacceptable harm** to the Pauli exclusion principle.

26 Particle-hole Excitations in the free electron gas and the Lindhard Function

In this section we look at collective modes. The main physical quantity we want to compute and understand for collective modes of the electron gas is the longitudinal dielectric constant. We know from linear response theory that the longitudinal dielectric constant is given by the retarded density-density correlation

$$\frac{\varepsilon_0}{\epsilon^L(\mathbf{q},\omega)} = 1 - \frac{1}{\varepsilon_0 q^2}\chi^R_{\rho\rho}(\mathbf{q},\omega) \tag{26.1}$$

The physical phenomenon of screening will manifest itself in the zero-frequency limit of the longitudinal dielectric constant $\epsilon^L(\mathbf{q},0)$. Interactions between electrons will be screened, hence it is important to know the dielectric constant. Plasma oscillations should come out from the finite frequency zeros of this same function $\epsilon^L(\mathbf{q},0)=0$.

We will start this section by a discussion of the **Lindhard function**, namely $\chi^R_{nn}(\mathbf{q},\omega)=\chi^R_{\rho\rho}(\mathbf{q},\omega)/e^2$ for the **free electron gas**. We will interpret the poles of this function. Then we introduce interactions with a simple physical discussion of **screening** and **plasma oscillations**. A diagrammatic calculation in the so-called **Random phase approximation** (RPA) will then allow us to recover in the appropriate limiting cases the phenomena of screening and of plasma oscillations.

It is noteworthy that even for the non-interacting electron gas, the density-density correlation function is not simply the product of two independent densities. Fundamentally, this is because even in the absence of interactions, the Pauli exclusion principle prohibits two electrons from being in the same state. This leads to correlations in the sense of quantum statistics. This is illustrated by Ref. Fig.(39-1) that shows that density excitation corresponds to the excitation of a particle-hole pair that is created and then destroyed in the same measurement process.

26.1 Definition and analytic continuation

Our plan is to evaluate the Matsubare response $\chi_{nn}(\mathbf{q},iq_n)$ and then obtain χ^R_{nn} through analytic continuation

$$\chi^R_{nn}(\mathbf{q},\omega) = \lim_{iq_n\to\omega+i\eta}\chi_{nn}(\mathbf{q},iq_n) \tag{26.2}$$

The Matsubare response in momentum-frequency space is

$$\begin{aligned}\chi_{nn}(\mathbf{q},iq_n) &= \int d^3\mathbf{r}e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\int_0^\beta d\tau e^{iq_n\tau}\left\langle T_\tau\left[\delta n(\mathbf{r},\tau)\delta n(\mathbf{r}',0)\right]\right\rangle \\ &= \frac{1}{\mathcal{V}}\int_0^\beta d\tau e^{iq_n\tau}\left\langle T_\tau\left[\delta n_{\mathbf{q}}(\tau)\delta n_{-\mathbf{q}}(0)\right]\right\rangle\end{aligned} \tag{26.3}$$

where the particle density operator and its momentum-space form is

$$\begin{aligned} n(\mathbf{r}) &\equiv \sum_\sigma \psi^\dagger_\sigma(\mathbf{r})\psi_\sigma(\mathbf{r}) \\ n_{\mathbf{q}} &\equiv \int d^3r\mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}}n(\mathbf{r}) \\ &= \sum_\sigma\int d^3r\mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}}\psi^\dagger_\sigma(\mathbf{r})\psi_\sigma(\mathbf{r}) \\ &= \sum_\sigma\int d^3r\mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}}\frac{1}{\mathcal{V}}\sum_{\mathbf{q}_1\mathbf{q}_2}e^{-i\mathbf{q}_1\cdot\mathbf{r}}e^{+i\mathbf{q}_2\cdot\mathbf{r}}c^\dagger_{\mathbf{q}_1\sigma}c_{\mathbf{q}_2\sigma} \\ &= \sum_{\mathbf{q}_1\mathbf{q}_2\sigma}c^\dagger_{\mathbf{q}_1\sigma}c_{\mathbf{q}_2\sigma}\delta_{\mathbf{q}+\mathbf{q}_1-\mathbf{q}_2} \\ &= \sum_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}\end{aligned} \tag{26.4}$$

Notice that

$$[\delta n_{\mathbf{q}},\delta n_{\mathbf{p}}] = [n_{\mathbf{q}},n_{\mathbf{p}}] \tag{26.5}$$

so for χ^R_{nn}, we can choose either case. For χ_{nn}, we shall choose the $\delta n\delta n$ case for simplicity in the calculation. We have

$$\delta n(\mathbf{q},t) = n(\mathbf{q},t) - \langle n(\mathbf{q},t)\rangle = n(\mathbf{q},t) - n(2\pi)^3\delta(\mathbf{q}) \tag{26.6}$$

or in discrete notation

$$\begin{aligned}\langle n_{\mathbf{q}}(\tau)\rangle &= \sum_{\mathbf{k}\sigma}\left\langle c^{\dagger}_{\mathbf{k}\sigma}(\tau)c_{\mathbf{k}+\mathbf{q}\sigma}(\tau)\right\rangle \\ &= \sum_{\mathbf{k}\sigma} e^{-(\zeta_{\mathbf{k}+\mathbf{q}}-\zeta_{\mathbf{k}})\tau}\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}\right\rangle \\ &= \delta_{\mathbf{q}}\sum_{\mathbf{k}\sigma}\left\langle c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right\rangle \\ &= \delta_{\mathbf{q}}N\end{aligned} \tag{26.7}$$

and $\langle n_{\mathbf{q}}(t)\rangle = \langle n_{-\mathbf{q}}(t)\rangle = \langle n_{\mathbf{q}}\rangle = \delta_{\mathbf{q}}N$ in fermi gas.

$$\langle \delta n_{\mathbf{q}}(\tau)\delta n_{-\mathbf{q}}\rangle = \langle (n_{\mathbf{q}}(\tau)-\langle n_{\mathbf{q}}\rangle)\,(n_{-\mathbf{q}}-\langle n_{-\mathbf{q}}\rangle)\rangle = \langle n_{\mathbf{q}}(\tau)n_{-\mathbf{q}}\rangle - \langle n\rangle\,\langle n\rangle \tag{26.8}$$

26.2 Density response for fermi gas

The density response can be expressed in terms of Green's function starting either from the Feynman or from the functional derivative approach. We shall arrive at the result in both ways.

26.2.1 Feynman's way

We write

$$\begin{aligned}\chi_{nn}(1-2) &= \langle \mathcal{T}\delta n(1)\delta n(2)\rangle \\ &= \langle \mathcal{T}n(1)n(2)\rangle - \langle \mathcal{T}n(1)\rangle\,\langle \mathcal{T}n(2)\rangle \\ &= \sum_{\sigma,\sigma'}\left[\left\langle \mathcal{T}\psi^{\dagger}_{\sigma}(1)\psi_{\sigma}(1)\psi^{\dagger}_{\sigma'}(2)\psi_{\sigma'}(2)\right\rangle - \mathcal{G}_{\sigma}(1,1^{+})\mathcal{G}_{\sigma'}(2,2^{+})\right] \\ &= \sum_{\sigma,\sigma'}\left[\left\langle \mathcal{T}\psi^{\dagger}_{\sigma}(1)\psi_{\sigma}(1)\psi^{\dagger}_{\sigma'}(2)\psi_{\sigma'}(2)\right\rangle_{0c} - \mathcal{G}_{\sigma}(1,1^{+})\mathcal{G}_{\sigma'}(2,2^{+})\right]\end{aligned} \tag{26.9}$$

Now set $V=0$, using Wick's theorem, the second term is cancelled

$$\begin{aligned}\chi^{0}_{nn}(1-2) &= \sum_{\sigma,\sigma'}\left[\left\langle \mathcal{T}\psi^{\dagger}_{\sigma}(1)\psi_{\sigma}(1)\psi^{\dagger}_{\sigma'}(2)\psi_{\sigma'}(2)\right\rangle_{0c} - \mathcal{G}^{0}_{\sigma}(1,1^{+})\mathcal{G}^{0}_{\sigma'}(2,2^{+})\right] \\ &= -\sum_{\sigma}\mathcal{G}_{\sigma}(2,1)\mathcal{G}_{\sigma}(1,2)\end{aligned} \tag{26.10}$$

$$\chi^{0}_{nn}(q) = -\sum_{\sigma}\sum_{k}\mathcal{G}_{\sigma}(k+q)\mathcal{G}_{\sigma}(k) \tag{26.11}$$

$$= -\sum_{\sigma}\int\frac{d^{3}\mathbf{k}}{(2\pi)^{3}}T\sum_{ik_n}\mathcal{G}^{0}_{\sigma}(\mathbf{k}+\mathbf{q},ik_n+iq_n)\mathcal{G}^{0}_{\sigma}(\mathbf{k},ik_n) \tag{26.12}$$

This is the so-called **Lindhard function**. It is also known as the **bubble diagram**.

Although we have not derived Feynman rules for χ_{nn}, it is clear that the last expression could have been written down directly from the diagram Ref. Fig.(39-1) if we had followed trivial generalizations of our old rules. There is even an overall minus sign for the closed loop and a sum over wave vectors, Matsubara frequency and spin inside the loop since these are not determined by momentum conservation. Now that we have obtained the zeroth order term it is clear how to apply Feynman rules for the terms of the perturbation series. But this is the subject of another subsection below.

26.2.2 Schwinger's way

Start from the expression for the four-point correlation function and setting $\phi=0$, and setting the arguments $1234\to 11^{+}2^{+}2$, we have

$$\frac{\delta\mathcal{G}(1,1^{+})}{\delta\phi(2^{+},2)} = \left\langle \mathcal{T}_{\tau}\psi(1)\psi^{\dagger}(1^{+})\psi^{\dagger}(2^{+})\psi(2)\right\rangle + \mathcal{G}(1,1^{+})\mathcal{G}(2,2^{+}) \tag{26.13}$$

If we sum over the spins associated with point 1 and the spins associated with point 2 and recall that once we sum over spins, we have $\sum_{\sigma_1} \mathcal{G}\left(1-1^{+}\right)=n$ where n is the average density, then

$$\begin{aligned}
-\sum_{\sigma_1,\sigma_2} \frac{\delta \mathcal{G}\left(1,1^{+}\right)}{\delta \phi\left(2^{+},2\right)} &= \sum_{\sigma_1,\sigma_2} \left\langle T_\tau \psi^{\dagger}\left(1^{+}\right) \psi(1) \psi^{\dagger}\left(2^{+}\right) \psi(2)\right\rangle - n^2 \\
&= \sum_{\sigma_1,\sigma_2} \langle T_\tau n(1) n(2)\rangle - n^2 \\
&= \langle T_\tau (n(1)-n)(n(2)-n)\rangle \\
&= \chi_{nn}(1-2)
\end{aligned} \tag{26.14}$$

We use the generalized RPA equation

$$\begin{aligned}
\frac{\delta \mathcal{G}\left(1,1^{+}\right)_\phi}{\delta \phi\left(2^{+},2\right)} =& \mathcal{G}(1,2)_\phi \mathcal{G}(2,1)_\phi \\
&+ \mathcal{G}(1,\overline{5})_\phi \left(V(\overline{5}-\overline{7}) \frac{\delta \mathcal{G}(\overline{7},\overline{7})_\phi}{\delta \phi\left(2^{+},2\right)} \right) \mathcal{G}(\overline{5},1)_\phi \\
&- \mathcal{G}(1,\overline{5})_\phi \left(V(\overline{5}-\overline{6}) \frac{\delta \mathcal{G}(\overline{5},\overline{6})_\phi}{\delta \phi\left(2^{+},2\right)} \right) \mathcal{G}(\overline{6},1)_\phi
\end{aligned} \tag{26.15}$$

for non-interacting system $V=0$, so only the first term survives, we have

$$\begin{aligned}
\chi_{nn}(1-2) &= -\sum_{\sigma_1,\sigma_2} \delta_{\sigma_1\sigma_2}\delta_{\sigma_1\sigma_2} \mathcal{G}_{\sigma_1}(1,2) \mathcal{G}_{\sigma_1}(2,1) \\
&= -\sum_{\sigma} \mathcal{G}^0_{\sigma}(1,2) \mathcal{G}^0_{\sigma}(2,1)
\end{aligned} \tag{26.16}$$

Taking the Fourier transform and using the convolution theorem, one obtains,

$$\begin{aligned}
\chi^0_{nn}(q) &= \int_1 e^{-iqx} \chi_{nn}(1) \\
&= -\sum_{\sigma} \sum_{k_1 k_2} \mathcal{G}^0_{\sigma}(k_1) \mathcal{G}^0_{\sigma}(k_2) \int_1 e^{-iqx} e^{ik_1 x_1} e^{-ik_2 x_2} \\
&= -\sum_{\sigma} \sum_{k_1 k_2} \mathcal{G}^0_{\sigma}(k_1) \mathcal{G}^0_{\sigma}(k_2) \delta(-q+k_1-k_2) \\
&= -\sum_{\sigma} \sum_{k_2} \mathcal{G}^0_{\sigma}(k_2+q) \mathcal{G}^0_{\sigma}(k_2) \\
&= -\sum_{\sigma} \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{ik_n} \mathcal{G}^0_{\sigma}(\mathbf{k}+\mathbf{q}, ik_n+iq_n) \mathcal{G}^0_{\sigma}(\mathbf{k}, ik_n)
\end{aligned} \tag{26.17}$$

26.3 Lindhard function

To compute

$$\chi^0_{nn}\left(\mathbf{q}, iq_n\right) = -\sum_{\sigma} \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{ik_n} \mathcal{G}^0_{\sigma}\left(\mathbf{k}+\mathbf{q}, ik_n+iq_n\right) \mathcal{G}^0_{\sigma}\left(\mathbf{k}, ik_n\right) \tag{26.18}$$

the sums over Matsubara frequency should be performed first and they are easy to do. The technique is standard. First introduce the notation $\zeta_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}} - \mu$, and use partial fractions

$$\begin{aligned}
\mathcal{G}^0_{\sigma}\left(\mathbf{k}+\mathbf{q}, ik_n+iq_n\right) \mathcal{G}^0_{\sigma}\left(\mathbf{k}, ik_n\right) &= \frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}} \frac{1}{ik_n-\zeta_{\mathbf{k}}} \\
&= \left[\frac{1}{ik_n-\zeta_{\mathbf{k}}} - \frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}} \right] \frac{1}{iq_n+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}}
\end{aligned} \tag{26.19}$$

the summation $\sum_\sigma$ only give a factor of 2, so

$$\chi^0_{nn}\left(\mathbf{q}, iq_n\right) = -2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{1}{iq_n+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}} T \sum_{ik_n} \left[\frac{1}{ik_n-\zeta_{\mathbf{k}}} - \frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}} \right] \tag{26.20}$$

we do not need a convergence factor for the whole summand, since it's of order $(ik_n)^{-2}$. Nevertheless, taking the partial fractions, we now need a convergence factor. But since we are evaluating a difference, as long as we choose the same convergence factor, we should get the same result

$$\begin{aligned} T\sum_{ik_n}\left[\frac{1}{ik_n-\zeta_{\mathbf{k}}}-\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}}\right] &= T\sum_{ik_n}\left[\frac{1}{ik_n-\zeta_{\mathbf{k}}}-\frac{1}{ik_n-\zeta_{\mathbf{k}+\mathbf{q}}}\right] \\ &= f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}}) \end{aligned} \tag{26.21}$$

notice that iq_n is a variable in χ_{nn}, so we should really use a different name $iq_{n'}$, only k_n is summed over. Since $\sum_{ik_n}$ run over all fermionic frequencies, adding a $iq_{n'}$ does not change the sum, so we can remove the iq_n in the summation. We have now

$$\chi^0_{nn}(\mathbf{q},iq_n) = -2\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{iq_n+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{26.22}$$

The retarded function is easy to obtain by analytic continuation. It is the so-called **Lindhard function**

$$\chi^{0R}_{nn}(\mathbf{q},\omega) = -2\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega+i\eta+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{26.23}$$

At zero temperature, the numerator is non-zero when $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ are not on the same side of the Fermi surface. The poles will then be located at $\omega=\zeta_{\mathbf{k}+\mathbf{q}}-\zeta_{\mathbf{k}}$. These poles are particle-hole excitations instead of single-particle excitations as in the case of the Green's function. The sign difference between $\zeta_{\mathbf{k}+\mathbf{q}}$ and $\zeta_{\mathbf{k}}$ comes from the fact that one of them plays the role of a particle while the other plays the role of a hole.

Diagrammatic form of particle-hole excitations: If we return to the diagram in Ref. Fig.(39-1), we should notice the following general feature. If we cut the diagram in two by a vertical line, we see that it is crossed by lines that go in opposite directions. Hence, we have a particle-hole excitation. In particle-particle or hole-hole excitations, the lines go in the same direction and the two single- particle energies $\zeta_{\mathbf{k}+\mathbf{q}}$ and $\zeta_{\mathbf{k}}$ add up instead of subtract.

26.3.1 Zero-temperature value of the Lindhard function: the particle-hole continuum

To evaluate the integral appearing in the Lindhard function, which is what Lindhard did, it is easier to evaluate the imaginary part first and then to obtain the real part using Kramers-Kronig. Let us begin

$$\Im\chi^{0R}_{nn}(\mathbf{q},\omega) = 2\pi\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left[f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})\right]\delta(\omega+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}) \tag{26.24}$$

with $\mathbf{k}\to\mathbf{k}-\mathbf{q}$ in the second term this becomes

$$\Im\chi^{0R}_{nn}(\mathbf{q},\omega) = 2\pi\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})\left[\delta(\omega+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}})-\delta(\omega+\zeta_{\mathbf{k}-\mathbf{q}}-\zeta_{\mathbf{k}})\right] \tag{26.25}$$

Doing the replacement $f(\zeta_{\mathbf{k}})=\theta(k_F-k)$, going to polar coordinates with $\mathbf{q}$ along the polar axis and doing the replacement $\varepsilon_{\mathbf{k}}=k^2/2m$, we have

$$\begin{aligned} \Im\chi^{0R}_{nn}(\mathbf{q},\omega) &= \frac{1}{(2\pi)}\int_0^{k_F}dkk^2\int_{-1}^{1}d(\cos\theta)\left[\delta\left(\omega+\frac{k^2}{2m}-\frac{|\mathbf{k}+\mathbf{q}|^2}{2m}\right)-\delta\left(\omega+\frac{|\mathbf{k}-\mathbf{q}|^2}{2m}-\frac{k^2}{2m}\right)\right] \\ &= \frac{1}{(2\pi)}\int_0^{k_F}dk\frac{mk}{q}\int_{-1}^{1}d(\cos\theta)\left[\delta\left(\frac{\omega-\varepsilon_{\mathbf{q}}}{kq/m}-\cos\theta\right)-\delta\left(\frac{\omega+\varepsilon_{\mathbf{q}}}{kq/m}-\cos\theta\right)\right] \end{aligned} \tag{26.26}$$

the angle θ is between $\mathbf{k}$ and $\mathbf{q}$. We have $\frac{\omega-\varepsilon_{\mathbf{q}}}{kq/m}<\frac{\omega+\varepsilon_{\mathbf{q}}}{kq/m}$, and the integrand is non-zero only when one of them is outside $[-1,1]$, there are two possibilities

$$\begin{aligned} \frac{\omega-\varepsilon_{\mathbf{q}}}{kq/m} &< -1 < \frac{\omega+\varepsilon_{\mathbf{q}}}{kq/m} < 1 \\ -1 &< \frac{\omega-\varepsilon_{\mathbf{q}}}{kq/m} < 1 < \frac{\omega+\varepsilon_{\mathbf{q}}}{kq/m} \end{aligned} \tag{26.27}$$

This strategy in fact allows one to do the integrals in any spatial dimension. One finds, for an arbitrary ellipsoidal dispersion

$$\varepsilon_{\mathbf{k}} = \sum_{i=1}^{d}\frac{k_i^2}{2m_i} \tag{26.28}$$

$$\Im\chi^{0R}_{nn}(\mathbf{q},\omega) = \frac{\prod_{i=1}^{d}(\sqrt{2m_i})}{2^d\pi^{(d-1)/2}\Gamma(\frac{d+1}{2})\sqrt{\varepsilon_{\mathbf{q}}}}\times \\ \left\{\theta\left(\mu-\frac{(\omega-\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right)\left[\mu-\frac{(\omega-\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right]^{\frac{d-1}{2}} - \theta\left(\mu-\frac{(\omega+\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right)\left[\mu-\frac{(\omega+\varepsilon_{\mathbf{q}})^2}{4\varepsilon_{\mathbf{q}}}\right]^{\frac{d-1}{2}}\right\} \tag{26.29}$$

The real part is also calculable but we do not quote it here. This functional form in low dimension is quite interesting. Figures Ref.(39-2)(39-3) and (39-4) show the imaginary part of the Lindhard function in, respectively, $d = 1, 2, 3$. The small plots on the right show a cut in wave vector at fixed frequency while the plots on the left show $\Im\chi^{0R}_{nn}(\mathbf{q},\omega)$ on the vertical axis, frequency going from left to right and wave vector going from back to front. In all cases, at finite frequency it takes a finite wave vector $\mathbf{q}$ to have absorption. If the wave vector is too large however the delta function cannot be satisfied and there is no absorption either. The one-dimensional case is quite special since at low frequency there is absorption only in a narrow wave vector band. This has a profound influence on the interacting case since it will allow room for collective modes to propagate without absorption. In fact, in the interacting one-dimensional case the collective modes become eigenstates. This leads to the famous **spin-charge separation**[10]. In two dimensions, there is a peak at $q = 2k_F$ that becomes sharper and sharper as the frequency decreases as we can more clearly see from the small plot on the right. By contrast, the three-dimensional function is smoother, despite a discontinuity in slope at $q = 2k_F$. The region in $\mathbf{q} - \omega$ space where there is absorption is referred to as the **particle-hole continuum**.

To understand the existence of the particle-hole continuum and its shape, it is preferable to return to the original expression 26.24. Since $\Im\chi^{0R}_{nn}(\mathbf{q},-\omega) = -\Im\chi^{0R}_{nn}(\mathbf{q},\omega)$ is odd in ω, we will focus on $\omega > 0$. Energy conservation then requires $\omega = \zeta_{\mathbf{k}+\mathbf{q}} - \zeta_{\mathbf{k}} > 0$. So non-vanishing part corresponds to $\zeta_{\mathbf{k}+\mathbf{q}} > 0$ and $\zeta_{\mathbf{k}} < 0$. Ref. In Fig.(39-5) we draw the geometry for $d = 3$. The two "spheres" represent the domain where $f(\zeta_{\mathbf{k}}), f(\zeta_{\mathbf{k}+\mathbf{q}})$ are non-vanishing, respectively. So the sphere-constraint is that we must be outside $\mathbf{k}$-sphere and inside $(\mathbf{k}+\mathbf{q})$-sphere. In addition, for a fixed $\mathbf{q}, \omega$, the delta function introduces an additional constraint

$$\omega = \zeta_{\mathbf{k}+\mathbf{q}} - \zeta_{\mathbf{k}} = \frac{q^2}{2m} + \frac{\mathbf{k}\cdot\mathbf{q}}{m} \tag{26.30}$$

so $\mathbf{k}\cdot\mathbf{q}$ is now a constant. Such a trajectory of $\mathbf{k}$ is on a plane. The value $\Im\chi$ is the area of the plane inside the $(\mathbf{k}+\mathbf{q})$-sphere and outside the $\mathbf{k}$-sphere.

Consider first the case $q > 2k_F$, the two spheres do not overlap. Hence, there is a minimum value for ω, given by the case where $\mathbf{k}+\mathbf{q}$ and $\mathbf{k}$ are antiparallel and $\mathbf{k}$ is on the Fermi surface of the occupied Fermi sphere. We find then,

$$\omega_{\min} = \frac{q^2}{2m} + \frac{-k_F q}{m} = \varepsilon_{\mathbf{q}} - v_F q; \quad q > 2k_F \tag{26.31}$$

There is also a maximum value of ω, namely when $\mathbf{k}$ and $\mathbf{q}$ are parallel and $\mathbf{k}$ is on the Fermi surface of the occupied sphere. This gives,

$$\omega_{\max} = \frac{q^2}{2m} + \frac{+k_F q}{m} = \varepsilon_{\mathbf{q}} + v_F q \quad ; \quad q > 2k_F \tag{26.32}$$

for $q < 2k_F$the two spheres may overlap, when we have a plane intersecting both spheres, we must exclude the overlap part. The domain of integration is now an annulus instead of a filled circle. When this occurs, there is a discontinuous change in slope of $\Im\chi^{0R}_{nn}(q,\omega)$. This occurs when the vectors $\mathbf{k}+\mathbf{q}$ and $\mathbf{k}$ are antiparallel to each other and when $k = q - k_F$,

$$\omega_{\text{change}} = \frac{q^2}{2m} + \frac{-(q-k_F)q}{m} = -\varepsilon_{\mathbf{q}} + v_F q \quad ; \quad q < 2k_F \tag{26.33}$$

the minimum is now changed to the point where $k = q/2$

$$\omega_{\min} = \frac{q^2}{2m} + \frac{-(q/2)q}{m} = 0 \quad ; \quad q < 2k_F \tag{26.34}$$

27 Interactions and Collective Modes in a simple way

Before we start the whole machinery to take into account interactions and perhaps make you lose track of the physics with too much formalism, it is helpful to recall some of the simple results that we should obtain.

[10] **Thierry Giamarchi. Quantum Physics in One Dimenaion. Clarendon Oxford, 2004.**

27.1 Expansion parameter in the presence of interactions: r_s

In the presence of interactions, it is convenient to define a dimensionless constant that measures the strength of interactions relative to the kinetic energy. If the kinetic energy is very large compared with the interaction strength, perturbative methods may have a chance. Let us begin by recalling some well known results. In the hydrogen atom, potential and kinetic energy are comparable. That defines a natural distance for interacting electrons, namely the **Bohr radius**. Let us remind ourselves of what this number is. Using the uncertainty principle, we have $\Delta k \sim a_0^{-1}$ so that the kinetic energy can be estimated as $1/\left(ma_o^2\right)$ and the value of a_0 itself is obtained by equating this to the potential energy

$$\begin{aligned} \frac{1}{ma_o^2} &= \frac{e^2}{4\pi\varepsilon_0 a_0} \\ a_0 &= \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.529\times10^{-10}m \sim 0.5\text{Å} \end{aligned} \tag{27.1}$$

In a metal, imagine each free electron take up a sphere of radius $r_s a_0$, the total volume is $V = N\frac{4\pi}{3}r_s^3 a_0^3$, so we can write the density of free electrons $n = N/V$ as

$$n = \left(\frac{4\pi}{3}r_s^3 a_0^3\right)^{-1} \tag{27.2}$$

density of electrons is related to the fermi wave-vector by

$$n = \frac{k_F^3}{3\pi^2} \tag{27.3}$$

so we can write r_s in terms of k_F:

$$r_s \equiv \left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{k_F a_0} \tag{27.4}$$

notice r_s is dimensionless. In a way, r_s is the average distance between electrons measured in units of the Bohr radius. Large r_s means that the electrons are far apart, hence that the kinetic energy is small. It's natural to then expect r_s to be a measure of the relative strength of the interactions. Indeed, considering the electrons close the Fermi surface,

$$\frac{\text{Potential}}{\text{Kinetic}} \sim \frac{\frac{e^2}{4\pi\varepsilon_0 r_s a_0}}{k_F^2/2m} \sim \frac{\frac{e^2}{4\pi\varepsilon_0}k_F}{k_F^2/2m} \sim \frac{m\frac{e^2}{4\varepsilon_0}}{k_F} \sim \frac{1}{k_F a_0} \sim r_s \tag{27.5}$$

It may be counterintuitive at first to think that interactions are less important at large densities but that is a consequence of the uncertainty principle, not a concept of classical mechanics.

27.2 Thomas-Fermi screening

Consider Poisson's equation for our electron gas in the presence of an external charge ρ_e. You can think of this external charge as being for example an impurity positive charge added to the medium. In the Landau gauge, where $\nabla\cdot\mathbf{A} = \mathbf{0}$, then $\nabla\cdot\mathbf{E} = -\nabla^2\phi$ and Maxwell's equation gives

$$-\nabla^2\phi(\mathbf{r}) = \frac{1}{\varepsilon_0}\left[\rho_e(\mathbf{r}) + \delta\rho(\mathbf{r})\right] \tag{27.6}$$

The quantity $\delta\rho(\mathbf{r})$ is the change in charge density of the background produced by the charged impurity

$$\delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \rho_0 = -e[n(\mathbf{r}) - n] \tag{27.7}$$

we need to find $n(\mathbf{r})$.

Assuming that the Fermi energy and the potential both vary slowly in space, at every point $\mathbf{r}$, we can assume a local fermi gas with $n(\mathbf{r})$ and $k_F^3(\mathbf{r})$ satisfying

$$\frac{n(\mathbf{r})}{n} = \frac{k_F^3(\mathbf{r})}{k_F^3} \tag{27.8}$$

The total Fermi-level energy E_F is now divided into kinetic and potential part

$$\frac{k_F^2(\mathbf{r})}{2m} + (-e\phi(\mathbf{r})) = E_F = \frac{k_F^2}{2m} \tag{27.9}$$

this gives

$$\frac{n(\mathbf{r})}{n} = \frac{k_F^3(\mathbf{r})}{k_F^3} = \left[\frac{k_F^2(\mathbf{r})/2m}{k_F^2/2m}\right]^{3/2} = \left(1 + \frac{e\phi(\mathbf{r})}{E_F}\right)^{3/2} \tag{27.10}$$

$$\begin{aligned}\delta\rho(\mathbf{r}) &= -en\left[\left(1 + \frac{e\phi(\mathbf{r})}{E_F}\right)^{3/2} - 1\right] \\ &\approx \frac{3}{2}\frac{ne^2}{E_F}\left(-\phi(\mathbf{r})\right)\end{aligned} \tag{27.11}$$

we have two definitions from linear response theory

$$\begin{aligned}\delta\rho(\mathbf{q},\omega) &= \chi_{\rho\rho}^{irr,R}(\mathbf{q},\omega)\left(-\phi(\mathbf{q},\omega)\right) \\ \delta\rho(\mathbf{q},\omega) &= \chi_{\rho\rho}^{R}(\mathbf{q},\omega)\left(-\phi_e(\mathbf{q},\omega)\right)\end{aligned} \tag{27.12}$$

we use the irreducible one $\chi_{\rho\rho}^{irr,R}(\mathbf{q},\omega)$, since it's the most direct one

$$\chi_{\rho\rho}^{irr,R}(\mathbf{q},\omega) = \frac{3}{2}\frac{ne^2}{E_F} \tag{27.13}$$

according to the sum rule, $\lim_{\mathbf{q}\to\mathbf{0}}\lim_{\omega\to 0}\chi_{nn}^{irr,R}(\mathbf{q},\omega) = \frac{\partial n}{\partial\mu}$, so we also have $\frac{\partial n}{\partial\mu} = \frac{3}{2}\frac{ne^2}{E_F}$. Since $\chi_{\rho\rho}^{irr,R}$ gives the density response to the **self-consistent potential** ϕ, it is called the irreducible susceptibility for reasons that will become clear in the next section.

The full **non-linear equation** for $\phi(\mathbf{r})$ is

$$-\nabla^2\phi(\mathbf{r}) = \frac{1}{\varepsilon_0}\rho_e(\mathbf{r}) - \frac{1}{\varepsilon_0}ne\left[\left(1 - \frac{(-e\phi(\mathbf{r}))}{E_F}\right)^{3/2} - 1\right] \tag{27.14}$$

in general it is important to solve this full non-linear equation because otherwise at short distances the impurity potential is unscreened $\phi(\mathbf{r}) \sim 1/r$ which leads to unphysical negative values of the density. Nevertheless, if we are interested only in long-distance properties, the linear approximation turns out to be excellent.

The linearized PDE is

$$\begin{aligned}-\nabla^2\phi(\mathbf{r}) &= \frac{1}{\varepsilon_0}\rho_e(\mathbf{r}) + \frac{1}{\varepsilon_0}\frac{3}{2}\frac{ne}{E_F}(-e\phi(\mathbf{r})) \\ q^2\phi(\mathbf{q},\omega) &= \frac{1}{\varepsilon_0}\left[\rho_e(\mathbf{q},\omega) - \chi_{\rho\rho}^{irr,R}(\mathbf{q},\omega)\phi(\mathbf{q},\omega)\right]\end{aligned} \tag{27.15}$$

$$\begin{aligned}\phi(\mathbf{q},\omega) &= \frac{1}{\varepsilon_0}\frac{\rho_e(\mathbf{q},\omega)}{q^2 + \chi_{\rho\rho}^{irr,R}(\mathbf{q},\omega)/\varepsilon_0} \\ &= \frac{1}{\varepsilon_0}\frac{\rho_e(\mathbf{q},\omega)}{q^2 + \frac{3}{2}\frac{ne^2}{E_F\varepsilon_0}} \\ &\equiv \frac{1}{\varepsilon_0}\frac{\rho_e(\mathbf{q},\omega)}{q^2 + q_{TF}^2} \\ &= \left[\varepsilon_0\frac{q^2 + q_{TF}^2}{q^2}\right]^{-1}\phi_e(\mathbf{q},\mathbf{r})\end{aligned} \tag{27.16}$$

where we have defined Thomas-Fermi wavevector

$$q_{TF}^2 = \frac{3}{2}\frac{ne^2}{\varepsilon_0 E_F} = \frac{e^2}{\varepsilon_0}\frac{\partial n}{\partial\mu} = \chi_{\rho\rho}^{irr,R}(\mathbf{q},\omega)/\varepsilon_0 \tag{27.17}$$

We can also define a Thomas-Fermi longitudinal dielectric constant by

$$\epsilon^L(\mathbf{q},\omega) = \varepsilon_0\frac{q^2 + q_{TF}^2}{q^2} = \varepsilon_0\left(1 + \frac{q_{TF}^2}{q^2}\right) \tag{27.18}$$

Let us pause to give a physical interpretation of this result. At small distances (large q) the charge is unscreened since $\varepsilon_L \to 1$. On the contrary, at large distance (small q) the sreening is very effective. In real space, one finds

an exponential decrease of the potential over a length scale q_{TF}^{-1}, the **Thomas-Fermi screening length**. Let us write this length in terms of r_s with $\hbar$ appearing explicitly now so that $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$,

$$\begin{aligned}\lambda^2 \equiv q_{TF}^{-2} &= \frac{2\varepsilon_0 E_F}{3ne^2} = \frac{2\varepsilon_0 k_F^2/2m}{3ne^2} = \frac{k_F^2 a_0}{12\pi n} \\ &= \frac{k_F^2 a_0^4}{12\pi}\left(\frac{4\pi}{3}r_s^3\right) = a_0^2\left(\frac{1}{9}\left(\frac{9\pi}{4}\right)^{2/3}\right) r_s\end{aligned} \tag{27.19}$$

we have

$$\lambda \sim a_0\sqrt{r_s} \tag{27.20}$$

We now discuss the two limits

$$\begin{aligned} &r_s \ll 1, \quad \frac{\text{potential}}{\text{kinetic}} \ll 1, \quad \lambda \gg a_0 r_s \\ &r_s \gg 1, \quad \frac{\text{potential}}{\text{kinetic}} \gg 1, \quad \lambda \ll a_0 r_s \end{aligned} \tag{27.21}$$

In the first case, kinetic energy dominates, the screening length is larger than the inter-electron distance, and the Thaomas-Fermi reasoning make sense. On the other hand, in the second case, the potential energy dominates, but the screening length is much smaller than the inter-electron distance. In this case, the free-electron Hamiltonian is no longer a good starting place for perturbation theory. In fact, for large enough r_s, electrons start to localize. Note however, we require r_s to be pretty large for this localization. For sodium, $r_s \sim 4$ while for aluminum, $r_s \sim 2$ but still, these are good metals.

27.3 Reducible and irreducible susceptibilities

The calculation of the longitudinal dielectric constant for a homogeneous isotropic medium proceeds, in the Landau gauge $\nabla \cdot \mathbf{A} = \mathbf{0}$, from the following equalities

$$q^2\phi(\mathbf{q},\omega) = \frac{1}{\varepsilon_0}\left(\rho_e(\mathbf{q},\omega) + \delta\rho(\mathbf{q},\omega)\right) \equiv \frac{1}{\varepsilon^L(\mathbf{q},\omega)}\rho_e(\mathbf{q},\omega) \tag{27.22}$$

Note the two different susceptibilities

$$\begin{aligned}\delta\rho(\mathbf{q},\omega) &= -\chi^R_{\rho\rho}(\mathbf{q},\omega)\phi_e(\mathbf{q},\omega) \\ \delta\rho(\mathbf{q},\omega) &= -\chi^{irr,R}_{\rho\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega)\end{aligned} \tag{27.23}$$

from the first definition, we have

$$\frac{1}{\varepsilon^L(\mathbf{q},\omega)} = \frac{1}{\varepsilon_0}\left(1 - V_{\mathbf{q}}\chi^R_{nn}(\mathbf{q},\omega)\right) \tag{27.24}$$

where $V_{\mathbf{q}} = e^2/\left(\varepsilon_0 q^2\right)$. From the second definition,

$$\frac{1}{\varepsilon^L(\mathbf{q},\omega)} = \frac{1}{\varepsilon_0}\frac{1}{1 + V_{\mathbf{q}}\chi^{irr,R}_{nn}(\mathbf{q},\omega)} \tag{27.25}$$

We see a relation between the susceptibility and irreducible susceptibility

$$\frac{1}{1 + V_{\mathbf{q}}\chi^{irr,R}_{nn}(\mathbf{q},\omega)} = 1 - V_{\mathbf{q}}\chi^R_{nn}(\mathbf{q},\omega) \tag{27.26}$$

which leads to

$$\chi^R_{nn}(\mathbf{q},\omega) = \frac{\chi^{irr,R}_{nn}(\mathbf{q},\omega)}{1 + V_{\mathbf{q}}\chi^{irr,R}_{nn}(\mathbf{q},\omega)} \tag{27.27}$$

In fact, this relation can be written in a Dyson equation form

$$\begin{aligned}\chi^R_{nn}(\mathbf{q},\omega) =& \chi^{irr,R}_{nn}(\mathbf{q},\omega) - \chi^{irr,R}_{nn}(\mathbf{q},\omega)V_{\mathbf{q}}\chi^{irr,R}_{nn}(\mathbf{q},\omega) \\ &+ \chi^{irr,R}_{nn}(\mathbf{q},\omega)V_{\mathbf{q}}\chi^{irr,R}_{nn}(\mathbf{q},\omega)V_{\mathbf{q}}\chi^{irr,R}_{nn}(\mathbf{q},\omega) + \ldots\end{aligned} \tag{27.28}$$

Classical electrodynamics thus imposes the above relation between the two different kinds of responses. We will see later in **Hedin's equations**, how we can preserve this structure in general. In the random phase approximation (RPA) that I will discuss in the next chapter, the above relation will be satisfied with $\chi^{irr,R}_{nn}(\mathbf{q},\omega)$ replaced by $\chi^{0,R}_{nn}(\mathbf{q},\omega)$, the non-interacting density-density correlation function. In general, the definition $\Pi^R_{nn}(\mathbf{q},\omega) \equiv -\chi^{irr,R}_{nn}(\mathbf{q},\omega)$ is used for the so-called **irreducible polarization** $\Pi^R_{nn}(\mathbf{q},\omega)$.

27.4 Plasma oscillations

Plasma oscillations are the density oscillations of a free electron gas. The physics of this is that because the system wants to stay neutral everywhere, electrostatic forces will want to bring back spontaneous electronic density fluctuations towards the uniform state but, because of the electron inertia, there is overshooting. Hence oscillations arise at a particular natural frequency, the so-called **plasma frequency**. In other words, it suffices to add inertia to our previous considerations to see the result come out.

We give a very simple minded macroscopic description valid only in the limit of very long wave length oscillations. Suppose there is a drift current

$$\mathbf{j} = -en\mathbf{v} \tag{27.29}$$

Taking the time derivative and using Newton's equations,

$$\frac{\partial \mathbf{j}}{\partial t} = -en\frac{\partial \mathbf{v}}{\partial t} = -\frac{en}{m}(-e\mathbf{E}) \tag{27.30}$$

Note that in Newton's equation we should use the total time derivative instead of the partial, but since we assume a uniform density ($\mathbf{q} = \mathbf{0}$) the total and partial derivative are identical. We are in a position where one more time derivative

$$\frac{\partial^2 \mathbf{j}}{\partial t^2} = \frac{ne^2}{m}\frac{\partial \mathbf{E}}{\partial t} \tag{27.31}$$

and an appeal to the longitudinal part of Maxwell's fourth equation

$$0 = \mu_0 \mathbf{j} + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \tag{27.32}$$

should give us the desired result, namely

$$\frac{\partial^2 \mathbf{j}}{\partial t^2} = -\frac{ne^2}{\varepsilon_0 m}\mathbf{j} \tag{27.33}$$

This equation has an oscillatory solution at a frequency ω_p:

$$\omega_p^2 \equiv \frac{ne^2}{\varepsilon_0 m} \tag{27.34}$$

the so-called plasma frequency. Since we know that the longitudinal dielectric constant vanishes at a collective mode, this gives us another expected limit of this function

$$\lim_{\omega \to \omega_p} \varepsilon^L(\mathbf{q} = \mathbf{0}, \omega) = \lim_{\omega \to \omega_p} a\left(\omega - \omega_p\right) \tag{27.35}$$

where a is an unknown, for the time being, positive constant. The sign is determined from the fact that the dielectric constant must return to a positive value equal to unity at very large frequency.

Alternatively, we can find the plasma frequency from oscillation of ρ

$$\begin{aligned} \frac{\partial \nabla \cdot \mathbf{j}}{\partial t} &= -\frac{en}{m}(-e\nabla \cdot \mathbf{E}) \\ -\frac{\partial^2 \rho}{\partial t^2} &= \frac{e^2 n}{\varepsilon_0 m}\rho \end{aligned} \tag{27.36}$$

28 Density Response in the presence of interactions

28.1 Density-Density correlations, RPA

As before, we will do this in both Feynman's way and Schwinger's way. The central problem is still to find out the susceptibility

$$\chi_{nn}\left(\mathbf{q}, iq_n\right) = \frac{1}{\mathcal{V}}\int_0^\beta d\tau e^{iq_n\tau}\left\langle T_\tau\left[\delta n_{\mathbf{q}}(\tau)\delta n_{-\mathbf{q}}(0)\right]\right\rangle \tag{28.1}$$

in the non-interacting case, we set $\langle ... \rangle$ to $\langle ... \rangle_0$. Now, we need to evaluate the expectation with respect to the full Hamiltonian.

28.1.1 Feynman's way

Recall that we had expression

$$\chi_{nn}(1-2)=\sum_{\sigma,\sigma'}\left[\left\langle \mathcal{T}\psi_\sigma^\dagger(1)\psi_\sigma(1)\psi_{\sigma'}^\dagger(2)\psi_{\sigma'}(2)\right\rangle_{0c}-\mathcal{G}_\sigma(1,1^+)\mathcal{G}_{\sigma'}(2,2^+)\right] \tag{28.2}$$

The second term remove all diagrams where $1,2$ are disconnected (Note that Linked Cluster theorem only remove bubble diagrams, so diagrams included in the second term would not be removed by the linked cluster theorem). Therefore, we only need to consider diagrams with neither bubbles or disconnected 1-2 type.

Ref. Fig.(41-1) shows all charge susceptibility diagrams to first order in the interaction. The four diagrams on the second line take into account self-energy effects on the single-particle properties. We will worry about this later. Of the two diagrams on the first line, the first one clearly dominates. Indeed, the dotted line leads to a factor $e^2/\left(\varepsilon_0 q^2\right)$ that diverges at small wave vectors. On the other hand, the contribution from the other diagram is proportional to

$$\begin{aligned}
&-\sum_\sigma\sum_{k,k'}\mathcal{G}_\sigma^0(k)\mathcal{G}_\sigma^0(k')\mathcal{G}_\sigma^0(k+q)\mathcal{G}_\sigma^0(k'+q)V(k-k')\\
=&-2\int\frac{d^3k}{(2\pi)^3}T\sum_{ik_n}\int\frac{d^3k'}{(2\pi)^3}T\sum_{ik'_n}\mathcal{G}_\sigma^0\left(\mathbf{k}+\mathbf{q},ik_n+iq_n\right)\mathcal{G}_\sigma^0\left(\mathbf{k},ik_n\right)\times\\
&\frac{-e^2}{\varepsilon_0\left|\mathbf{k}-\mathbf{k}'\right|^2}\mathcal{G}_\sigma^0\left(\mathbf{k}'+\mathbf{q},ik'_n+iq_n\right)\mathcal{G}_\sigma^0\left(\mathbf{k}',ik'_n\right)
\end{aligned} \tag{28.3}$$

which is a convergent integral with no singularity at $q=0$. (In the book there is one less minus sign)

For a very short range potential, namely a wave-vector independent potential, the situation would have been completely different since the contribution of the last diagram would have been simply minus half of the contribution of the first one, the only differences being the additional fermion loop in the first one that leads to a sign difference and a factor of two for spin. We will come back on this in our study of the Hubbard model.

Let us thus concentrate on the most important contribution at long wave lengths namely the first diagram. In addition to being divergent as $q\to 0$, it has additional pathologies. Indeed, it has double poles at the particle-hole excitations of the non-interacting problem while the Lehmann representation shows us that it should not. This problem sounds familiar.However, we can solve this problem by summing an infinite subset of diagrams. Taking a simple example

$$\begin{aligned}
&\frac{1}{1-x}\times\frac{1}{1-V\frac{1}{1-x}}=\frac{1}{1-V-x}, \qquad \text{has first order pole}\\
&\frac{1}{1-x}\times\left(1+V\frac{1}{1-x}+V\frac{1}{1-x}V\frac{1}{1-x}\right)=\frac{1}{1-x}+\frac{V}{(1-x)^2}+\frac{V^2}{(1-x)^3}, \qquad \text{has first, second, third order poles}
\end{aligned} \tag{28.4}$$

This subset of diagrams is illustrated in Ref. Fig.(41-2). This is the famous **random phase approximation** (RPA). One also meets the terminology **ring diagrams** (in the context of free energy calculations) or, more often, one also meets the name **bubble diagrams**. The full susceptibility is represented by adding a triangle to one of the external vertices. That triangle represents the so-called **dressed three point vertex**. The reason for this name will come out more clearly later. The full series, represented schematically on the first two lines of the figure, may be summed to infinity by writing down the equation on the last line. This equation looks like a particle-hole version of the Dyson equation. The undressed bubble plays the role of an irreducible susceptibility. It is irreducible with respect to cutting one interaction line.

From our calculation of the susceptibility for non-interacting electrons we know that Feynman's rules apply for the diagrams on Ref. Fig.(41-2). Each bubble is associated with a factor $\chi_{nn}^0\left(\mathbf{q},iq_n\right)$, a quantity defined in such a way that it contains the minus sign associated with the fermion loop. The dashed interaction lines each lead to a factor $-V_{\mathbf{q}}=-e^2/\left(\varepsilon_0 q^2\right)$, the minus sign being associated with the fact that one more $V_{\mathbf{q}}$ means one higher order in perturbation theory (remember the $(-1)^n$ rule). The sum over bubbles, represented by the last line on Ref. Fig.(41-2) is

$$\begin{aligned}
\chi_{nn}(\mathbf{q},iq_n)&=\chi_{nn}^0(\mathbf{q},iq_n)+\chi_{nn}^0(\mathbf{q},iq_n)\left(-V_{\mathbf{q}}\right)\chi_{nn}(\mathbf{q},iq_n)\\
\chi_{nn}(\mathbf{q},iq_n)&=\frac{\chi_{nn}^0(\mathbf{q},iq_n)}{1+V_{\mathbf{q}}\chi_{nn}^0(\mathbf{q},iq_n)}
\end{aligned} \tag{28.5}$$

with $V_{\mathbf{q}}=\frac{e^2}{\varepsilon_0 q^2}$.

28.1.2 Schwinger's way

In Schwinger's formalism, we are already performing the interacting average, so the formula still applies

$$\chi_{nn}(1-2) = -\sum_{\sigma_1,\sigma_2} \frac{\delta \mathcal{G}\left(1,1^+\right)}{\delta\phi\left(2^+,2\right)} \tag{28.6}$$

and Fourier transforming, we obtain in the case where the irreducible vertex is obtained from functional derivatives of the Hartree-Fock self-energy the set of diagrams in Fig. 37-7

$$\begin{aligned}\frac{\delta \mathcal{G}\left(1,1^+\right)_\phi}{\delta\phi\left(2^+,2\right)} =& \mathcal{G}(1,2)_\phi \mathcal{G}(2,1)_\phi \\ &- \mathcal{G}(1,\overline{5})_\phi \left(V(\overline{5}-\overline{6}) \frac{\delta \mathcal{G}(\overline{5},\overline{6})_\phi}{\delta\phi\left(2^+,2\right)} \right) \mathcal{G}(\overline{6},1)_\phi \\ &+ \mathcal{G}(1,\overline{5})_\phi \left(V(\overline{5}-\overline{7}) \frac{\delta \mathcal{G}(\overline{7},\overline{7})_\phi}{\delta\phi\left(2^+,2\right)} \right) \mathcal{G}(\overline{5},1)_\phi\end{aligned} \tag{28.7}$$

the middle diagram has two internal momentum: k, k' to be integrated over, while the last diagram has only one internal momentum k. At small q, the contribution from the middle diagram is not singular because the Coulomb potential is integrated over, by contrast, the last diagram has a $1/q^2$ from the interaction potential. Therefore, we only keep the last diagram. The integral equation

$$\frac{\delta \mathcal{G}\left(1,1^+\right)_\phi}{\delta\phi\left(2^+,2\right)} = \mathcal{G}(1,2)_\phi \mathcal{G}(2,1)_\phi + \mathcal{G}(1,\overline{5})_\phi \mathcal{G}(\overline{5},1)_\phi \left(V(\overline{5}-\overline{7}) \frac{\delta \mathcal{G}(\overline{7},\overline{7}^+)_\phi}{\delta\phi\left(2^+,2\right)} \right) \tag{28.8}$$

Notice that $\chi_{nn} = \frac{\delta \mathcal{G}}{\delta \bar{\phi}}$, $\chi^0_{nn} = \mathcal{G}\mathcal{G}$, we have

$$\begin{aligned}-\sum_{\sigma_1\sigma_2} \frac{\delta \mathcal{G}\left(1,1^+\right)_\phi}{\delta\phi\left(2^+,2\right)} &= -\sum_{\sigma_1\sigma_2} \mathcal{G}(1,2)_\phi \mathcal{G}(2,1)_\phi - \left(-\sum_{\sigma_1\sigma_2} \mathcal{G}(1,\overline{5})_\phi \mathcal{G}(\overline{5},1)_\phi \right) \left(V(\overline{5}-\overline{7}) \left(-\frac{\delta \mathcal{G}(\overline{7},\overline{7}^+)_\phi}{\delta\phi\left(2^+,2\right)} \right) \right) \\ \chi_{nn}(1-2) &= \chi^0_{nn}(1-2) - \chi^0_{nn}(1-\bar{5}) V(\bar{5}-\bar{7}) \chi_{nn}(\bar{7}-2)\end{aligned} \tag{28.9}$$

A Fourier Transform gives the same result as the Feynman calculation

$$\begin{aligned}\chi_{nn}(q) &= \chi^0_{nn}(q) - \chi^0_{nn}(q) V_{\mathbf{q}} \chi_{nn}(q) \\ \chi_{nn}(q) &= \frac{\chi^0_{nn}(q)}{1 + V_{\mathbf{q}} \chi^0_{nn}(q)} = \frac{1}{\chi^0_{nn}(q)^{-1} + V_{\mathbf{q}}}\end{aligned} \tag{28.10}$$

This is the so-called **Random Phase Approximation**, or **RPA**. The last form of the equality highlights the fact that the irreducible vertex, here $V_{\mathbf{q}}$, plays the role of an irreducible self-energy in the particle-hole channel. The analytical continuation will be trivial.

Note that we have written $\chi^0_{nn}(q)$ for the bubble diagram, i.e. the first term on the right-hand side of the equation in Ref. Fig. 37-7 even though everything we have up to now in the Schwinger formalism are **dressed Green's functions**. The reason is that neglecting the middle diagram on the right-hand side of the equality is like neglecting the contribution from the Fock, or exchange self-energy in Ref. Fig. 37-6. The only term left then is is the Hartree term that we argued should vanish because of the neutralizing background. Hence, the Green's functions are bare ones and the corresponding susceptibility is the Lindhard function.

28.2 Dielectric constant and related physical properties

Using our previous results for the imaginary part of the susceptibility for non-interacting particles, the real part can be found from the Hilbert transform. From this we obtain the explicit expression for the real and imaginary parts of the dielectric function in three dimensions at zero temperature. Recall that longitudinal dielectric constant and charge susceptibility are related by

$$\frac{1}{\epsilon^L(\mathbf{q},\omega)} = \frac{1}{\varepsilon_0}\left(1 - V_{\mathbf{q}} \chi^R_{nn}(\mathbf{q},\omega)\right) = \frac{1}{\varepsilon_0\left(1 + V_{\mathbf{q}} \chi^{0R}_{nn}(\mathbf{q},\omega)\right)} \tag{28.11}$$

or

$$\epsilon^L(\mathbf{q},\omega) = \varepsilon_0 \left(1 + V_{\mathbf{q}} \chi^{0R}_{nn}(\mathbf{q},\omega)\right) \tag{28.12}$$

For positive frequencies, one finds, with definition $\epsilon_1 \equiv \Re\epsilon$, $\epsilon_2 \equiv \Im\epsilon$,

$$\frac{\epsilon_1^L(\mathbf{q},\omega)}{\varepsilon_0} = 1 + \frac{q_{TF}^2}{q^2}\left\{\frac{1}{2} + \frac{k_F}{4q}\left[\left(1 - \frac{(\omega-\varepsilon_q)^2}{q^2 v_F^2}\right)\ln\left|\frac{\omega - v_F q - \varepsilon_q}{\omega + v_F q - \varepsilon_q}\right| + \left(1 - \frac{(\omega+\varepsilon_q)^2}{q^2 v_F^2}\right)\ln\left|\frac{\omega + v_F q + \varepsilon_q}{\omega - v_F q + \varepsilon_q}\right|\right]\right\}$$

$$\epsilon_2^L(\mathbf{q},\omega) = \begin{cases} \frac{\pi}{2}\frac{\omega}{v_F q}\frac{q_{TF}^2}{q^2} & \omega \le v_F q - \varepsilon_q \\ \frac{\pi k_F}{4q}\frac{q_{TF}^2}{q^2}\left(1 - \frac{(\omega-\varepsilon_q)^2}{q^2 v_F^2}\right) & v_F q - \varepsilon_q \le \omega \le \varepsilon_q + v_F q \\ 0 & \omega \ge \varepsilon_q + v_F q \\ \frac{\pi k_F}{4q}\frac{q_{TF}^2}{q^2}\left(1 - \frac{(\omega-\varepsilon_q)^2}{q^2 v_F^2}\right) & \varepsilon_q - v_F q \le \omega \le \varepsilon_q + v_F q \end{cases} \tag{28.13}$$

where in the first three cases $q < 2k_F$ and in the last case $q > 2k_F$. This calculation is not obvious. The integral is done at length in Fetter and Walecka [11]. We will see below that we can find the interesting limiting cases for the integrals entering the calculation of the Lindhard function rather easily, except for the logarithm. That logarithm is important for **Friedel's oscillations**. It comes basically from the Hilbert transform of the Heaviside-θ function. Recall in our geometric arguments with Fermi spheres that discontinuities in the slope of the non-interacting charge susceptibility occur when $q = 2k_F$.

We can simplify the expression using natural units

$$\frac{\epsilon_1^L(\mathbf{q},\omega)}{\varepsilon_0} = 1 + \frac{r_0}{q^2}\left\{\frac{1}{2} + \frac{1}{4q}\left[\left(1 - \left(\frac{\omega - q^2}{2q}\right)^2\right)\ln\left|\frac{\omega - 2q - q^2}{\omega + 2q - q^2}\right| + \left(1 - \left(\frac{\omega + q^2}{2q}\right)^2\right)\ln\left|\frac{\omega + 2q + q^2}{\omega - 2q + q^2}\right|\right]\right\}$$

$$\epsilon_2^L(\mathbf{q},\omega) = \begin{cases} \frac{\pi}{4}\frac{\omega}{q^3} r_0 & \omega \le v_F q - \varepsilon_q \\ \frac{\pi}{4q^3} r_0 \left(1 - \left(\frac{\omega - q^2}{2q}\right)^2\right) & v_F q - \varepsilon_q \le \omega \le \varepsilon_q + v_F q \\ 0 & \omega \ge \varepsilon_q + v_F q \\ \frac{\pi}{4q^3} r_0 \left(1 - \left(\frac{\omega - q^2}{2q}\right)^2\right) & \varepsilon_q - v_F q \le \omega \le \varepsilon_q + v_F q \end{cases}$$

$$[q] = k_F, \quad [\omega] = E_F, \quad q_{TF}^2/k_F^2 = r_0 = 4(\frac{2}{3})^{2/3}\pi^{-4/3} r_s \tag{28.14}$$

now we only have one parameter r_0 or equivalently r_s which is of order 1.

We now analyze these results to extract five important physical ingredients:

1. There is a particle-hole continuum but the poles are simply shifted from their old positions instead of becoming poles of high-order.
2. There is screening at low frequency.
3. There are Friedel oscillations in space.
4. There are plasma oscillations in time
5. At long wavelengths the plasma oscillations exhaust the f-sum rule

28.2.1 Particle-hole continuum

Let us first think of a finite system with $2M$ discrete poles in $\chi^{0R}_{nn}(\mathbf{q},\omega)$ to see that these have been shifted. The number of simple poles is even because the function is odd. The spectral representation tells us, using the fact

[11] Fetter and Walecka Quantum Theory of many-particle systems (2003) p165

that,$\chi''_{nn}(\mathbf{q},\omega')$ is odd w.r.t ω:

$$\begin{aligned}\chi^{0R}_{nn}(\mathbf{q},\omega) &= \int \frac{d\omega'}{\pi}\frac{\chi^{0\prime\prime}_{nn}(\mathbf{q},\omega')}{\omega'-\omega-i\eta} = \int \frac{d\omega'}{\pi}\frac{\omega'\chi^{0\prime\prime}_{nn}(\mathbf{q},\omega')}{(\omega')^2-(\omega+i\eta)^2} \\ &= \sum_{i=1}^{M}\frac{A_i}{u_i^2-(\omega+i\eta)^2} \\ &= \frac{\sum_{i=1}^{M}A_i\prod_{j\neq i}\left((\omega+i\eta)^2-v_j^2\right)}{\prod_{i=1}^{M-1}\left(u_i^2-(\omega+i\eta)^2\right)} \\ &= \frac{B\prod_{i=1}^{M-1}\left((\omega+i\eta)^2-v_i^2\right)}{\prod_{i=1}^{M}\left(u_i^2-(\omega+i\eta)^2\right)}\end{aligned} \tag{28.15}$$

where A_i is positive because $\omega'\chi^{0\prime\prime}_{nn}(\mathbf{q},\omega')$ is positive, and u_i are positions of the delta functions in $\omega'\chi^{0\prime\prime}_{nn}(\mathbf{q},\omega')$. The parameters A_i and u_i then are respectively the residue and the location of each pole in $\chi^{0R}_{nn}(\mathbf{q},\omega)$. We have combined the sum of fractions on a common denominator so that the numerator of the last expression has one less power of $(\omega+i\eta)^2$. We do not need to specify the values of B and v_i. Using this expression for the non-interacting susceptibility, the RPA susceptibility is

$$\chi^{R}_{nn}(\mathbf{q},\omega) = \frac{B\prod_{i=1}^{M-1}\left((\omega+i\eta)^2-v_i^2\right)}{\prod_{i=1}^{M}\left(u_i^2-(\omega+i\eta)^2\right)+V_{\mathbf{q}}B\prod_{i=1}^{M-1}\left((\omega+i\eta)^2-v_i^2\right)} \tag{28.16}$$

The denominator can be rewritten as a polynomial of order M in $(\omega+i\eta)^2$, but the zeros of this polynomial, corresponding to the poles of the retarded susceptibility, have shifted. To find out the location of the poles of the charge excitations, at least qualitatively, it suffices to look for the domain where the imaginary part is non vanishing. Using our RPA result

$$\Im\left(\frac{x+iy}{1+x+iy}\right) = \frac{y}{(1+x)^2+y^2} \tag{28.17}$$

$$\Im\chi^{R}_{nn}(\mathbf{q},\omega) = \frac{\Im\chi^{0R}_{nn}(\mathbf{q},\omega)}{\left(1+V_{\mathbf{q}}\Re\chi^{0R}_{nn}(\mathbf{q},\omega)\right)^2+\left(V_{\mathbf{q}}\Im\chi^{0R}_{nn}(\mathbf{q},\omega)\right)^2}. \tag{28.18}$$

In a finite system, suppose $\Im\chi^{0R}_{nn}(\mathbf{q},\omega)$ diverge at some frequency ω_0, since $\Im\chi^{R}_{nn}(\mathbf{q},\omega)$ contain a $\left(\Im\chi^{0R}_{nn}\right)^2$ in the denominator, this does not in general leads to a divergence. In order that $\Im\chi^{R}_{nn}$ to diverges, we need both $\left(\Im\chi^{0R}_{nn}\right)^2$ and $\left(1+V_{\mathbf{q}}\Re\chi^{0R}_{nn}(\mathbf{q},\omega)\right)^2$ to vanish at some frequency and faster than $\Im\chi^{0R}_{nn}$. If we take the limit $\Im\chi^{0R}_{nn}\to 0$ first, we approach the delta function limit of the Lorentzian:

$$\Im\chi^{R}_{nn}(\mathbf{q},\omega) \to \pi\delta\left(1+V_{\mathbf{q}}\Re\chi^{0R}_{nn}(\mathbf{q},\omega)\right) \tag{28.19}$$

The new poles are the locations of the new delta functions, namely, the solution of

$$\begin{aligned}\frac{1}{V_{\mathbf{q}}}+\Re\chi^{0R}_{nn}(\mathbf{q},\omega) &= \frac{1}{V_{\mathbf{q}}}+\sum_{i=1}^{M}\frac{A_i}{u_i^2-\omega^2} \\ &= \frac{1}{V_{\mathbf{q}}}+\sum_{i=1}^{M}\frac{A_i}{2u_i}\left(\frac{1}{u_i-\omega}+\frac{1}{u_i+\omega}\right)=0\end{aligned} \tag{28.20}$$

The solution of this equation may in principle be found graphically as illustrated in Fig.(41-4). I have taken the simple case $2M=6$ for clarity. In reality, $M\to\infty$ and the separation between each discrete pole of $\Re\chi^{0R}_{nn}(\mathbf{q},\omega)$ is inversely proportional to a power of the size of the system $1/\mathcal{V}$. The poles of non-interacting χ^0 are represented by the divergent frequencies of the function $\Re\chi^{0R}_{nn}$, which are asymptotes of the lines, while the interacting poles are located at the intersections between the function $\Re\chi^{0R}_{nn}$ and a horizontal line $-1/V_{\mathbf{q}}$. We see that except for the last two symmetrically located solutions at large frequency, all the new solutions are very close to those of the non-interacting system. And they must be at a location where the non-interacting $\Im\chi^{0R}_{nn}(\mathbf{q},\omega)$ vanishes.

In summary then, the particle-hole continuum is basically at the same place as it was in the non-interacting system, even though the residues may have changed. The two solutions at large frequency correspond to plasma oscillations, as we will see later. They are well separated from the particle-hole continuum for small q where $1/V_{\mathbf{q}}$

is very small. However, at large wave vector it is quite possible to find that the high frequency poles become very close again to the particle-hole continuum.

Since $\Im\left(\epsilon^L(\mathbf{q},\omega)/\varepsilon_0\right)^{-1} = 1 + V_{\mathbf{q}}\Im\chi^R_{nn}(\mathbf{q},\omega)$ the zeros of the dielectric constant are at the same location as the poles of $\chi^R_{nn}(\mathbf{q},\omega)$ and, from what we just said, these poles are located basically in the same $(\omega,\mathbf{q})$ domain as the particle- hole continuum of the non-interacting system, except for possibly a pair of poles (**plasma pole**). This situation is illustrated schematically in Fig.(41-5), that generalizes Fig.(39-6).

28.2.2 Screening

At zero frequency, namely for a static charge perturbation, using the RPA expression for dielectric function 28.13, we see that the imaginary part of the dielectric constant ϵ_2^L vanishes[12], while the real part becomes

$$\frac{\epsilon_1^L(\mathbf{q},0)}{\varepsilon_0} = 1 + \frac{q_{TF}^2}{q^2}\frac{\epsilon_1^L(\mathbf{q},\omega)}{\varepsilon_0} = 1 + \frac{q_{TF}^2}{q^2}\left\{\frac{1}{2} + \frac{k_F}{2q}\left[\left(1 - \frac{q^2}{(2k_F)^2}\right)\ln\left|\frac{q+2k_F}{q-2k_F}\right|\right]\right\} \tag{28.21}$$

In the long wave length limit $q/2k_F \to 0$, we recover the Thomas-Fermi result

$$g(x) = \frac{1}{2} + \frac{1}{2x}\left(1 - \frac{1}{4}x^2\right)\ln\left|\frac{1+\frac{1}{2}x}{1-\frac{1}{2}x}\right| \tag{28.22}$$

$$\begin{aligned} g(x) &\approx 1 + O\left(x^2\right) \quad x \ll 1 \\ g(x) &\approx \frac{1}{2} + \frac{1}{4}(x-2)\ln\left[\frac{1}{4}|x-2|\right] \quad |x-2| \ll 1 \\ g(x) &\sim \frac{4}{3}x^{-2} \quad x > 1 \end{aligned} \tag{28.23}$$

$$\lim_{q/2k_F\to 0}\frac{\epsilon_1^L(\mathbf{q},0)}{\varepsilon_0} = 1 + \frac{q_{TF}^2}{q^2} \tag{28.24}$$

Alternatively, we can also obtain this result from the Lindhard function

$$\chi^{0R}_{nn}(\mathbf{q},\omega) = -2\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f\left(\zeta_{\mathbf{k}}\right) - f\left(\zeta_{\mathbf{k}+\mathbf{q}}\right)}{\omega + i\eta + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}} \tag{28.25}$$

$$\begin{aligned} \lim_{\mathbf{q}\to 0}\frac{\epsilon_1^L(\mathbf{q},0)}{\varepsilon_0} &= \lim_{\mathbf{q}\to 0}\left[1 - 2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}}\right] \\ &= \left[1 - 2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{\partial f\left(\zeta_{\mathbf{k}}\right)}{\partial\zeta_{\mathbf{k}}}\right] \\ &= 1 + V_{\mathbf{q}}\frac{\partial}{\partial\mu}\left[2\int\frac{d^3\mathbf{k}}{(2\pi)^3}f\left(\zeta_{\mathbf{k}}\right)\right] \\ &= 1 + \frac{e^2}{\varepsilon_0 q^2}\frac{\partial n}{\partial\mu} \\ &= 1 + \frac{q_{TF}^2}{q^2} \end{aligned} \tag{28.26}$$

the corresponding potential

$$\begin{aligned} V_{\text{eff}}(\mathbf{r}) &= \int\frac{d^3q}{(2\pi)^3}V_{\text{eff}}(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}} \\ &= \int\frac{d^3q}{(2\pi)^3}\frac{V(\mathbf{q})}{\varepsilon^L(\mathbf{q},\omega=0)}e^{i\mathbf{q}\cdot\mathbf{r}} \\ &= \int\frac{d^3q}{(2\pi)^3}\frac{e^2}{q^2}\frac{1}{\varepsilon_0(1+\frac{q_{TF}^2}{q^2})}e^{i\mathbf{q}\cdot\mathbf{r}} \\ &= \frac{e^2}{\varepsilon_0}\int\frac{d^3q}{(2\pi)^3}\frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{q^2+q_{TF}^2} \\ &= \frac{e^2}{4\pi\varepsilon_0}\frac{e^{-q_{TF}r}}{r} \end{aligned} \tag{28.27}$$

[12]Note that $q = 2k_F$ corresponds to $\varepsilon_q = v_F q$. The fourth case where $q > 2k_F$ clearly does not include $\omega = 0$. Among the first three cases where $q < 2k_F$ and $\varepsilon_q < v_F q$, only the first case includes $\omega = 0$, but the first case is proportional to ω, so $\Im\epsilon_2^L(\mathbf{q},\omega=0) = 0$.

is then a Yukawa potential or **screened Coulomb potential**.

28.2.3 Friedel Oscillations

The approximation we have done above is incorrect. We have taken part of $q \to 0$ and left the other part unchanged, which is in general not valid. We can perform a more careful Fourier Transform[13] with the general $\frac{\epsilon_1^L(\mathbf{q},0)}{\varepsilon_0}$,

$$\begin{aligned} V_{eff}(\mathbf{r}) &= \int \frac{d^3q}{(2\pi)^3} \frac{V(\mathbf{q})}{\varepsilon^L(\mathbf{q},\omega=0)} e^{i\mathbf{q}\cdot\mathbf{r}} \\ &= \int \frac{d^3q}{(2\pi)^3} \frac{e^2}{\varepsilon_0} \left[q^2 + q_{TF}^2 \left\{ \frac{1}{2} + \frac{k_F}{2q} \left[\left(1 - \frac{q^2}{(2k_F)^2} \right) \ln \left| \frac{q+2k_F}{q-2k_F} \right| \right] \right\} \right]^{-1} e^{i\mathbf{q}\cdot\mathbf{r}} \\ &= \frac{e^2}{\varepsilon_0(2\pi)^2} \int_{-\infty}^{\infty} dq_1 e^{iq_1 r} \int_0^{\infty} dq_r q_r \left[q^2 + q_{TF}^2 \left\{ \frac{1}{2} + \frac{k_F}{2q} \left[\left(1 - \frac{q^2}{(2k_F)^2} \right) \ln \left| \frac{q+2k_F}{q-2k_F} \right| \right] \right\} \right]^{-1} \\ &= ... \end{aligned} \tag{28.28}$$

and obtain a better approximation

$$\lim_{r\to\infty} V_{\text{eff}}(r) \propto \frac{2\xi}{(4+\xi)^2} \frac{\cos(2k_F r)}{r^3} \tag{28.29}$$

with $\xi = q_{TF}^2/(2k_F^2)$. These are so-called **Friedel oscillations**. Returning to Ref.Fig. (39-5) you will recall that in Fourier space there are discontinuity in slopes at $q = 2k_F$. Friedel oscillations are the real-space manifestation of these discontinuity in slope. In other words they come from the real-space version of the logarithm at $q = 2k_F$. They manifest themselves physically in several ways. For example they broaden NMR lines and they give rise to an effective interaction $J\mathbf{S}_1 \cdot \mathbf{S}_2$ between magnetic impurities whose amplitude J oscillates in sign. This is the so-called **RKKY interaction**. The change in sign of J with distance is a manifestation of Friedel's oscillations.

(**?**)The Friedel oscillations originate in the **sharpness of the Fermi surface**. At finite temperature, where the Fermi surface broadens, they are damped as $e^{-k_F r(\Delta/E_F)}$ where Δ is of order T. Another way to write this last result is $e^{-r/\xi_{th}}$ where the thermal de Broglie wavelength is of order v_F/T in our units. Restoring physical units, that length is defined by setting the thermal energy uncertainty $k_B T$ equal to $v_F \hbar \Delta k$ and identifying the spread in wave vector around k_F as $\Delta k \sim \xi_{th}^{-1}$. We will encounter this length in other contexts as well.

28.2.4 Plasma and Landau Damping

We have already suggested in Fig.(41-4) that at small q, a large frequency pole far from the particle-hole continuum appears. Let us look at this parameter range. Taking $v_F q/\omega$ as a small parameter, $\epsilon_2^L(\mathbf{q},\omega)$ is infinitesimal at the plasmon pole but vanishes everywhere else in its vicinity. On the other hand the limiting form of $\epsilon_1^L(\mathbf{q},\omega)$ may be obtained directly from

$$\begin{aligned} \frac{\epsilon^L(\mathbf{q},\omega)}{\varepsilon_0} &= 1 + V_{\mathbf{q}} \chi_{nn}^{0R}(\mathbf{q},\omega) \\ &= 1 - 2V_{\mathbf{q}} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega + i\eta + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}} \end{aligned} \tag{28.30}$$

[13] A.L. Fetter and J.D. Walecka, op. cit., p.178

when the frequency is large and outside the particle-hole continuum, we can write

$$\begin{aligned}
\lim_{\mathbf{q}\ll\mathbf{k}_F}\lim_{\omega\gg\varepsilon_q+\mathbf{v}_F q}\frac{\varepsilon_1^L(\mathbf{q},\omega)}{\varepsilon_0} &= \lim_{\mathbf{q}\to 0,\omega\gg\varepsilon_q+\mathbf{v}_F q}\left[1-2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}}\right] \\
&= \lim_{\mathbf{q}\ll\mathbf{k}_F}\left[1+2V_{\mathbf{q}}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega^2}(\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}})\right] \\
&= \lim_{\mathbf{q}\ll\mathbf{k}_F}\left[1+\frac{4V_{\mathbf{q}}}{\omega^2}\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})(\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}})\right] \\
&= \lim_{\mathbf{q}\ll\mathbf{k}_F}\left[1-\frac{4V_{\mathbf{q}}}{\omega^2}\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})\frac{2\mathbf{k}\cdot\mathbf{q}+q^2}{2m}\right] \\
&= 1-\frac{2V_{\mathbf{q}}n}{\omega^2}\frac{q^2}{2m} \\
&= 1-\frac{\omega_P^2}{\omega^2}
\end{aligned} \tag{28.31}$$

with the value of $\omega_p^2=\frac{ne^2}{\varepsilon_0 m}$. One can continue the above approach to higher order or proceed directly with a tedious Taylor series expansion in powers of $v_F q/\omega$:

$$\frac{1}{\omega+\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}}}=\frac{1}{\omega}+\frac{(\zeta_{\mathbf{k}+\mathbf{q}}-\zeta_{\mathbf{k}})}{\omega^2}+\frac{(\zeta_{\mathbf{k}+\mathbf{q}}-\zeta_{\mathbf{k}})^2}{\omega^3}+\frac{(\zeta_{\mathbf{k}+\mathbf{q}}-\zeta_{\mathbf{k}})^3}{\omega^4}+... \tag{28.32}$$

odd orders of ω vanishes due to the symmetry properties of $(f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}}))(\zeta_{\mathbf{k}+\mathbf{q}}-\zeta_{\mathbf{k}})$, the next even order is

$$\begin{aligned}
&\frac{2V_{\mathbf{q}}}{\omega^4}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left(f(\zeta_{\mathbf{k}})-f(\zeta_{\mathbf{k}+\mathbf{q}})\right)(\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}})^3 \\
=&\frac{4V_{\mathbf{q}}}{\omega^4}\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})(\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{q}})^3 \\
=&-\frac{4V_{\mathbf{q}}}{\omega^4}\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})\left(\frac{\mathbf{k}\cdot\mathbf{q}}{m}+\frac{q^2}{2m}\right)^3 \\
\approx&-\frac{4V_{\mathbf{q}}}{\omega^4}\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})3\left(\frac{\mathbf{k}\cdot\mathbf{q}}{m}\right)^2\frac{q^2}{2m} \\
=&-3\frac{\omega_p^2}{\omega^2}\times\frac{1}{\omega^2}\left[\frac{1}{n}2\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})\left(\frac{\mathbf{k}\cdot\mathbf{q}}{m}\right)^2\right] \\
=&-3\frac{\omega_p^2}{\omega^2}\times\frac{1}{\omega^2 m^2}\left[\frac{1}{n}2\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})\left(k_x^2q_x^2+k_y^2q_y^2+k_z^2q_z^2\right)\right] \\
=&-3\frac{\omega_p^2}{\omega^2}\times\frac{1}{\omega^2 m^2}\left[\frac{q^2}{3}\frac{\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})k^2}{\int\frac{d^3\mathbf{k}}{(2\pi)^3}f(\zeta_{\mathbf{k}})}\right] \\
=&-3\frac{\omega_p^2}{\omega^2}\times\frac{1}{\omega^2 m^2}\left[\frac{q^2}{3}\frac{k_F^5/5}{k_F^3/3}\right] \\
=&-\frac{3}{5}\frac{\omega_p^2}{\omega^2}\times\frac{(v_F q)^2}{\omega^2}
\end{aligned} \tag{28.33}$$

In summary, the high ω expansion gives

$$\lim_{\omega\gg\varepsilon_q+\mathbf{v}_F q}\frac{\varepsilon_1^L(\mathbf{q}\to 0,\omega)}{\varepsilon_0}=1-\frac{\omega_p^2}{\omega^2}-\frac{3}{5}\frac{\omega_p^2}{\omega^2}\frac{(v_F q)^2}{\omega^2}+\dots \tag{28.34}$$

Several physical remarks follow directly from this result

- Even at long wavelength $q\to 0$, the interaction becomes unscreened at sufficiently high frequency. More specifically,

$$\frac{\varepsilon_1^L\left(\mathbf{q}\to 0,\omega\gg\omega_p\right)}{\varepsilon_0}\to 1 \tag{28.35}$$

- The collective plasma oscillation that we expected does show up. Indeed, $\varepsilon_1(\mathbf{q}\to 0,\omega)=0$ when

$$\begin{aligned} 0&=\omega^2-\omega_p^2-\frac{3}{5}\frac{\omega_p^2}{\omega^2}\left(v_F q\right)^2+\dots \\ \omega^2&\approx\omega_p^2+\frac{3}{5}\left(v_F q\right)^2+\dots \end{aligned} \tag{28.36}$$

  Letting the right-had side be called ω_q, we have in the vicinity of this solution $\omega\approx\omega_q$

$$\frac{\varepsilon_1^L(\mathbf{q}\to 0,\omega)}{\varepsilon_0}\approx 1-\frac{\omega_q^2}{\omega^2}\approx\frac{2}{\omega_q}\left(\omega-\omega_q\right) \tag{28.37}$$

  which is precisely the form we had obtained from macroscopic considerations. We now know that the unknown constant we had at this time has the value $a=2/\omega_q$.

Fig.(41-6) shows a plot of both the real and the imaginary parts of the dielectric constant for small wave vector ($q\ll q_{TF}$). We see that the dielectric constant is real and very large at zero frequency, representing screening, whereas the vanishing of the real part at large frequency leads to the plasma oscillations, the so-called plasmon. Given the scale of the figure, it is hard to see the limiting behavior $\varepsilon_1(\mathbf{q},\infty)\to 1$ but the zero crossing is illustrated by the maximum in $\Im(1/\varepsilon)$. There is another zero crossing of ε_1 but it occurs in the particle-hole continuum where ε_2 is large. Hence this is an over-damped mode.

When q is sufficiently large that the plasmon enters the particle-hole continuum, damping becomes very large. This mechanism for damping is known as **Landau damping**.

28.2.5 f-sum

Let us check if the f-sum rule is satisfied, recall that it takes the form

$$2\int_0^\infty\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega)=\frac{nq^2}{m} \tag{28.38}$$

from relation

$$\varepsilon_0/\epsilon^L(\mathbf{q},\omega)=1-V_{\mathbf{q}}\chi^R_{nn}(\mathbf{q},\omega) \tag{28.39}$$

we have

$$\int_0^\infty\frac{d\omega}{2\pi}\omega\Im\left[\frac{\varepsilon_0}{\varepsilon^L(\mathbf{q}\to 0,\omega)}\right]=-V_{\mathbf{q}}\frac{nq^2}{4m}=-\frac{ne^2}{4m\varepsilon_0}=-\frac{\omega_p^2}{4} \tag{28.40}$$

We can check our small q approximation

$$\int_0^\infty\frac{d\omega}{2\pi}\omega\Im\frac{1}{\frac{2}{\omega_q}\left(\omega-\omega_q\right)+i\eta}=\int_0^\infty\frac{d\omega}{2\pi}\omega(-\pi)\frac{\omega_q}{2}\delta\left(\omega-\omega_q\right)=-\frac{\omega_q^2}{4} \tag{28.41}$$

This means that at $q=0$, the plasmon exhaust the f-sum rule. Nothing else is necessary to satisfy this sum rule. On the other hand, for $q\neq 0$, one can check that the particle-hole continuum gives a contribution

$$-\frac{\omega_p^2}{4}+\frac{\omega_q^2}{4}=\frac{3}{20}\left(v_F q\right)^2 \tag{28.42}$$

as necessary to satisfy the f-sum rule.

One of the key general problems in many-body theory is to devise approximations that satisfy conservation laws in general and the f-sum rule in particular. The RPA is such an approximation. This is non-trivial. It is a consequence of the fact that RPA is consistent with charge conservation. We will discuss this problem in more details later.

29 Hartree-Fock

Our strategy in this section will be as follows

1. Show the failure of Hartree-Fock

2. Understand the failure by the consistency relations between the self-energy and density fluctuations

3. Cure the problem using the screened interaction in the calculation, discuss the physical interpretation

4. Derive fermi-liquid scattering rate

It is useful to derive the result from the variational principle as well as directly from a Green's function point of view. Since Hartree-Fock is sometimes actually quite good, it is advisable to develop a deep understanding of this approach.

29.1 Variational principle

In this section we derive the variational principle for thermodynamic systems. We start from a general inequality between any two density matrices ϱ, ϱ'

$$S = -\operatorname{Tr}[\varrho \ln \varrho] \leq -\operatorname{Tr}[\varrho \ln \varrho'] \tag{29.1}$$

Proof: Let $|m\rangle$ and $|m'\rangle$ be the basis that diagonalize respectively ϱ and ϱ'. Then by inserting the closure relation, and defining $p_m = \langle m|\varrho|m\rangle$ with the analogous definition for p'_m, we find

$$\begin{aligned}
\operatorname{Tr}\left[-\varrho \ln \varrho + \varrho \ln \varrho'\right] &= \sum_{m,m'} \langle m| \left[-\varrho \ln \varrho + \varrho \ln \varrho'\right] |m'\rangle \langle m'| m\rangle \\
&= \sum_{m,m'} \left(-p_m \ln p_m + p_m \ln p'_{m'}\right) \langle m \mid m'\rangle \langle m' \mid m\rangle \\
&= \sum_{m,m'} \langle m \mid m'\rangle \langle m' \mid m\rangle \, p_m \ln \frac{p'_{m'}}{p_m}.
\end{aligned} \tag{29.2}$$

we have $\langle m \mid m'\rangle \langle m' \mid m\rangle \, p_m \geq 0$. Using the identity $\ln y \leq y - 1$, we can write

$$\begin{aligned}
\operatorname{Tr}\left[-\varrho \ln \varrho + \varrho \ln \varrho'\right] &\leq \sum_{m,m'} \langle m \mid m'\rangle \langle m' \mid m\rangle \left(p'_{m'} - p_m\right) \\
&= \operatorname{Tr}(\rho') - \operatorname{Tr}(\rho) = 0
\end{aligned} \tag{29.3}$$

the equality is taken when $\langle m \mid m'\rangle = 0$ or $p'_{m'} = p_m$ for all $|m\rangle, |m'\rangle$.

Now take a simple density matrix $\varrho = \varrho_0 = Z_{\tilde{0}}^{-1} e^{-\beta(\tilde{H}_0 - \mu N)}$ and a complicated density matrix $\varrho' = Z^{-1} e^{-\beta(H-\mu N)}$, the inequality gives

$$\begin{aligned}
-\operatorname{Tr}[\varrho_0 \ln \varrho_0] &\leq -\operatorname{Tr}\left[\varrho_0 \ln \frac{e^{-\beta(H-\mu N)}}{Z}\right] \\
-\operatorname{Tr}[\varrho_0 \ln \varrho_0] &\leq \frac{1}{T} \operatorname{Tr}\left[\varrho_0 (H - \mu N)\right] + \ln Z \\
-T \ln Z &\leq \operatorname{Tr}\left[\varrho_0 (H - \mu N)\right] + T \operatorname{Tr}[\varrho_0 \ln \varrho_0]
\end{aligned} \tag{29.4}$$

or

$$-T \ln Z \leq -T \ln Z_{\tilde{0}} + \left\langle H - \tilde{H}_0 \right\rangle_{\tilde{0}} \tag{29.5}$$

where $\langle O \rangle_{\tilde{0}}$ refers to an average of the operator O with the density matrix ϱ_0. This inequality is called **Feynman variational principle** or **Bogoliubov's inequality**. Since it holds for the entropy holds for arbitrary $\tilde{H}_0$, so if we can solve a class of parametrized$\tilde{H}_0$, we can then minimize the RHS to find the one closest to the exact Hamiltonian.

29.2 Hartree-Fock from Variational principle

In Hartree-Fock theory, we give ourselves a trial one-particle Hamiltonian and use the variational principle to find the parameters. In the electron gas case the true non-interacting part of the Hamiltonian is

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} = \sum_{\mathbf{k},\sigma} \frac{k^2}{2m} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \tag{29.6}$$

The interacting part, written in Fourier space, takes the form

$$H - H_0 = \frac{1}{2\mathcal{V}} \sum_{\mathbf{k},\sigma} \sum_{\mathbf{k}',\sigma'} \sum_{\mathbf{q}\neq 0} c^\dagger_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',\sigma'} V_{\mathbf{q}} c_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma}, \qquad V_{\mathbf{q}} = \frac{e^2}{\varepsilon_0 q^2} \tag{29.7}$$

where we have removed the $\mathbf{q} = 0$ mode, as required by neutrality. In this notation, $\mathbf{q}$ is often referred to as the "**transfer variable**" while $\mathbf{k}, \mathbf{k}'$ are the **band variables**. To apply the variational principle, one takes

$$\tilde{H}_0 = \sum_{\mathbf{k},\sigma} \tilde{\epsilon}_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \tag{29.8}$$

with variational parameter $\tilde{\epsilon}_{\mathbf{k}}$. Using the Feynman variational principle, we minimize the right hand-side of

$$-T \ln Z \leq -T \ln Z_0 + \left\langle H - \tilde{H}_0 \right\rangle \tag{29.9}$$

The partition function is given by

$$\begin{aligned} -T \ln Z_0 &= -T \ln \mathrm{Tr} \left(e^{-\beta(\tilde{H}_0 - \mu N)} \right) \\ &= -T \ln \prod_{\mathbf{k}\sigma} \mathrm{Tr}_{\mathbf{k}} \left(e^{-\beta(\tilde{\epsilon}_{\mathbf{k}} - \mu) n_{\mathbf{k}\sigma}} \right) \\ &= -T \sum_{\mathbf{k},\sigma} \ln \left(1 + e^{-\beta(\tilde{\epsilon}_{\mathbf{k}} - \mu)} \right) \end{aligned} \tag{29.10}$$

The second part can be evaluated using Wick's theorem

$$\begin{aligned} \left\langle H - \tilde{H}_0 \right\rangle_0 &= \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}}) \left\langle c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \right\rangle + \frac{1}{2\mathcal{V}} \sum_{\mathbf{k},\sigma} \sum_{\mathbf{k}',\sigma'} \sum_{\mathbf{q}\neq 0} V_{\mathbf{q}} \left\langle c^\dagger_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',\sigma'} c_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma} \right\rangle \\ &= \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}}) \left\langle c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \right\rangle \\ &\quad + \frac{1}{2\mathcal{V}} \sum_{\mathbf{k},\sigma} \sum_{\mathbf{k}',\sigma'} \sum_{\mathbf{q}\neq 0} V_{\mathbf{q}} \left\{ \left\langle c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}+\mathbf{q},\sigma} \right\rangle \left\langle c^\dagger_{\mathbf{k}',\sigma'} c_{\mathbf{k}'-\mathbf{q},\sigma'} \right\rangle - \left\langle c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}'-\mathbf{q},\sigma'} \right\rangle \left\langle c^\dagger_{\mathbf{k}',\sigma'} c_{\mathbf{k}+\mathbf{q},\sigma} \right\rangle \right\} \end{aligned} \tag{29.11}$$

We have $\left\langle c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma'} \right\rangle = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} f(\tilde{\zeta}_{\mathbf{k}})$ with $f(\tilde{\zeta}_{\mathbf{k}}) = (e^{\beta(\tilde{\epsilon}_{\mathbf{k}} - \mu)} + 1)^{-1}$, so

$$\left\langle H - \tilde{H}_0 \right\rangle_0 = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}}) f(\tilde{\zeta}_{\mathbf{k}}) - \frac{1}{\mathcal{V}} \sum_{\mathbf{k}\neq\mathbf{k}'} V_{\mathbf{k}'-\mathbf{k}} f(\tilde{\zeta}_{\mathbf{k}}) f(\tilde{\zeta}_{\mathbf{k}'}) \tag{29.12}$$

overall ,the RHS is

$$\mathrm{RHS} = \sum_{\mathbf{k}} \left\{ -2T \ln \left(1 + e^{-\beta\tilde{\zeta}_{\mathbf{k}}} \right) + 2 \left(\zeta_{\mathbf{k}} - \tilde{\zeta}_{\mathbf{k}} \right) f(\tilde{\zeta}_{\mathbf{k}}) \right\} - \frac{1}{\mathcal{V}} \sum_{\mathbf{k}\neq\mathbf{k}'} V_{\mathbf{k}'-\mathbf{k}} f(\tilde{\zeta}_{\mathbf{k}}) f(\tilde{\zeta}_{\mathbf{k}'}) \tag{29.13}$$

now, treating $\tilde{\epsilon}_{\mathbf{k}}$ as parameters, we differentiate RHS w.r.t them and set them equal to zero

$$\begin{aligned} 0 = \frac{\partial \mathrm{RHS}}{\partial \tilde{\epsilon}_{\mathbf{k}}} &= 2 \frac{e^{-\beta\tilde{\zeta}_{\mathbf{k}}}}{1 + e^{-\beta\tilde{\zeta}_{\mathbf{k}}}} - 2 f(\tilde{\zeta}_{\mathbf{k}}) + 2 \left(\zeta_{\mathbf{k}} - \tilde{\zeta}_{\mathbf{k}} \right) f'(\tilde{\zeta}_{\mathbf{k}}) - f'(\tilde{\zeta}_{\mathbf{k}}) \frac{2}{\mathcal{V}} \sum_{\mathbf{k}'\neq\mathbf{k}} V_{\mathbf{k}'-\mathbf{k}} f(\tilde{\zeta}_{\mathbf{k}'}) \\ &= 2 f'(\tilde{\zeta}_{\mathbf{k}}) \left[\left(\zeta_{\mathbf{k}} - \tilde{\zeta}_{\mathbf{k}} \right) - \frac{1}{\mathcal{V}} \sum_{\mathbf{k}'\neq\mathbf{k}} V_{\mathbf{k}'-\mathbf{k}} f(\tilde{\zeta}_{\mathbf{k}'}) \right] \end{aligned} \tag{29.14}$$

since $f'(x) = \frac{d}{dx}\frac{1}{e^{\beta x}-1} = -\beta\frac{e^{\beta x}}{(e^{\beta x}-1)^2} \neq 0$, the bracket must be equal to zero, so

$$\tilde{\epsilon}_{\mathbf{k}} - \epsilon_{\mathbf{k}} = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}'\neq\mathbf{k}} V_{\mathbf{k}'-\mathbf{k}} f(\tilde{\zeta}_{\mathbf{k}'}) = \frac{1}{\mathcal{V}}\int \frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{e^2}{\varepsilon_0\left\|\mathbf{k}-\mathbf{k}'\right\|^2}\frac{1}{e^{\beta(\tilde{\epsilon}_{\mathbf{k}}-\mu)}+1} \tag{29.15}$$

As usual the chemical potential is determined by fixing the number of particles.
Before we evaluate this integral let us obtain this same result from the Green's function point of view.

29.3 Hartree-Fock from Green's functions

The above equation may be obtained directly from the Schwinger or Feynman approaches. First, recall that the Hartree term disappears because it involves $V_{q=0} = 0$ that vanishes because of the neutralizing background. The Fock term gives, in Schwinger's formalism(with dressed Green's functions)

$$\begin{aligned}\Sigma^{(1)}(\mathbf{k}) &= -\int \frac{d^3\mathbf{q}}{(2\pi)^3} T\sum_{q_n} \mathcal{G}_\sigma(\mathbf{k}-\mathbf{q})V(\mathbf{q}) \\ &= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} T\sum_{k'_n} e^{ik'_n 0^+}\mathcal{G}_\sigma(\mathbf{k}')V(\mathbf{k}-\mathbf{k}')\end{aligned} \tag{29.16}$$

from Dyson's equation, $\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}$, we can write the dressed Green's function to first order

$$\mathcal{G}_\sigma(\mathbf{k}) = \frac{1}{\mathcal{G}_0^{-1}(\mathbf{k}) - \Sigma^{(1)}(\mathbf{k})} = \frac{1}{ik_n - \zeta_{\mathbf{k}} - \Sigma^{(1)}(\mathbf{k})} \tag{29.17}$$

this gives another self-consistent equation

$$\begin{aligned}\Sigma^{(1)}(\mathbf{k}) &= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} T\sum_{k'_n} e^{ik'_n 0^+}\frac{e^2}{\varepsilon_0\left\|\mathbf{k}-\mathbf{k}'\right\|^2}\frac{1}{ik'_n - \zeta_{\mathbf{k}'} - \Sigma^{(1)}(\mathbf{k}')} \\ &= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{e^2}{\varepsilon_0\left\|\mathbf{k}-\mathbf{k}'\right\|^2} f\left(\zeta_{\mathbf{k}'} + \Sigma^{(1)}(\mathbf{k}')\right) \\ &= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{e^2}{\varepsilon_0\left\|\mathbf{k}-\mathbf{k}'\right\|^2} f(\tilde{\zeta}_{\mathbf{k}'})\end{aligned} \tag{29.18}$$

The old particle with dispersion $\epsilon_{\mathbf{k}}$ then looks like a new particle with dispersion

$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k}) \tag{29.19}$$

so we arrive at the same self-consistent HF equation

$$\tilde{\epsilon}_{\mathbf{k}} - \epsilon_{\mathbf{k}} = -\int \frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{e^2}{\varepsilon_0\left\|\mathbf{k}-\mathbf{k}'\right\|^2} f\left(\tilde{\zeta}_{\mathbf{k}'}\right) \tag{29.20}$$

From the point of view of non-interacting Green's functions, it looks as if the perturbation expansion for the full Green's function, illustrated by a thick arrow in Ref. Fig.(42-2), was written in terms of a perturbation series that involves the full Green's function itself. Iterating shows that in this approximation we have a self- energy that resums the infinite subset of diagrams illustrated on the bottom part of this same figure. In the Feynman approach, one commonly says that all the rainbow diagrams have been summed. In principle this Hartree-Fock Green's function may be used in further perturbative calculations. We just have to be careful not to double-count the diagrams we have already included.

29.4 Hartree-Fock from renormalized perturbation theory

We want to do perturbation theory but using this time for the Hamiltonian

$$H = \tilde{H}_0 + \left(H_0 - \tilde{H}_0 + V\right) \tag{29.21}$$

That is a trick that I will use repeatedly when we study broken symmetries and phase transitions. The unperturbed Hamiltonian is now $\tilde{H}_0$, some quadratic Hamiltonian. In addition to the usual perturbation V, there is now a translationally invariant one-body potential $H_0 - \tilde{H}_0$. One determines the self-energy in such a way that $\tilde{H}_0$ becomes the best "effective medium" in the sense that to first order in $\left(H_0 - \tilde{H}_0 + V\right)$ the self-energy calculated in this effective medium vanishes completely. This is illustrated in Ref. Fig.(42-3). This kind of approach is also known as **renormalized perturbation theory**.

The effect of a one-body potential on the Green's function is easy to evaluate,

$$\mathcal{G}(1,2) = -\left\langle T_\tau \exp\left\{-\frac{1}{2}V(\bar{1})\psi^\dagger(\bar{1})\psi(\bar{1})\right\}\psi(1)\psi^\dagger(2)\right\rangle_c \tag{29.22}$$

with trivial Feynman rules and connected Feynman diagrams, generating diagrams in the same way as Dyson's equation

$$\mathcal{G}(\mathbf{k}) = \mathcal{G}_0(\mathbf{k}) + \mathcal{G}_0(\mathbf{k})V(\mathbf{k})\mathcal{G}(\mathbf{k}) \tag{29.23}$$

so the only effect of this one-particle potential is to add $V(\mathbf{k})$ to the self-energy. In our case, if

$$H_0 - \tilde{H}_0 = \sum_{\mathbf{k}\sigma}\left(\epsilon_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}}\right) c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} \tag{29.24}$$

the only effect of this perturbation is adding $\epsilon_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}}$ to the self energy $\Sigma(\mathbf{k})$. The so-called Hartree diagram (or tadpole diagram) with one loop does not contribute because it is proportional to $V_{\mathbf{q}=0} = 0$. The Hartree term is in a sense the classical contribution coming from the interaction of the electron with the average charge density. The last diagram on the right of the figure is the Fock term that comes from exchange and is a quantum effect. Algebraically,

$$\widetilde{\Sigma} = \epsilon_{\mathbf{k}} - \widetilde{\epsilon}_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k}) = 0 \tag{29.25}$$

Using the expression for the exchange, or Fock, diagram $\Sigma^{(1)}(\mathbf{k})$,

$$\Sigma^{(1)}(\mathbf{k}) = -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} T\sum_{ik'_n} \frac{e^2}{\varepsilon_0\left|\mathbf{k}-\mathbf{k}'\right|^2}\tilde{\mathcal{G}}^0\left(\mathbf{k}', ik'_n\right)e^{ik'_n\eta} \tag{29.26}$$

this then give the same self-consistency equation for $\tilde{\epsilon}_{\mathbf{k}}$.

29.5 Hartree-Fock incorrectly predicts zero effective mass

To evaluate our expression for the Hartree-Fock self-energy $\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k})$ we need the chemical potential. As usual in the grand-canonical ensemble, the chemical potential is determined by requiring that we have the correct density. Let us suppose then that we have a density n,

$$\begin{aligned} n &= 2\int \frac{d^3\mathbf{k}}{(2\pi)^3} T\sum_{ik_n}\tilde{\mathcal{G}}^0\left(\mathbf{k}, ik_n\right)e^{ik_n 0^+} \\ &= 2\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{1}{e^{\beta\left(\epsilon_{\mathbf{k}}+\Sigma^{(1)}(\mathbf{k})-\mu\right)}+1} \\ \lim_{T\to 0} n &= 2\int \frac{d^3\mathbf{k}}{(2\pi)^3}\theta(\mu - \epsilon_{\mathbf{k}} - \Sigma^{(1)}(\mathbf{k})) \\ &= 2\int \frac{d^3\mathbf{k}}{(2\pi)^3}\theta(k_F - |\mathbf{k}|) \end{aligned} \tag{29.27}$$

where k_F is the momentum at which the $\mu - \epsilon_{\mathbf{k}} - \Sigma^{(1)}(\mathbf{k})$ vanishes, so it is defined as the solution of

$$\epsilon_{k_F} + \Sigma^{(1)}(k_F) - \mu = 0 \tag{29.28}$$

k_F defined in this way given exactly the same relation $n = k_F^3/(3\pi^2)$ as the Fermi gas. This is an elementary example of **Luttinger's theorem** that we will discuss in a later chapter. This theorem says that the volume

enclosed by the Fermi surface is independent of interactions. Clearly, if $\mu_0 = \epsilon_{k_F}$ is the value of the chemical potential in the non-interacting system, then the interacting chemical potential is

$$\mu = \mu_0 + \Sigma^{(1)}(k_F) \tag{29.29}$$

we now perform the self-consistent integral for $\Sigma^{(1)}(\mathbf{k})$,

$$\begin{aligned}
\Sigma^{(1)}(\mathbf{k}) &= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} \frac{e^2}{\varepsilon_0 \left\|\mathbf{k}-\mathbf{k}'\right\|^2} f\left(\zeta_{\mathbf{k}'} + \Sigma^{(1)}(\mathbf{k}')\right) \\
&= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} \frac{e^2}{\varepsilon_0 \left\|\mathbf{k}-\mathbf{k}'\right\|^2} \frac{1}{e^{\beta\left(\epsilon_{\mathbf{k}}+\Sigma^{(1)}(\mathbf{k})-\mu\right)}+1} \\
\lim_{T\to 0} \Sigma^{(1)}(\mathbf{k}) &= -\int \frac{d^3\mathbf{k}'}{(2\pi)^3} \frac{e^2}{\varepsilon_0 \left\|\mathbf{k}-\mathbf{k}'\right\|^2} \theta(k_F - |\mathbf{k}|) \\
&= -\frac{e^2}{\varepsilon_0 4\pi^2} \int_0^{k_F} dk' k'^2 \int_{-1}^{1} \frac{d\cos\theta}{k^2 + k'^2 - 2kk'\cos\theta} \\
&= -\frac{e^2}{4\pi^2\varepsilon_0} \int_0^{k_F} dk' \frac{k'}{k} \ln\left|\frac{k+k'}{k-k'}\right| \\
&= -\frac{e^2}{4\pi^2\varepsilon_0} k_F \left[y \int_0^{1/y} dx \left(x \ln\left|\frac{x+1}{x-1}\right| \right) \right]
\end{aligned} \tag{29.30}$$

with $x = k'/k$, $y = k/k_F$. There is a singularity at $x = 1$. We will evaluate this integral as a principle-value integral, since we should ignore the $k \neq k'$ term corresponding to $q = 0$.

$$\Sigma^{(1)}_{T=0}(\mathbf{k}) = -\frac{e^2}{4\pi^2\varepsilon_0} k_F \left[1 + \frac{1-y^2}{2y} \ln\left|\frac{1+y}{1-y}\right| \right], \qquad y = k/k_F \tag{29.31}$$

At $y = 1$, we have

$$\Sigma^{(1)}_{T=0}(k_F) = -\frac{e^2}{4\pi^2\varepsilon_0} k_F \tag{29.32}$$

The ratio of this term to the zeroth order term, namely the kinetic energy $k_F^2/2m$ is of order r_s

$$\frac{\Sigma^{(1)}_{T=0}(k_F)}{\text{K.E.}} = \frac{-\frac{e^2}{4\pi^2\varepsilon_0} k_F}{k_F^2/2m} \propto \frac{1}{k_F a_0} \propto r_s \tag{29.33}$$

where we used $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$ and $r_s \equiv \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{k_F a_0}$. We also have

$$\mu = \frac{k_F^2}{2m} - \frac{e^2}{4\pi^2\varepsilon_0} k_F, \qquad n = \frac{k_F^3}{3\pi^2} \tag{29.34}$$

Up to here everything seems to be consistent, except if we start to ask about the effective mass. The plot of the self-energy suggests that there is an anomaly in the slope at $y = 1$ or $k = k_F$. This reflects itself in the effective mass. Indeed, using the general formula

$$\frac{m}{m^*} = \lim_{\mathbf{k}\to\mathbf{k}_F} \frac{1 + \frac{\partial}{\partial\zeta_{\mathbf{k}}} \Re\Sigma^R(\mathbf{k}, E_{\mathbf{k}} - \mu)}{1 - \frac{\partial}{\partial\omega} \Re\Sigma^R(\mathbf{k},\omega)\big|_{\omega = E_{\mathbf{k}} - \mu}} = 1 + \frac{dk}{d\zeta_{\mathbf{k}}} \frac{\partial\Sigma^{(1)}(\mathbf{k})}{\partial k}\bigg|_{k=k_F} \tag{29.35}$$

$$\begin{aligned}
\frac{m}{m^*} &= \lim_{k\to k_F} \frac{1 + \frac{1}{v_{\mathrm{F}}} \frac{\partial \Re\Sigma(k,\omega)}{\partial k}\Big|_{\omega = E_{\mathbf{k}} - \mu}}{1 - \frac{\partial \Re\Sigma(k,\omega)}{\partial\omega}\Big|_{\omega = E_{\mathbf{k}} - \mu}} \\
&= 1 + \frac{1}{v_{\mathrm{F}}} \frac{\partial\Sigma^{(1)}(\mathbf{k})}{\partial k}|_{k=k_F} \\
&= 1 - \frac{1}{v_{\mathrm{F}}} \frac{e^2}{4\pi^2\varepsilon_0} \lim_{y\to 1} \frac{d}{dy} \left[1 + \frac{1-y^2}{2y} \ln\left|\frac{1+y}{1-y}\right| \right]
\end{aligned} \tag{29.36}$$

We have already seen that the function $1+\frac{1-y^2}{2y}\ln\left|\frac{1+y}{1-y}\right|$ has a point with infinite slope at $y=1$. Taking $y<1$, for example, we have

$$\begin{aligned}\lim_{y\to 1^-}\frac{d}{dy}\left[\frac{1-y^2}{2y}\ln\left(\frac{1+y}{1-y}\right)\right] &= \lim_{y\to 1^-}\frac{1}{y}-\frac{1+y^2}{2y^2}\ln\left(\frac{1+y}{1-y}\right)\\ &= 1-\ln 2+\lim_{y\to 1^-}\ln(1-y)\\ &= -\infty\end{aligned} \tag{29.37}$$

This corresponds to the unphysical result $m^*=0$. An effective mass smaller than the bare mass is possible but rather unusual. In general, interactions will make quasiparticles look heavier.

The physical reason for the failure of Hartree-Fock is the following. It is correct to let the electron have exchange interaction of the type included in rainbow diagrams do, but it is incorrect to neglect the fact that the other electrons in the background will also react to screen this interaction. We discuss this in more details below.

30 Consistency Relations

We have found an expression for the density fluctuations that appears correct since it has all the correct Physics. It was a non-trivial task since we had to sum an infinite subset of diagrams. We will see that it is also difficult to obtain the correct expression for the self-energy without a bit of physical hindsight. We might have thought that the variational principle would have given us a good starting point but we will see that in this particular case it is a disaster. The following theorems will help us to understand why this is so and will suggest how to go around the difficulty. We thus go back to some formalism again to show that there is a general relation between self-energy and charge fluctuations. We will have a good approximation for the self-energy only if it is consistent with our good approximation for the density fluctuations. We also take this opportunity to show how to obtain the self-energy since just a few additional lines will suffice

Recall the equations of motion for Green's function, without source field

$$\left(\frac{\partial}{\partial\tau_1}-\frac{\nabla_1^2}{2m}-\mu\right)\mathcal{G}(1,2)=-\delta(1-2)+\left\langle T_\tau\left[\psi^\dagger\left(\overline{2^+}\right)V(1-\overline{2})\psi(\overline{2})\psi(1)\psi^\dagger(2)\right]\right\rangle_\phi \tag{30.1}$$

In Fourier space, this will be the Dyson's equation $\mathcal{G}_0^{-1}\mathcal{G}=1+\Sigma\mathcal{G}$. The self-energy is then related to the four-point correlation function through

$$\int_{1''}\Sigma(1,1'')\,\mathcal{G}(1'',2)=-\left\langle T_\tau\left[\int_{1'}\psi^\dagger\left(1'^+\right)V(1'-1)\,\psi(1')\,\psi(1)\psi^\dagger(2)\right]\right\rangle \tag{30.2}$$

(note that here $\int_1=\sum_{\sigma_1}\int d^3\mathbf{x}_1\int_0^\beta d\tau$)
we now take the limit $2\to 1^+$, the RHS becomes

$$\left\langle T_\tau\left[\int_{1'}\psi^\dagger(1^+)\psi^\dagger(1'^+)V(1'-1)\psi(1')\psi(1)\right]\right\rangle \tag{30.3}$$

recall the definition for the average of potential energy

$$2\langle V\rangle=\sum_{\sigma_1}\int d^3\mathbf{x}_1\int_{1'}\left\langle T_\tau\left[\psi^\dagger\left(1^+\right)\psi^\dagger\left(1'\right)V\left(1'-1\right)\psi\left(1'\right)\psi(1)\right]\right\rangle \tag{30.4}$$

we may as well put an extra summation $\int_0^\beta d\tau_1$ on both hand-sides. Time translational symmetry allows us to argue that $\langle V\rangle$ is independent of time, so

$$\begin{aligned}2\langle V\rangle\beta &= \int_1\int_{1''}\Sigma(1,1'')\,\mathcal{G}\left(1'',1^+\right)\\ &= \int_1\int_{1''}\left\langle T_\tau\left[\psi^\dagger\left(1^+\right)\psi^\dagger\left(1'\right)V\left(1'-1\right)\psi\left(1'\right)\psi(1)\right]\right\rangle\end{aligned} \tag{30.5}$$

The right-hand side is in turn related to the density-density correlation function. To see this, it suffices to return to space spin and time indices and to recall that the potential is instantaneous and spin independent so that when

we exchange the equal-time operators

$$\begin{aligned}
2\langle V\rangle\beta &= \int_{1'}\int_{1}\left\langle \psi^{\dagger}\left(1^{+}\right)\psi^{\dagger}\left(1'^{+}\right)V\left(1'-1\right)\psi\left(1'\right)\psi(1)\right\rangle \\
&= -\beta\sum_{\sigma_1,\sigma_1'}\int d^{3}\mathbf{x}_{1'}\int d^{3}\mathbf{x}_{1}\left\langle \psi_{\sigma_{1'}}^{\dagger}\left(\mathbf{x}_{1'}\right)v\left(\mathbf{x}_{1'}-\mathbf{x}_{1}\right)\psi_{\sigma_1}\left(\mathbf{x}_{1}\right)\right\rangle \delta_{\sigma_1,\sigma_{1'}}\delta\left(\mathbf{x}_{1'}-\mathbf{x}_{1}\right) \\
&\quad +\beta\sum_{\sigma_1,\sigma_{1'}}\int d^{3}\mathbf{x}_{1'}\int d^{3}\mathbf{x}_{1}\left\langle \psi_{\sigma_{1'}}^{\dagger}\left(\mathbf{x}_{1'}\right)\psi_{\sigma_{1'}}\left(\mathbf{x}_{1'}\right)v\left(\mathbf{x}_{1'}-\mathbf{x}_{1}\right)\psi_{\sigma_1}^{\dagger}\left(\mathbf{x}_{1}\right)\psi_{\sigma_1}\left(\mathbf{x}_{1}\right)\right\rangle \\
&= -\beta v(0)n\mathcal{V}+\beta\int d^{3}\mathbf{x}_{1'}\int d^{3}\mathbf{x}_{1}\left\langle n(\mathbf{x}_{1'})v\left(\mathbf{x}_{1'}-\mathbf{x}_{1}\right)n(\mathbf{x}_{1})\right\rangle
\end{aligned} \tag{30.6}$$

Recall that the definition for Matsubara susceptibility is

$$\chi_{nn}(\mathbf{x}_1,\tau_1;\mathbf{x}_2,\tau_2)=\langle\mathcal{T}_{\tau}n(\mathbf{x}_1,\tau_1)n(\mathbf{x}_2,\tau_2)\rangle \tag{30.7}$$

so we have

$$\begin{aligned}
&\int d^{3}\mathbf{x}_{1'}\int d^{3}\mathbf{x}_{1}\left\langle n\left(\mathbf{x}_{1'}\right)v\left(\mathbf{x}_{1'}-\mathbf{x}_{1}\right)n\left(\mathbf{x}_{1}\right)\right\rangle \\
=&\int d^{3}\mathbf{x}_{1'}\int d^{3}\mathbf{x}_{1}v\left(\mathbf{x}_{1'}-\mathbf{x}_{1}\right)\chi_{nn}\left(\mathbf{x}_{1'},0;\mathbf{x}_{1}0\right) \\
=&\mathcal{V}\int d^{3}(\mathbf{x}_{1'}-\mathbf{x}_{1})v(\mathbf{x}_{1'}-\mathbf{x}_{1})\chi_{nn}\left(\mathbf{x}_{1'}-\mathbf{x}_{1},0\right) \\
=&\mathcal{V}\int d^{3}\mathbf{x}\int\frac{d^{3}q_2}{(2\pi)^{3}}e^{i\mathbf{q}_2\cdot\mathbf{x}}V_{\mathbf{q}_2}\int\frac{d^{3}q_1}{(2\pi)^{3}}e^{i\mathbf{q}_1\cdot\mathbf{x}}\chi_{nn}\left(\mathbf{q}_1,0\right) \\
=&\int\frac{d^{3}q}{(2\pi)^{3}}V_{\mathbf{q}}\left[\lim_{\tau\to0}\mathcal{V}\chi_{nn}(\mathbf{q},\tau)\right] \\
=&\mathcal{V}\int\frac{d^{3}q}{(2\pi)^{3}}V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n)\right]
\end{aligned} \tag{30.8}$$

$$\begin{aligned}
2\langle V\rangle\beta &= -n\mathcal{V}\beta v(0)+\beta\mathcal{V}\int\frac{d^{3}q}{(2\pi)^{3}}V_{\mathbf{q}}T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n) \\
&= \beta\mathcal{V}\left\{\int\frac{d^{3}q}{(2\pi)^{3}}V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n)-n\right]\right\}
\end{aligned} \tag{30.9}$$

we have also

$$\begin{aligned}
\int_{1}\int_{1''}\Sigma\left(1,1''\right)\mathcal{G}\left(1'',1^{+}\right) &= \beta\mathcal{V}\left\{\int\frac{d^{3}q}{(2\pi)^{3}}V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n)-n\right]\right\} \\
\int_{1''}\Sigma\left(1,1''\right)\mathcal{G}\left(1'',1^{+}\right) &= \frac{1}{2}\int\frac{d^{3}q}{(2\pi)^{3}}V_{\mathbf{q}}\left[T\sum_{iq_n}\chi_{nn}(\mathbf{q},iq_n)-n\right]
\end{aligned} \tag{30.10}$$

where we used the spatial temporal translational invariance of $\Sigma\left(1,1''\right)\mathcal{G}\left(1'',1^{+}\right)$.

31 GW Curing of Hartree Fock

In this Section, we present the solution to the failure of Hartree-Fock that was found by Gell-Man and Brueckner. The Physics is that the interaction appearing in Hartree-Fock theory should be screened. Or equivalently, the self-energy that we find should be consistent with the density fluctuations found earlier since $\Sigma\mathcal{G}$ is simply related to the density fluctuations. The resulting expression that we will find is also known as the GW approximation.

31.1 Schwinger's way

In Schwinger's formalism, we already have an expression

$$\Sigma(1,\overline{2})\mathcal{G}\left(\overline{2},1^{+}\right)=V(1-\overline{2})\left\langle T_{\tau}\left[\psi^{\dagger}(\overline{2}^{+})\psi(\overline{2})\psi^{\dagger}(1^{+})\psi(1)\right]\right\rangle \tag{31.1}$$

It shows that we should have an approximation for the self-energy that, when multiplied by $\mathcal{G}$, gives the density-density correlation function. That is a very general result, or sum-rule, is a sort of consistency relation between one- and two-particle properties. This is a very important property that we will use also later in the context of non-perturbative treatments of the Hubbard model.

Returning to the self-energy expansion

$$\begin{aligned}\Sigma(1,3)_{\phi}=&-V(1-3)\mathcal{G}\left(1,3^{+}\right)_{\phi}-V(1-\overline{2})\mathcal{G}(1,\overline{4})_{\phi}\frac{\delta\Sigma(\overline{4},3)_{\phi}}{\delta\mathcal{G}(\overline{5},\overline{6})_{\phi}}\frac{\delta\mathcal{G}(\overline{5},\overline{6})_{\phi}}{\delta\phi\left(\overline{2^{+}},\overline{2}\right)}\\&+V(1-\overline{2})\mathcal{G}\left(\overline{2},\overline{2^{+}}\right)_{\phi}\delta(1-3).\end{aligned} \tag{31.2}$$

and replace the irreducible vertex $\delta\Sigma/\delta\mathcal{G}$ by the one shown in Fig. 41-3 that we used to compute the density-density correlation function illustrated in Fig. 37-7. Note that as before in the RPA approximation, we keep the most divergent diagrams which are proportional to $V_{\mathbf{q}}$. The final result is illustrated in Fig. 44-5. We just need to replace the functional derivative of the Green function appearing at the bottom right by the RPA series illustrated in Fig. 41-3. Recalling that the Hartree term vanishes, the final result is

$$\begin{aligned}\Sigma_{RPA}\left(\mathbf{k},ik_{n}\right)&=\Sigma^{(2)}\left(\mathbf{k},ik_{n}\right)\\&=-\sum_{q}\mathcal{G}(k+q)V(q)-\sum_{q}\mathcal{G}(k+q)V(q)V(q)\chi_{nn}(q)\\&=-\int\frac{d^{3}\mathbf{q}}{(2\pi)^{3}}T\sum_{iq_{n}}V_{\mathbf{q}}\left[1-\frac{V_{\mathbf{q}}\chi_{nn}^{0}\left(\mathbf{q},iq_{n}\right)}{1+V_{\mathbf{q}}\chi_{nn}^{0}\left(\mathbf{q},iq_{n}\right)}\right]\mathcal{G}\left(\mathbf{k}+\mathbf{q},ik_{n}+iq_{n}\right)\\&=-\int\frac{d^{3}\mathbf{q}}{(2\pi)^{3}}T\sum_{iq_{n}}\frac{V_{\mathbf{q}}}{1+V_{\mathbf{q}}\chi_{nn}^{0}\left(\mathbf{q},iq_{n}\right)}\mathcal{G}\left(\mathbf{k}+\mathbf{q},ik_{n}+iq_{n}\right)\end{aligned} \tag{31.3}$$

where the first term comes from the Fock contribution.Using our result for the longitudinal dielectric constant that follows from the density fluctuations in the RPA approximation

$$\Sigma^{(2)}(k)=-\int\frac{d^{3}\mathbf{q}}{(2\pi)^{3}}T\sum_{iq_{n}}\frac{V_{\mathbf{q}}}{\varepsilon_{L}\left(\mathbf{q},iq_{n}\right)/\varepsilon_{0}}\mathcal{G}\left(\mathbf{k}+\mathbf{q},ik_{n}+iq_{n}\right)e^{ik_{n}\eta} \tag{31.4}$$

comparing this with the Hartree-Fock approximation

$$\Sigma^{(1)}(k)=-\int\frac{d^{3}\mathbf{q}}{(2\pi)^{3}}T\sum_{iq_{n}}V_{\mathbf{q}}\mathcal{G}\left(\mathbf{k}+\mathbf{q},ik_{n}+iq_{n}\right)e^{ik_{n}\eta} \tag{31.5}$$

the effective interaction entering the Fock term should be the screened one instead of the bare one. The two are equal only at very high frequency. The screened potential

$$W(q)=\frac{V_{\mathbf{q}}}{\varepsilon_{L}\left(\mathbf{q},iq_{n}\right)/\varepsilon_{0}}=\frac{e^{2}}{\varepsilon_{L}\left(\mathbf{q},iq_{n}\right)q^{2}} \tag{31.6}$$

is often denotes W which means the integrand is $W\mathcal{G}^{0}$, hence the name **GW approximation**.

In the book we used $\mathcal{G}=\mathcal{G}^{0}$, is this necessary? Why didn't we use this in the Hartree-fock approximation for self-energy?

32 Physics in Single-particle Properties

In this Chapter, we interpret the results of calculations based on formulas of the previous Chapter, and compare with experiments. In particular, after a look at the overall picture, we will recover theoretically the Fermi liquid regime, and compare with experiment.

32.1 Single-particle spectral weight

The real-part and the absolute value of the imaginary part of the RPA self-energy at zero temperature are plotted in Fig.(45-1) as a function of frequency for three different wave vectors. In the Hartree-Fock approximation, the self-energy was completely frequency independent. The result here is quite different. The screened interation contains the **plasmons** and has a drastic effect on single-particle properties. There are several points worth mentioning.

1. $\Im\Sigma(\mathbf{k},\omega=0)=0$ for all wave vectors. This is true only at zero temperature. This property will play a key role in the derivation of Luttinger's theorem later.

2. The straight line that appears on the plots is $\omega-\varepsilon_{\mathbf{k}}$. The intersection of this straight line with $\Re\Sigma$, which is defined on the figure to contain the chemical potential, corresponds (in our notation) to the solution of the equation
$$\omega-\varepsilon_{\mathbf{k}}=\Re\Sigma^R(\mathbf{k},\omega)-\mu \tag{32.1}$$
which determines the position of maxima in the spectral weight,
$$\begin{aligned} A(\mathbf{k},\omega) &= -2\Im G^R(\mathbf{k},\omega) \\ &= \frac{-2\Im\sum^R(\mathbf{k},\omega)}{\left(\omega-\zeta_{\mathbf{k}}-\Re\sum^R(\mathbf{k},\omega)\right)^2+\left(\Im\sum^R(\mathbf{k},\omega)\right)^2} \end{aligned} \tag{32.2}$$
maxima that we identify as quasiparticles. Let us look at the solution near $\omega=0$. These correspond to a peak in the spectral weight Fig.(45-2). At the Fermi wave vector, the peak is located precisely where the imaginary part of the self-energy vanishes, hence the peak is a delta function. On the other hand, away from $k=k_F$, the maximum is located in a region where the imaginary part is not too large, hence the quasiparticle has a finite lifetime. Recall that to have the quasiparticle shape described by Fermi liquid theory
$$A(\mathbf{k},\omega)\approx 2\pi Z_{\mathbf{k}}\left[\frac{1}{\pi}\frac{\Gamma_{\mathbf{k}}(\omega)}{\left(\omega-E_{\mathbf{k}}+\mu\right)^2+\left(\Gamma_{\mathbf{k}}(\omega)\right)^2}\right]+inc \tag{32.3}$$
it is necessary that at the crossing point, the slope of $\Re\Sigma^R(\mathbf{k},\omega)$ be negative because it is necessary that
$$Z_{\mathbf{k}}=\frac{1}{1-\frac{\partial}{\partial\omega}\Re\Sigma^R(\mathbf{k},\omega)\big|_{\omega=E_{\mathbf{k}}-\mu}}\in[0,1] \tag{32.4}$$
if the previous formula is to make sense.

3. indicated on Fig. 45-1, there is a threshold-like feature at $\omega_p=\pm 1$where $Im\Sigma^R$ becomes large. This is when the one-particle excitations can emit or absorb real plasmons.

4. From the previous discussion, we see that the two maxima away from $\omega=0$ at $k=k_F$ do not correspond to quasiparticle solutions. The weight near the maxima away from $\omega=0$ come from scattering rates $\Im\Sigma^R$ that are large, but not too large compared with the value of $\omega-\zeta_{\mathbf{k}}-\Re\Sigma^R(\mathbf{k},\omega)$. At the threshold where $\Im\Sigma^R$ is really large, the spectral weight in fact vanishes. Note that the maxima away from $\omega=0$ at $k=k_F$ are near the value of ω where the quasiparticle condition is almost satisfied.

5. For the figure on the right, $k=1.4k_F$, the peak nearest $\omega=0$ corresponds to a quasiparticle solution. Note however that for wave vectors so far from the Fermi surface, the width of the peak starts to be quite a bit larger. The maxima further away all occur in regions where $\Im\Sigma^R$ is large and the quasiparticle condition is almost satisfied.

6. For $k=0.6k_F$, there seems to be an additional quasiparticle solution, namely a solution where $\frac{\partial}{\partial\omega}\Re\Sigma^R$ is negative and $\Im\Sigma^R$ is not too large, located at an energy ω_p below the main quasiparticle energy. Since the free-electron band is bounded from below, $\Im\Sigma^R$ vanishes at sufficiently negative frequency, allowing a new solution to develop when interactions are sufficiently strong. This solution looks like a bound state.

32.2 Simplifying the expression for Σ''

In this section, we write the imaginary part of the self-energy in a form that is easy to interpret physically. The evaluation in the Fermi-liquid limit is given in the following section. Here we want to first show that the imaginary part of the self-energy defined by

$$\Sigma^R(\mathbf{k},\omega) = \Sigma'(\mathbf{k},\omega) + i\Sigma''(\mathbf{k},\omega) \tag{32.5}$$

may be written in the form

$$\Sigma''(\mathbf{k},\omega) = -\frac{m}{2|k|}\int\frac{d^2q_\perp}{(2\pi)^2}\int\frac{d\omega'}{\pi}\left[n_B(\omega')+f(\omega+\omega')\right]V_{\mathbf{q}}^2\chi''_{nn}\left(q_\perp,q_\parallel,\omega'\right) \tag{32.6}$$

where $q_\parallel$ is the solution of the equation

$$\frac{|k|}{m}q_\parallel + \frac{q_\parallel^2}{2m} = \left[\omega+\omega'-\left(\frac{k^2}{2m}-\mu+\frac{q_\perp^2}{2m}\right)\right] \tag{32.7}$$

To prove this, recall that RPA self-energy is

$$\begin{aligned}\Sigma_{RPA}(\mathbf{k},ik_n) &= -\sum_q \mathcal{G}(k+q)V(q) - \sum_q \mathcal{G}(k+q)V(q)V(q)\chi_{nn}(q)\\ &= -\int\frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{iq_n}V_{\mathbf{q}}\left[1-\frac{V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)}{1+V_{\mathbf{q}}\chi^0_{nn}(\mathbf{q},iq_n)}\right]\mathcal{G}(\mathbf{k}+\mathbf{q},ik_n+iq_n)\\ &= \Sigma_{HF}(\mathbf{k}) + \int\frac{d^3\mathbf{q}}{(2\pi)^3}T\sum_{iq_n}\left[V_{\mathbf{q}}\chi^{RPA}_{nn}(\mathbf{q},iq_n)V_{\mathbf{q}}\right]\mathcal{G}(\mathbf{k}+\mathbf{q},ik_n+iq_n)\end{aligned} \tag{32.8}$$

the first part at $T=0$ is the Hartree-Fock approximation. The important points are that

1. it is the only contribution that survives at $\omega\to\infty$
2. the imaginary part comes only from the second term

To find the imaginary part, let us concentrate on this last expression and use the spectral representation for χ^{RPA}_{nn},

$$\chi_{nn}(\mathbf{q},z) = \int\frac{d\omega'}{\pi}\frac{\chi''_{nn}(\mathbf{q},\omega')}{\omega'-z} \tag{32.9}$$

$$\chi^{RPA}_{nn}(\mathbf{q},iq_n) = \lim_{z\to iq_n}\int\frac{d\omega'}{\pi}\frac{\chi''_{nn}(\mathbf{q},\omega')}{\omega'-z} = \int\frac{d\omega'}{\pi}\frac{\chi''_{nn}(\mathbf{q},\omega')}{\omega'-iq_n} \tag{32.10}$$

We have (Here we have taken $\mathcal{G}\to\mathcal{G}_0$)

$$\Sigma_{RPA}(\mathbf{k},ik_n) - \Sigma_{HF}(\mathbf{k}) = \int\frac{d^3\mathbf{q}}{(2\pi)^3}\int\frac{d\omega'}{\pi}T\sum_{iq_n}\left[V_{\mathbf{q}}\frac{\chi''_{nn}(\mathbf{q},\omega')}{\omega'-iq_n}V_{\mathbf{q}}\right]\frac{1}{ik_n+iq_n-\zeta_{\mathbf{k}+\mathbf{q}}} \tag{32.11}$$

we do the Matsubara summation first

$$\begin{aligned}-T\sum_{iq_n}\frac{1}{iq_n-\omega'}\frac{1}{iq_n+ik_n-\zeta_{\mathbf{k}+\mathbf{q}}} &= -T\sum_{iq_n}\left[\frac{1}{iq_n-\omega'}-\frac{1}{iq_n+ik_n-\zeta_{\mathbf{k}+\mathbf{q}}}\right]\frac{1}{ik_n+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}}\\ &= \left[T\sum_{iq_n}\frac{-e^{ik_n0^+}}{iq_n-\omega'}+T\sum_{iq_n}\frac{e^{ik_n0^+}}{iq_n+ik_n-\zeta_{\mathbf{k}+\mathbf{q}}}\right]\frac{1}{ik_n+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}}\\ &= \left[n_B(\omega')+f(\zeta_{\mathbf{k}+\mathbf{q}})\right]\frac{1}{ik_n+\omega'-\zeta_{\mathbf{k}+\mathbf{q}}}\end{aligned} \tag{32.12}$$

we have

$$\begin{aligned}
\Sigma_{RPA}\left(\mathbf{k}, ik_n\right) - \Sigma_{HF}(\mathbf{k}) &= \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} \left[n_B(\omega') + f(\zeta_{\mathbf{k}+\mathbf{q}})\right] \frac{V_{\mathbf{q}}\chi''_{nn}(\mathbf{q},\omega')V_{\mathbf{q}}}{ik_n + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}} \\
\Sigma^R_{RPA}\left(\mathbf{k}, \omega\right) - \Sigma^R_{HF}(\mathbf{k}) &= \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} \left[n_B(\omega') + f(\zeta_{\mathbf{k}+\mathbf{q}})\right] \frac{V_{\mathbf{q}}\chi''_{nn}(\mathbf{q},\omega')V_{\mathbf{q}}}{\omega + i\eta + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}} \\
\Sigma''\left(\mathbf{k}, ik_n\right) &= \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} \left[n_B(\omega') + f(\omega+\omega')\right] V_{\mathbf{q}}\chi''_{nn}(\mathbf{q},\omega')V_{\mathbf{q}}(-\pi)\delta(\omega + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}) \\
&= -\int \frac{d^2\mathbf{q}_\perp}{(2\pi)^2} \int \frac{d\omega'}{\pi} \left[n_B(\omega') + f(\omega+\omega')\right] \left\{ \int \frac{dq_\parallel}{2} \delta(\omega + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}) V^2_{\mathbf{q}} \chi''_{nn}(\mathbf{q},\omega') \right\}
\end{aligned} \tag{32.13}$$

where we've defined $q_\parallel$ by the direction parallel to the wave vector $\mathbf{k}$ and calling $q_\perp$ the other directions. Given a fixed $\mathbf{q}_\perp$, ω and ω',the integral over $q_\parallel$ can be performed, first note

$$\delta(\omega + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}) = \left| \frac{d\zeta_{\mathbf{k}+\mathbf{q}}}{dq_\parallel} \right|^{-1} \delta(q_\parallel - q^0_\parallel) = \frac{m}{k + q^0_\parallel} \delta(q_\parallel - q^0_\parallel) \tag{32.14}$$

where $q^0_\parallel$ is a solution of the following equation

$$\begin{aligned}
\left[\omega + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}\right]_{q_\parallel = q^0_\parallel} &= 0 \\
\omega + \omega' - \frac{k^2 + 2kq^0_\parallel + (q^0_\parallel)^2 + q^2_\perp}{2m} + \mu &= 0 \\
\frac{|k|}{m} q^0_\parallel + \frac{\left(q^0_\parallel\right)^2}{2m} &= \omega + \omega' - \left(\frac{k^2}{2m} - \mu + \frac{q^2_\perp}{2m} \right)
\end{aligned} \tag{32.15}$$

so the integral in {...} is

$$\left[\frac{m}{2k + 2q^0_\parallel} V^2_{\mathbf{q}} \chi''_{nn}(\mathbf{q},\omega') \right]_{q_\parallel = q^0_\parallel} \tag{32.16}$$

(somehow the denomenator is changed to $2k$ in the book?)

We then obtain, assuming that we are in a region of frequency where the delta function has a solution, the desired result

$$\Sigma''(\mathbf{k},\omega) = -\frac{m}{2|k|} \int \frac{d^2q_\perp}{(2\pi)^2} \int \frac{d\omega'}{\pi} \left[n_B\left(\omega'\right) + f\left(\omega+\omega'\right)\right] V^2_{\mathbf{q}} \chi''_{nn}\left(q_\perp, q_\parallel, \omega'\right) \tag{32.17}$$

In the zero temperature limit, $f\left(\omega+\omega'\right) = \theta\left(-\omega-\omega'\right)$ and $n_B\left(\omega'\right) = -\theta\left(-\omega'\right)$ so that if we take $\omega > 0$ then the integral over ω' extends over the interval $-\omega < \omega' < 0$ where $n_B\left(\omega'\right) + f\left(\omega+\omega'\right)$ takes the value -1. At low temperature, the contributions to Σ'' will come mostly from this same frequency interval since this is where the combination $n_B\left(\omega'\right) + f\left(\omega+\omega'\right) \neq 0$. This immediately allows us to understand why the imaginary part of the self-energy in Fig.(45-1) above starts to be large when the frequency becomes of the order of the plasma frequency. This is only when ω is that large that the contributions from $\omega' \approx \omega_p$ in χ''_{nn} can start to contribute. This is where the quasiparticles can start to absorb or emit plasmons.

It is easier to interpret the physical meaning of the imaginary part by concentrating on the case $\omega > 0$ and then performing a change of variables $\omega' \to -\omega'$. Then the integration window at $T = 0$ becomes $-\omega < -\omega' < 0$, or $\omega > \omega' > 0$. Using

$$n_B\left(-\omega'\right) = -\left(1 + n_B\left(\omega'\right)\right) \tag{32.18}$$

and $\chi''_{nn}\left(\mathbf{q},-\omega'\right) = -\chi''_{nn}\left(\mathbf{q},\omega'\right) = -\chi''_{nn}\left(-\mathbf{q},\omega'\right)$, the imaginary part of the self-energy becomes

$$\begin{aligned}
\Sigma''(\mathbf{k},\omega) &= -\pi \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} \left[n_B(\omega') + f(\omega+\omega')\right] V^2_{\mathbf{q}} \chi''_{nn}(\mathbf{q},\omega') \delta(\omega + \omega' - \zeta_{\mathbf{k}+\mathbf{q}}) \\
&= -\pi \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\omega'}{\pi} \left[\left(1 + n_B\left(\omega'\right)\right) - f\left(\omega-\omega'\right)\right] V^2_{\mathbf{q}} \chi''_{nn}\left(\mathbf{q},\omega'\right) \delta\left(\omega - \omega' - \zeta_{\mathbf{k}+\mathbf{q}}\right) \\
&= -\int \frac{d^3\mathbf{q}}{(2\pi)^3} \left[1 + n_B(\omega - \zeta_{\mathbf{k}+\mathbf{q}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})\right] V^2_{\mathbf{q}} \chi''_{nn}(\mathbf{q}, \omega - \zeta_{\mathbf{k}+\mathbf{q}}) \\
&= -\int \frac{d^3\mathbf{q}}{(2\pi)^3} V^2_{\mathbf{q}} \chi''_{nn}(-\mathbf{q}, \omega - \zeta_{\mathbf{k}+\mathbf{q}}) \left[\left(1 + n_B(\omega - \zeta_{\mathbf{k}+\mathbf{q}})\right)\left(1 - f(\zeta_{\mathbf{k}+\mathbf{q}})\right) + n_B(\omega - \zeta_{\mathbf{k}+\mathbf{q}}) f(\zeta_{\mathbf{k}+\mathbf{q}})\right]
\end{aligned} \tag{32.19}$$

The first term $(1+n_B(\omega-\zeta_{\mathbf{k}+\mathbf{q}}))(1-f(\zeta_{\mathbf{k}+\mathbf{q}}))$ represents the decay of a particle of energy ω and wave vector $\mathbf{k}$ into an empty particle state of energy $\zeta_{\mathbf{k}+\mathbf{q}}$ and momentum $\mathbf{k}+\mathbf{q}$, plus a bosonic excitation (particle-hole continuum or plasmon) of energy $\omega-\zeta_{\mathbf{k}+\mathbf{q}}$ and momentum $-\mathbf{q}$. The second term $n_B(\omega-\zeta_{\mathbf{k}+\mathbf{q}})f(\zeta_{\mathbf{k}+\mathbf{q}})$ represents the case where the incident state is a hole of energy ω and wave vector $\mathbf{k}$ that decays into another hole of energy $\zeta_{\mathbf{k}+\mathbf{q}}$ and momentum $\mathbf{k}+\mathbf{q}$ by absorbing a boson of energy $\omega-\zeta_{\mathbf{k}+\mathbf{q}}$ and momentum $-\mathbf{q}$. The latter is in some sense the first process but time reversed. This is illustrated in Fig.(45-3). "Scattering-in" terms that represent repopulation of the state $\mathbf{k}$ occur in transport equations, or two-body response functions, not here.

32.3 Fermi liquid results

We now demonstrate the frequency dependence $\Sigma''(\mathbf{k}_F,\omega;T=0)\propto\omega^2$, which is essential in the establishment of quasiparticles in Fermi liquid theory. We will also find out the temperature dependence $\Sigma''(\mathbf{k}_F,\omega=0;T)\propto T^2$. Consider the imaginary part of self energy at $\mathbf{k}=k_F$

$$\Sigma''(k_F,\omega)=-\frac{1}{2v_F}\int\frac{d^2q_\perp}{(2\pi)^2}\int\frac{d\omega'}{\pi}\left[n_B(\omega')+f(\omega+\omega')\right]V_{\mathbf{q}}^2\chi''_{nn}(q_\perp,q_\parallel,\omega') \tag{32.20}$$

(here it may be argued that $q_\parallel^0\ll k_F$ so we ignore this factor in $k+q_\parallel^0$)

$$v_Fq_\parallel+\frac{q_\parallel^2}{2m}=\left[\omega+\omega'-\frac{q_\perp^2}{2m}\right] \tag{32.21}$$

The key to understanding the Fermi liquid regime is in the relative width in frequency of $\chi''_{nn}(\mathbf{q},\omega')/\omega'$ vs the width of the combined Bose and Fermi functions. In general, the function $n_B(\omega')+f(\omega+\omega')$ depends on ω' on a scale $\max(\omega,T)$ while far from a phase transition, $\chi''_{nn}(\mathbf{q},\omega')/\omega'$ depends on frequency only on the scale of the Fermi energy.

At the $\omega'\to0$ limit, we can assume $\chi''_{nn}(\mathbf{q},\omega')/\omega'$ to be independent of frequency. To see this, using the fact that $\Im\chi^{0R}_{nn}(\mathbf{q},0)=0$ from the explicit expression

$$\begin{aligned}\lim_{\omega\to0}\Im\frac{\chi}{\omega}&=\lim_{\omega\to0}\frac{1}{\omega}\Im\frac{\chi^0}{1+V_{\mathbf{q}}\chi^0}\\&=\lim_{\omega\to0}\frac{\Im\chi^0/\omega}{\left(1+V_{\mathbf{q}}\Re\chi^0\right)^2+\left(V_{\mathbf{q}}\Im\chi^0\right)^2}\\&=\frac{\lim_{\omega\to0}\Im\chi^0/\omega}{\left(1+V_{\mathbf{q}}\Re\chi^0\right)^2}\end{aligned} \tag{32.22}$$

so we have

$$\lim_{\omega\to0}\Im\chi^R_{nn}(\mathbf{q},\omega)/\omega=\frac{\lim_{\omega\to0}\Im\chi^{0R}_{nn}(\mathbf{q},\omega)/\omega}{\left(1+V_{\mathbf{q}}\Re\chi^{0R}_{nn}(\mathbf{q},0)\right)^2} \tag{32.23}$$

it suffices that the Lindhard function $\Im\chi^{0R}_{nn}(\mathbf{q},\omega)$ has the property that $\Im\chi^{0R}_{nn}(\mathbf{q},\omega)/\omega$ is independent of frequency at low frequency. This is indeed the case, as can be checked from equation 28.13

$$\frac{\Im\chi^{0R}_{nn}(\mathbf{q},\omega)}{\omega}=\frac{\Im\epsilon^L(\mathbf{q},\omega)}{\omega\varepsilon_0V_{\mathbf{q}}}=\frac{\pi}{2}\frac{1}{\varepsilon_0V_{\mathbf{q}}}\frac{1}{v_Fq}\frac{q_{TF}^2}{q^2} \tag{32.24}$$

for $q<2k_F$ and $\omega\le v_Fq-\varepsilon_q$. We will assume this constant in the frequency range over which $n_B(\omega')+f(\omega+\omega')$ differs from zero. We also have that

$$V_{\mathbf{q}}^2\frac{\Im\chi^R_{nn}(\mathbf{q},\omega)}{\omega}=\frac{\pi}{2}\frac{V_{\mathbf{q}}}{\varepsilon_0}\frac{1}{v_Fq}\frac{q_{TF}^2}{q^2}=\frac{\pi}{2}\frac{e^2}{\varepsilon_0^2}\frac{1}{v_Fq^3}\frac{q_{TF}^2}{q^2} \tag{32.25}$$

so the integral, defined as $A(k_F)$ is then dependent only on $q_\parallel$

$$\begin{aligned}A(k_F)&\equiv\int\frac{d^2q_\perp}{(2\pi)^2}\lim_{\omega'\to0}\frac{V_{\mathbf{q}}^2\chi''_{nn}\left(q_\perp,q_\parallel(q_\perp,v_F);\omega'\right)}{\omega'}\\&=\frac{\pi}{2}\frac{e^2}{\varepsilon_0^2v_F}\frac{1}{(2\pi)^2}\frac{1}{q_{TF}}\int\frac{d^2q_\perp}{q_{TF}^2}\frac{1}{(q_\perp^2/q_{TF}^2+q_\parallel^2/q_{TF}^2)^{5/2}}\end{aligned} \tag{32.26}$$

which in turn depends on ω and ω', satisfying

$$\begin{aligned}(q_\parallel + k_F)^2 &= 2m(\omega+\omega') + k_F^2 - q_\perp^2 \approx k_F^2 - q_\perp^2 \\ q_\parallel &= k_F\left[\sqrt{1-q_\perp^2/k_F^2} - 1\right]\end{aligned} \tag{32.27}$$

where in the small frequency limit, $\omega, \omega' \ll E_F = \frac{k_F^2}{2m}$, so $q_\parallel$ would be independent of ω, ω'. In this sense,

$$A(k_F) = \frac{\pi}{2}\frac{e^2}{\varepsilon_0^2 v_F}\frac{1}{(2\pi)^2}\frac{1}{q_{TF}}\int \frac{d^2q_\perp}{q_{TF}^2}\frac{1}{(q_\perp^2/q_{TF}^2 + k_F^2/q_{TF}^2\left(\sqrt{1-q_\perp^2/k_F^2}-1\right)^2)^{5/2}} \tag{32.28}$$

which we shall not evaluate right now. The remaining part of the integral is

$$\Sigma''(k_F,\omega) = -\frac{A(k_F)}{2v_F}\int\frac{d\omega'}{\pi}\left[n_B(\omega') + f(\omega+\omega')\right]\omega' \tag{32.29}$$

we can evaluate the frequency integral exactly,

$$\int_{-\infty}^{\infty} d\omega'\left[n_B(\omega') + f(\omega+\omega')\right]\omega' = \frac{1}{2}\left[\omega^2 + (\pi T)^2\right] \tag{32.30}$$

so we finally have

$$\Sigma''(k_F,\omega) \approx -\frac{A(\mathbf{k}_F)}{4\pi v_F}\left[\omega^2 + (\pi T)^2\right] \tag{32.31}$$

(in the book there is one less π in the denominator)

We now just quote without proof some of the results of further calculations of Fermi liquid parameters. The solution of the quasiparticle equation

$$E_\mathbf{k} - \mu - \varepsilon_\mathbf{k} = \Re\Sigma^R(\mathbf{k}, E_\mathbf{k}-\mu) - \mu \tag{32.32}$$

gives

$$E_\mathbf{k} = \varepsilon_\mathbf{k} - 0.17 r_s\left(\ln r_s + 0.2\right)\frac{k_F k}{2m} + cst \tag{32.33}$$

The effective mass appearing in this expression is now obviously finite and given

$$m^* = \frac{m}{1 - 0.08 r_s\left(\ln r_s + 0.2\right)} \tag{32.34}$$

If we evaluate the scattering rate for $\omega = E_\mathbf{k} - \mu$ we find

$$\Gamma_\mathbf{k}\left(E_\mathbf{k}-\mu\right) = 0.25 r_s^{1/2}\frac{\left(k-k_F\right)^2}{2m} \tag{32.35}$$

Quinn and Ferrell write the following physically appealing form

$$\Gamma_\mathbf{k}\left(\zeta_\mathbf{k}\right) Z_\mathbf{k}^{-1} = \frac{\sqrt{3}\pi^2}{128}\omega_p\left(\frac{\zeta_\mathbf{k}}{E_F}\right)^2 \tag{32.36}$$

The scattering rate is proportional to the plasma frequency, but reduced by an important phase space factor. The more general results, beyond leading order in r_s can be found in Eqs.(8.92-8.93) of Giuliani and Vignale "Quantum theory of the electron liquid".

Fig.(45-4) gives the value of the Σ' and Σ'' evaluated at the frequency corresponding to the quasiparticle position. The important point is that the real-part of the self-energy is weakly wave vector dependent up to about $k = 2k_F$. The imaginary part on the other hand vanishes as expected on the Fermi surface, while away from it remains relatively small on the scale of the Fermi energy. This justifies a posteriori the success of the free electron picture of solids.

32.4 Comparison with experiments

We are finally ready to compare the predictions of this formalism to experiments. The results shown in the present section are taken from G.D. Mahan, op. cit., Sec.5.8.

The first quantity that comes to mind to compare with experiment is the effective mass. This quantity can in principle be obtained from cyclotron resonance or from specific heat measurements. It turns out however that the theoretical prediction for m^*/m differs from unity by only about 10%. But what makes comparisons with experiment for this quantity very difficult is that there are two other contributions to the effective mass in real materials. First there are **band structure effects**. These are small in sodium but large in lithium and many other metals. The second additional contribution to the effective mass comes from **electron-phonon interactions**. We will see in the next chapter that these effects can be quite large. So we need to wait.

A striking prediction of many body theory is that the size of the jump in momentum distribution at the Fermi level at zero temperature should be quite different from unity. Fig.(45-5) illustrates the prediction for sodium at $r_s = 3.97$. The following Table of expected jumps is from Hedin[8].

r_s	Z_{RPA}
0	1
1	0.859
2	0.768
3	0.700
4	0.646
5	0.602
6	0.568

(32.37)

Unfortunately even through photoemission we do not have access directly to this jump in three dimensional materials, as we discussed in the previous chapter. Another probe that gives indirect access to this jump is Compton scattering. In Compton scattering, a photon scatters off an electron, leaving with a different energy an momentum along with an electron in a new momentum state. This is really as if photons scattered-off electrons as billiard balls, conserving energy and momentum. Photons are scattered inelastically from all the electrons in the solid. The contribution from conduction electrons can be extracted by subtraction. In the so-called "sudden approximation", the cross section for photon scattering is proportional to

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \int d^3\mathbf{k} n_{\mathbf{k}} \delta\left(\omega + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}\right) \tag{32.38}$$

where ω is the energy and $\mathbf{q}$ the wave vector transferred by the photon and $n_{\mathbf{k}} = \left\langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \right\rangle$. We do not need $(1 - n_{\mathbf{k}+\mathbf{q}})$ to insure that the final electron state is empty because the energy transfer is so large, as we see in the experimental results, that we are sure the state will be empty. Changing to polar coordinates, we see that

$$\begin{aligned} \frac{d^2\sigma}{d\omega d\Omega} &\propto \int k^2 dk d(\cos\theta) n_{\mathbf{k}} \delta\left(\omega - \varepsilon_{\mathbf{q}} - \frac{kq}{m}\cos\theta\right) \\ &\propto \int k^2 dk n_k \int_{-1}^{1} d(\cos\theta) \delta\left(Q - k\cos\theta\right) \\ &\propto \int k dk \frac{m}{q} n_k \theta(k - |Q|) \end{aligned} \tag{32.39}$$

where

$$Q \equiv \frac{m}{q}\left(\varepsilon_q - \omega\right) \tag{32.40}$$

in terms of Q, we have

$$\frac{d^2\sigma}{d\omega d\Omega} \propto \frac{1}{q}\int_{|Q|}^{\infty} n_k k dk \tag{32.41}$$

For free electrons, $n_k = \theta(k_F - k)$, this gives

$$\frac{d^2\sigma}{d\omega d\Omega} \propto J(Q) \propto \frac{1}{2q}\left(k_F^2 - Q^2\right)\theta\left(k_F - Q\right) \tag{32.42}$$

In this case then, the slope is discontinuous at $k_F = Q$ as illustrated on the left of Fig.(45-6). In the interacting case, the change in slope at k_F remains theoretically related to Z. Also, one expects a signal above k_F as illustrated on the left of the figure. Experimental results for sodium, $r_s = 3.96$, are given on the right of the figure along with the theoretical prediction. This metal is the one closest to the free electron model. The experimentalists have verified that Q is a good scaling variable, in other words that the cross section depends mainly on Q. Also, the existence of a tail above k_F is confirmed. However, the agreement with theory is not excellent.

The experimental results for the mean free path are more satisfactory. Let the mean free path $\ell_{\mathbf{k}}$ be defined by

$$\frac{1}{\ell_{\mathbf{k}}} = \frac{\Gamma_{\mathbf{k}}}{v_{\mathbf{k}}} = \frac{1}{\tau_{\mathbf{k}} v_{\mathbf{k}}} = -\frac{2}{v_{\mathbf{k}}} \Im\Sigma\left(\mathbf{k}, \zeta_{\mathbf{k}}\right) \tag{32.43}$$

Fig.(45-7) presents the results of experiments on aluminum, $r_s = 2.07$. If one takes into account only scattering by plasmons one obtains the dashed line. The full RPA formula, including the contribution from the particle-hole continuum, was obtained numerically by Lundqvist for $r_s = 2$ and is in excellent agreement with experiment.

The cross section for inelastic electron scattering, that is proportional to $\Im\left(1/\varepsilon^L\right)$, is shown in Fig. (45-8) for aluminum. The plasma resonance at low momentum transfer is visible around 15eV for the larger nanoparticles. You can even see the two plasmon peak around 30eV. The resonance is much larger than the particle-hole continuum, as we saw in the theoretical plot of Fig.(41-6). The small peak at small frequency is a surface plasmon. In Ref. [227] you can find an analysis of the width of the plasmon. It comes, in particular, from the decay of the plasmon in other conduction-electron bands.

33 Free Energy Calculations

The diagram rules for the free energy are more complicated than for the Green's function. For those that have followed the Feynman track, we have seen in the previous chapter the form of the linked-cluster theorem for the free-energy. It is given by a sum of connected diagrams. However, in doing the Wick contractions for a term of order n, there will be $(n-1)!$ identical diagrams instead of $n!$. This means that there will be an additional $1/n$ in front of diagrams of order n, by contrast with what happened for Green's functions. This makes infinite resummations a bit more difficult (but not undoable!).

33.1 Free energy and consistency between one and two-particle quantities

I first start with a general theorem to compute the free energy and show that it can be obtained either directly from the density fluctuations or from the self-energy and the Green's function, which we know already are related. This trick is apparently due to Pauli[14]. Assume $K = H_0 + \lambda V - \mu N$ parametrized by λ, we have

$$-\frac{1}{\beta}\frac{\partial \ln Z}{\partial \lambda} = -\frac{1}{\beta}\frac{1}{Z}\frac{\partial Tr\left[e^{-\beta(H_0+\lambda V-\mu N)}\right]}{\partial \lambda} = \frac{1}{Z}\,\mathrm{Tr}\left[e^{-\beta(H_0+\lambda V-\mu N)}V\right] = \frac{1}{\lambda}\langle \lambda V\rangle_\lambda \tag{33.1}$$

we can treat the above equation as a differential equation with respect to λ, define free energy $\Omega = -T\ln Z$, we have

$$\frac{d}{d\lambda}\Omega = \frac{1}{\lambda}\langle \lambda V\rangle_\lambda, \qquad \Omega(\lambda = 0) = \Omega_0 = -T\ln Z_0 \tag{33.2}$$

suppose we are able to calculate the RHS for every $\lambda \in [0,1]$, we would then obtain $\Omega(\lambda)$ in this range. Our final goal is to obtain $\Omega(\lambda = 1)$, this is then written as an integral over λ

$$\Omega = -T\ln Z = -T\ln Z_0 + \int_0^1 \frac{d\lambda}{\lambda}\langle \lambda V\rangle_\lambda \tag{33.3}$$

The expectation value of the potential energy may be obtained by writing down directly a diagrammatic expansion, or by using what we already know, namely the **density correlations**. Indeed we have shown in a previous section how the potential energy may be obtained from density correlations,

$$\begin{aligned}\Omega =& -T\ln Z = -T\ln Z_0 \\ &+ \frac{\mathcal{V}}{2}\int_0^1 d\lambda \int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}} \left[T\sum_{iq_n} \chi^\lambda_{nn}\left(\mathbf{q}, iq_n\right) - n\right]\end{aligned} \tag{33.4}$$

[14] A.L. Fetter and J.D. Walecka, op. cit., p.69

Using our previous relation between self-energy and potential energy, the coupling-constant integration may also be done with

$$\Omega = -T \ln Z_0 + \frac{T}{2} \int_0^1 \frac{d\lambda}{\lambda} \int_1 \int_{1''} \Sigma_\lambda \left(1, 1''\right) \mathcal{G}_\lambda \left(1'', 1^+\right) \tag{33.5}$$

where the subscript λ reminds oneself that the interaction Hamiltonian must be multiplied by a coupling constant λ.

33.2 Free energy for the Coulomb gas in the RPA approximation

In the zero temperature limit, we have that

$$\begin{aligned} E_{\text{tot}}^{RPA}(T=0) - \mu N &= \lim_{T\to 0} \Omega \\ &= \lim_{T\to 0} \left\{-T \ln Z_0\right\} + \lim_{T\to 0} \left\{ \frac{\mathcal{V}}{2} \int_0^1 d\lambda \int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}} \left[T \sum_{iq_n} \chi_{nn}^{\lambda}\left(\mathbf{q}, iq_n\right) - n \right] \right\} \end{aligned} \tag{33.6}$$

the first part is

$$\begin{aligned} \lim_{T\to 0} \left\{-T \ln Z_0\right\} &= \lim_{T\to 0} \left\{ -T \ln \mathrm{Tr} \left(e^{-\beta(H_0 - \mu N)} \right) \right\} \\ &= \lim_{T\to 0} \left\{ -T \sum_{k,\sigma} \ln \left(1 + e^{-\beta \xi_k}\right) \right\} \\ &= -\frac{d}{d\beta} \left[\sum_{k,\sigma} \ln \left(1 + e^{-\beta \xi_k}\right) \right]_{\beta\to\infty} \\ &= \sum_{k,\sigma} \xi_k f_{T=0}(\xi_k) \\ &= 2\mathcal{V} \int_{k<k_F} \frac{d^3k}{(2\pi)^3} \left(\frac{k^2}{2m} - \mu \right) \end{aligned} \tag{33.7}$$

To evaluate the second term, we relate χ to χ'' using the spectral representation

$$T \sum_{iq_n} \chi_{nn}(\mathbf{q}, iq_n) = T \sum_{iq_n} \int \frac{d\omega'}{\pi} \frac{\chi''_{nn}(\mathbf{q}, \omega')}{\omega' - iq_n} = \int \frac{d\omega'}{\pi} n_B(\omega') \chi''_{nn}\left(\mathbf{q}, \omega'\right) \tag{33.8}$$

In the zero temperature limit, $\lim_{T\to 0} n_B(\omega') = -\theta(-\omega')$ and we have

$$\begin{aligned} \lim_{T\to 0} \int \frac{d\omega'}{\pi} n_B(\omega') \chi''_{nn}\left(\mathbf{q}, \omega'\right) &= -\int_{-\infty}^{0} \frac{d\omega'}{\pi} \chi''_{nn}(\mathbf{q}, \omega') \\ &= \int_0^{\infty} \frac{d\omega'}{\pi} \chi''_{nn}(\mathbf{q}, -\omega') \\ &= -\int_0^{\infty} \frac{d\omega'}{\pi} \chi''_{nn}(\mathbf{q}, \omega') \end{aligned} \tag{33.9}$$

so that the expression for the ground state energy becomes

$$\frac{E_{\text{tot}}^{RPA}(T=0) - \mu N}{\mathcal{V}} = 2 \int_{k<k_F} \frac{d^3k}{(2\pi)^3} \left(\frac{k^2}{2m} - \mu \right) + \frac{1}{2} \int_0^1 d\lambda \int \frac{d^3q}{(2\pi)^3} V_{\mathbf{q}} \left[-\Im \int_0^{\infty} \frac{d\omega'}{\pi} \frac{\chi_{nn}^{0R}(\mathbf{q}, \omega')}{1 + \lambda V_{\mathbf{q}} \chi_{nn}^{0R}(\mathbf{q}, \omega')} - n \right] \tag{33.10}$$

The coupling constant integration is easy to perform

$$\begin{aligned} &\int_0^1 d\lambda V_{\mathbf{q}} \left[-\Im \int_0^{\infty} \frac{d\omega'}{\pi} \frac{\chi_{nn}^{0R}\left(\mathbf{q}, \omega'\right)}{1 + \lambda V_{\mathbf{q}} \chi_{nn}^{0R}\left(\mathbf{q}, \omega'\right)} - n \right] \\ &= -V_{\mathbf{q}} n - \int_0^{\infty} \frac{d\omega'}{\pi} \Im \left\{ \ln \left[1 + V_{\mathbf{q}} \chi_{nn}^{0R}\left(\mathbf{q}, \omega'\right) \right] \right\} \end{aligned} \tag{33.11}$$

$$\frac{E_{\rm tot}^{RPA}(T=0)-\mu N}{\mathcal{V}}=2\int_{k<k_F}\frac{d^3k}{(2\pi)^3}\left(\frac{k^2}{2m}-\mu\right)+\frac{1}{2}\int\frac{d^3q}{(2\pi)^3}V_{\mathbf{q}}\left[-V_{\mathbf{q}}n-\int_0^\infty\frac{d\omega'}{\pi}\Im\left\{\ln\left[1+V_{\mathbf{q}}\chi_{nn}^{0R}\left(\mathbf{q},\omega'\right)\right]\right\}\right] \tag{33.12}$$

The rest of the calculation is tedious. One finds at zero temperature, [15]

$$\frac{E_{Tol}^{RPA}(T=0)}{N}=\frac{2.21}{r_s^2}-\frac{0.916}{r_s}+0.0622\ln r_s-0.142+\mathcal{O}\left(r_s,r_s\ln r_s\right) \tag{33.13}$$

[15] G.D. Mahan, op. cit., p.391.

Part VI
Hubbard Model and Mott Physics

The jellium model is clearly a gross caricature of real solids. It does a good job nevertheless for simple metals, like sodium or aluminum. But it is important to have more realistic models that take into account the presence of a lattice of ions.The best methods today to find the electronic charge distribution are based on **Density Functional Theory** (**DFT**), that we explain very schematically in the first Chapter of this Part. These methods give a band structure that, strictly speaking, should not be interpreted as single-particle excitations. Nevertheless, for elements in the top rows of the periodic table, the band structure found from DFT works well. If we include the long-range Coulomb interaction with the GW approximation described above, then results for band gaps for example can be quite good. For narrow-band materials however, such as transition metal oxides that include d-electrons, this is not enough. We will explore the rich Physics contained in a simple model, the **Hubbard model**, that was proposed to understand **narrow band materials**. That model adds to the band structure an on-site interaction term U that is supposed to represent the screened Coulomb interaction. We will see that in such a short-range interaction model, spin excitations that had basically disappeared from the electron-gas problem, will now play a prominent role. Even when the interaction is not too strong, we will see why the perturbative methods that we have described in the previous Part are of limited validity. When the interaction is not too strong, we can treat the problem non-perturbatively using the Two-Particle-Self-Consistent approach and others. The Hubbard model will also allow us to understand why certain materials that are predicted to be good metals by band structure theory are in fact insulators. Insulating behavior can be induced by the interaction U when it is **larger than the bandwidth**. Such interaction-induced insulators are known as **Mott insulators**. And the transition between the metallic and the insulating phase that occurs as a function of U is called the **Mott transition**. The best known method to treat materials that are close to a Mott transition is Dynamical Mean-Field Theory and its cluster generalizations, that we will explain. High-temperature superconductors and layered organic conductors are examples of systems that display Mott insulating phases. In the next Part we will use the Hubbard model to introduce broken symmetry states with ferromagnetism as an example. In this Part, we restrict ourselves to the normal paramagnetic state.

34 Density Functional Theory

The presence of a static lattice of ions creates bands, as we know from one-electron theory. How do we generalize this to the many-body case with electron-electron interactions. In particular, how do we go beyond Hartree-Fock theory? Modern versions of band structure calculations, now more frequently referred to as **electronic structure calculations**, are based on **Density Functional Theory** (**DFT**). This is a ground state or thermal equilibrium method that is also used for molecules. We begin by describing the general method, then its implementation for band-structure calculations and then fnite temperature generalizations.

34.1 The ground state energy is a functional of the local density

DFT is based on a simple theorem of Hohenberg and Kohn[16].

Theorem: When there is a unique ground state, its ground state energy is a unique functional of the single-electron density.

We present the version of Levy[17] and Lieb [18]. In both cases, we use the variational principle for the ground state: the ground state wave function is the one which minimizes the energy

$$E[\Psi] = \langle \Psi | H | \Psi \rangle \tag{34.1}$$

with constraint $\langle \Psi | \Psi \rangle = 1$. Consider a Hamiltonian

$$H = T_{kin} + V_c + V_l \tag{34.2}$$

[16] P. Hohenberg and W. Kohn, Phys. Rev. 136B, 864 (1964).
[17] M. Levy, Proc. Natl. Acad. Sci., USA 79, 6062 (1979)
M. Levy, Phys. Rev. A 26, 1200 (1982).
[18] E. Lieb. Physics as Natural Philosophy, page 111. 1982

where T_{kin} is the kinetic energy, V_c is the Coulomb interaction between electrons and V_l is the interaction between the electrons and ions. Let $n_l(\mathbf{r}')$ be the charge density of the lattice, we can write

$$\begin{aligned}\langle\Psi|\, V_l\,|\Psi\rangle &= \langle\Psi|\int d^3\mathbf{r}\int d^3\mathbf{r}'\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\frac{e^2}{4\pi\varepsilon_0\,|\mathbf{r}-\mathbf{r}'|}n_l(\mathbf{r}')\,|\Psi\rangle \\ &= \int d^3\mathbf{r}\,\langle\Psi|\,\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\,|\Psi\rangle\int d^3\mathbf{r}'\frac{e^2}{4\pi\varepsilon_0\,|\mathbf{r}-\mathbf{r}'|}n_l(\mathbf{r}') \\ &= \int d^3\mathbf{r}n(\mathbf{r})V_l(\mathbf{r})\end{aligned} \tag{34.3}$$

where in the last line I have defined the lattice potential

$$V_l(\mathbf{r}) \equiv \int d^3\mathbf{r}'\frac{e^2}{4\pi\varepsilon_0\,|\mathbf{r}-\mathbf{r}'|}n_l(\mathbf{r}') \tag{34.4}$$

and the one-body electronic density

$$n(\mathbf{r}) \equiv \int d^3\mathbf{r}\,\langle\Psi\,|\psi^\dagger(\mathbf{r})\psi(\mathbf{r})|\,\Psi\rangle \tag{34.5}$$

Hohenberg and Kohn first proved that in the ground state, $V_l(\mathbf{r})$ leads to a unique density $n(\mathbf{r})$. That shows that the ground state energy is a **unique functional** of $n(\mathbf{r})$ since $V_l(\mathbf{r})$ determines the Hamiltonian (kinetic energy and electron-electron interactions are always the same). That theorem, that assumes that the **ground state is unique**, is proven by contradiction as follows. Assume that the potentials $V_l(\mathbf{r})$ and $V_l'(\mathbf{r})$ lead to the same density $n(\mathbf{r})$. The many-particle wave functions $|\Psi\rangle$ and $|\Psi'\rangle$ must be different since they correspond to different Schrödinger equations. The variational property then tells us that

$$\begin{aligned}E' &= \langle\Psi'\,|H'|\,\Psi'\rangle < \langle\Psi\,|H'|\,\Psi\rangle = \langle\Psi\,|H - V_\ell + V_\ell'|\,\Psi\rangle \\ E' &< E + \int d\mathbf{r}n(\mathbf{r})\,[V_l'(\mathbf{r}) - V_l(\mathbf{r})]\end{aligned} \tag{34.6}$$

equivalently, exchange the prime and unprimed quantities,

$$E < E' + \int d\mathbf{r}n(\mathbf{r})\,[V_l(\mathbf{r}) - V_l'(\mathbf{r})] \tag{34.7}$$

Adding the two equations, we have that

$$E + E' < E + E' \tag{34.8}$$

which cannot be true since the ground state is unique by hypothesis, so E is not equal to E'. This proves that two different lattice potentials $V_l(\mathbf{r})$ and $V_l'(\mathbf{r})$ cannot correspond to the same density $n(\mathbf{r})$.This is equivalent to saying that the ground state energy is a unique functional of the density.

A more illuminating approach is that of Levy and Lieb [2, 3] [134]. If we take the set of all normalized wave functions, the variational principle can be formulated as

$$E = \min_\Psi\,\langle\Psi\,|T_{kin} + V_c + V_l|\,\Psi\rangle \tag{34.9}$$

We now perform the minimization in two steps. First with respect to all wave functions that have the same one-particle density, then with respect to the one- particle density

$$\begin{aligned}E &= \min_n\min_{\Psi\to n}\,\langle\Psi\,|T_{kin} + V_c + V_l|\,\Psi\rangle \\ E &= \min_n\left[\left(\min_{\Psi\to n}\,\langle\Psi\,|T_{kin} + V_c|\,\Psi\rangle\right) + \int d^3\mathbf{r}n(\mathbf{r})V_l(\mathbf{r})\right] \\ &= \min_n\left[F[n] + \int d^3\mathbf{r}n(\mathbf{r})V_l(\mathbf{r})\right].\end{aligned} \tag{34.10}$$

where we have defined

$$F[n] = \min_{\Psi\to n}\,\langle\Psi\,|T_{kin} + V_c|\,\Psi\rangle \tag{34.11}$$

That functional of $n(\mathbf{r})$ contains kinetic energy and Coulomb interaction between electrons. It is independent of the lattice potential and is thus a universal property of the inhomogeneous electron gas. We say inhomogeneous because we have to find this function for densities that depend on position. We can then write

$$E\left[V_l\right] = \min_{n(\mathbf{r})} \left[F[n] + \int d^3\mathbf{r} n(\mathbf{r}) V_l(\mathbf{r}) \right] \tag{34.12}$$

From that point of view, the Hohenberg-Kohn ground state energy E is a functional of the external potential and is the Legendre transform of the Levy-Lieb functional F with

$$\frac{\delta E\left[V_l\right]}{\delta V_l(\mathbf{r})} = n(\mathbf{r}) \tag{34.13}$$

which can in principle be inverted to write $V_l(\mathbf{r})$ as a function of $n(\mathbf{r})$ and then write $E\left[V_l\right]$ as a functional of $n(\mathbf{r})$, namely $E\left[V_l[n(\mathbf{r})]\right]$. The inverse Legendre transform leads to

$$\frac{\delta F[n]}{\delta n(\mathbf{r})} = -V_l(\mathbf{r}) \tag{34.14}$$

We have shown that a) the ground state energy depends only on $n(\mathbf{r})$ instead of the whole wave function. b) The functional $F[n]$ is universal in the sense that it depends only on $n(\mathbf{r})$ and nothing else. If we can find the exact $F[n]$ for all possible $n(\mathbf{r})$, it can be applied to all situations. When the density does not vary too violently, we can just find out the functional $F[n]$ by solving the inhomogeneous electron gas by whatever method we can, Monte Carlo for example.

34.2 The Kohn-Sham approach

Our task is to find out the functional form of $F[n] = \min_{\Psi\to n} \langle \Psi \left| T_{kin} + V_c \right| \Psi \rangle$, which contains both kinetic term and Coulomb interaction term. This functional in principle exist, but we would need to search among all possible Ψ compatible with $n(\mathbf{r})$. The only term that does not need minimization is the Hartree term

$$\frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{e^2 n(\mathbf{r}) n(\mathbf{r}')}{4\pi\varepsilon_0 \left|\mathbf{r} - \mathbf{r}'\right|} \tag{34.15}$$

which is already written in terms of $n(\mathbf{r})$. To perform the minimization practically, we must therefore restrict to special types of Ψ which makes it possible for us to compute $\langle \Psi \left| T_{kin} + V_c \right| \Psi \rangle$. If Ψ is a slater determinant of single-particle orbitals, as in band theory, we would be able to evaluate the integral.

Kohn and Sham [116] proposed to expand the density in terms of orthogonal one-body orbitals for N particles in a paramagnetic state:

$$n(\mathbf{r}) = \sum_{i=1,\sigma}^{N/2} \left| \phi_{i,\sigma}^{KS}(\mathbf{r}) \right|^2 \tag{34.16}$$

If the wave function was simply obtained by filling these orthogonal orbitals $\phi_{KS}(\mathbf{r})$ up to the Fermi level, and the many-body wavefunction is simply a slater determinant of these functions, the corresponding kinetic energy would be easy to compute

$$T_{KS} = \langle \Psi_{KS} \left| T_{kin} \right| \Psi_{KS} \rangle = \sum_{i=1,\sigma} \int d^3\mathbf{r} \phi_{i,\sigma}^{KS}(\mathbf{r}) \left(\frac{-\nabla^2}{2m} \right) \phi_{i,\sigma}^{KS}(\mathbf{r}) \tag{34.17}$$

The Kohn-Sham method then proposes to write for the universal functional

$$F[n] = \min_{\Psi_{KS}\to n} \langle \Psi_{KS} \left| T_{kin} \right| \Psi_{KS} \rangle + \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{e^2 n(\mathbf{r}) n(\mathbf{r}')}{4\pi\varepsilon_0 \left|\mathbf{r} - \mathbf{r}'\right|} + E_{xc}[n] \tag{34.18}$$

The above equation defines the exchange correlation functional $E_{xc}[n]$. Going back to the definition of $F[n]$, we see that

$$\begin{aligned} E_{xc}[n] = & \min_{\Psi\to n} \langle \Psi \left| T_{kin} + V_c \right| \Psi \rangle - \min_{\Psi_{KS}\to n} \langle \Psi_{KS} \left| T_{kin} \right| \Psi_{KS} \rangle \\ & - \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{e^2 n(\mathbf{r}) n(\mathbf{r}')}{4\pi\varepsilon_0 \left|\mathbf{r} - \mathbf{r}'\right|} \end{aligned} \tag{34.19}$$

Note that the Kohn-Sham expression for the kinetic energy is not exact. Years of experience have yielded good approximations for the universal functional $E_{xc}[n]$. The simplest approximation, the **Local Density Approximation** (**LDA**) reads, for real orbitals,

$$\begin{aligned} E_{xc}^{LDA}[n] = &- \frac{1}{2} \min_{\Psi_{KS}\to n} \sum_{\sigma,\sigma'} \sum_{i,j}^{N/2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \delta_{\sigma,\sigma'} \frac{e^2 \phi_{i,\sigma}^{KS}(\mathbf{r}) \phi_{j,\sigma}^{KS}(\mathbf{r}) \phi_{i,\sigma'}^{KS}(\mathbf{r}') \phi_{j,\sigma'}^{KS}(\mathbf{r}')}{4\pi\varepsilon_0 |\mathbf{r}-\mathbf{r}'|} \\ &+ \int d^3\mathbf{r} C^X n^{4/3}(\mathbf{r}). \end{aligned} \tag{34.20}$$

The first term is the Kohn-Sham exchange energy computed from $\left\langle \Psi \left| \hat{V}_c \right| \Psi \right\rangle$ with the Kohn-Sham wave function. Instead of minimizing with respect to the KohnSham orbitals restricted to a given density and then with respect to the density, one now treat $F[n] \to F^{LDA}[\{\phi_{i\sigma}^{KS}\}]$ and thus

$$\begin{aligned} E[V_l] &= \min_{n(\mathbf{r})} \left[F[n] + \int d^3\mathbf{r} n(\mathbf{r}) V_l(\mathbf{r}) \right] \\ &= \min_{n(\mathbf{r})} \min_{\{\phi_i^{KS}\}\to n} \left[F[\{\phi^{KS}\}] + \int d^3\mathbf{r} n(\mathbf{r}) V_l(\mathbf{r}) \right] \\ &= \min_{\phi_i^{KS}} \left[F[\{\phi^{KS}\}] + \int d^3\mathbf{r} n(\mathbf{r}) V_l(\mathbf{r}) \right] \end{aligned} \tag{34.21}$$

this transforms the problem into minimizing with respect to the Kohn-Sham orbitals $\phi_{i\sigma}^{KS}$. We can then take functional derivatives with respect to these orbitals and obtain equations that have the structure of the integro-differential Hartree-Fock equation. What has been achieved is that we have an auxiliary non-interacting electron problem, obeying Fermi-statistics obviously, that should give a good approximation to the ground-state energy and ground-state density.

The eigenenergies or Kohn-Sham orbitals cannot be interpreted as exact single-particle excitations. They may however serve as a starting point for further calculations using many-body theory, as I explain in the next Chapter on the Hubbard model.

DFT is based on the existence of a universal functional of the density. However, this functional is unknown, so a major part of the work in that field has been to improve the quality of the functional. A well known example is the Perdew, Burke, Ernzerhof functional[19]. Another well known author in that field that has helped make DFT a truly first principles approach is Marvin L. Cohen [221]. Note that going beyond the LDA approximation leads to more general functionals of $n(\mathbf{r})$ that can depend for example on derivatives of the density, for example the Laplacian of the density or the square of the gradient (to make sure we that $F[n]$ is a scalar) etc.

Another direction for improvement by Car and Parrinello [50] has been to combine **molecular dynamics** with DFT to go beyond the pair-potential approximation, thereby making possible the simulation of both covalently bonded and metallic systems and allowing the application of density-functional theory to much larger systems than previously feasible.

I note without proof for now that there is an exact expression for the exchange correlation energy $E_{xc}[n]$. Given the density $n(\mathbf{r})$ we can write this exchange correlation energy as follows [120],

$$E_{xc}(\mathbf{r}) = \frac{\delta \Phi_{DFT}^{xc}[n]}{\delta n(\mathbf{r})} \tag{34.22}$$

where

$$\Phi_{DFT}^{xc}[n] = T \sum_{iq_n} \int d^3\mathbf{r} \int d^3\mathbf{r}' \int_0^1 d\lambda \frac{\chi_{\rho\rho}^{\lambda}(\mathbf{r},\mathbf{r}';iq_n)}{4\pi\varepsilon_0 |\mathbf{r}-\mathbf{r}'|} \tag{34.23}$$

where the charge density is $\rho(\mathbf{r}) = \sqrt{\lambda} e n(\mathbf{r})$ and the corresponding susceptibility $\chi_{\rho\rho}^{\lambda}(\mathbf{r},\mathbf{r}';iq_n)$ is calculated for a Coulomb potential where the electric charge is λe^2. One uses this expression to find more accurate exchange-correlation functionals.

[19] John P. Perdew, Kieron Burke, and Matthias Ernzerhof. Generalized gradi- ent approximation made simple [phys. rev. lett. 77, 3865 (1996)]. Phys. Rev. Lett., 78:1396ñ1396, Feb 1997.

34.3 DFT and many-body perturbation theory

DFT has been designed to find ground states. The eigenenergies of the Kohn Sham orbitals are just the result of a parametrization of the density. There is nothing in the theory that guarantees that they represent single-particle excited states. To find excited states and even improve ground state energies, it was proposed to use the many-body perturbation method developed for the electron gas. The idea is to expand the field operators $\psi_\sigma(\mathbf{r})$ using the Kohn-Sham orbitals. In that basis, the effect of interactions is minimized, but it is still there. One can then use any many-body method to find excited states and other interesting properties. The first method to use is the RPA to find the dielectric constant. The corresponding self-energy with the screened interaction is referred to in this context as the GW approximation. These calculations can be seen as an approximation for the exact equations of Hedin who also performed the first full calculation for the electron gas.

One had to wait till the mid 80's to see applications to real materials [20]. As shown in Fig. (53-1), spectacular agreement with experiment for band gaps has been achieved in the latest version of the approach[21]. In that approach, a quasiparticle approximation is taken for the Green's function, which is determined self-consistently. This helps remove the influence of the choice of basis for the Kohn-Sham orbitals.

Yet, this approach fails for late transition metals oxides, which are insulators, but predicted to be metals by DFT based methods. A partial remedy for this was to include an orbital-dependent potential U, that acts only on the d or f orbitals, the so-called **LDA+U method**. In order of increasing localization of the orbitals, meaning larger interactions, we find: $5d, 4d, 3d, 4f$, and $5f$. Within a given row of the periodic table, moving from left to right also increases localization. But what is U? That takes me to the next topic.

34.4 Model Hamiltonians

In parallel efforts to understand properties of materials, the study of simple Hamiltonians revealed very rich physics. One of the first difficult problems that was tackled was that of the **Kondo Hamiltonian**. That Hamiltonian was suggested by Nobel Prize winner PW Anderson in his study of a model, now known as the **Anderson impurity model**, that introduced a double occupancy cost U for electrons on an impurity with localized orbital[22]. In the Kondo problem, an isolated impurity with a local moment is hybridized antiferromagnetically with a conduction-electron sea. At high temperature, this local moment is free. At low temperature, there is a crossover to a state where the localized moment essentially disappears by forming a highly entangled singlet state with the conduction sea. A full solution of that problem had to wait for the renormalization group of Nobel Prize winner Ken Wilson[23]. The solution to this problem explained in particular the **resistivity minimum found in dilute alloys**.

Another important model was proposed independently in 1964 by Hubbard, Kanamori and Gutwiller. Known today as the **Hubbard model**, this model has two non-commuting terms. A term that represents electrons moving on a lattice with one orbital per site. That term is diagonal in a plane-wave basis. The other term represents the energy cost U associated with double occupancy and is diagonal in the site basis. This model was proposed to understand emergent phases of matter such as ferromagnetism. But in the end, it revealed itself as a way to explain **antiferromagnetism** and the **metal-insulator transition**, or **Mott transition**. The latter problem was by far the most difficult one. The interaction-induced metal insulator transition was proposed by Peierls and Mott around 1937 as an explanation for the discrepancy between the band picture of solids and observation in materials such as NiO.

Early explanations of the Mott transition at half-filling, all based on the Hubbard model, included a) Hubbard who proposed that the original density of states is split in two by U so that when U is small enough, a metal is recovered [24] b) Brinkmann and Rice who suggested that the effective mass of electrons diverges at the transition[25], a result recovered by the modern slave-boson approach of Kotliar and Ruckenstein [26] c) Slater who associated the transition to an emergent long-range antiferromagnetic order[27]. The latter explanation is invalid for what are called

[20] Mark S. Hybertsen and Steven G. Louie. First-principles theory of quasi-particles: Calculation of band gaps in semiconductors and insulators. Phys. Rev. Lett., 55:1418ñ1421, Sep 1985.

[21] M. van Schilfgaarde, Takao Kotani, and S. Faleev. Quasiparticle self- consistent gw theory. Phys. Rev. Lett., 96:226402, Jun 2006.

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[23] Kenneth G. Wilson. The renormalization group: Critical phenomena and the kondo problem. Rev. Mod. Phys., 47:773ñ840, Oct 1975.

[24] J. Hubbard and Brian Hilton Flowers. Electron correlations in narrow energy bands iii. an improved solution. Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences, 281(1386):401ñ419, 1964.

[25] W. F. Brinkman and T. M. Rice. Application of gutzwillerís variational method to the metal-insulator transition. Phys. Rev. B, 2:4302ñ4304, Nov 1970.

[26] Gabriel Kotliar and Andrei E. Ruckenstein. New functional integral ap- proach to strongly correlated fermi systems: The gutzwiller approximation as a saddle point. Phys. Rev. Lett., 57:1362ñ1365, Sep 1986.

[27] J. C. Slater. Magnetic e§ects and the hartree-fock equation. Phys. Rev., 82:538ñ541, May 1951.

today Mott insulators in a paramagnetic state.

35 The Hubbard Model

Let me step back. Suppose we have one-body states, obtained either from Hartree-Fock or from Density Functional Theory (DFT). The latter is a much better approach than Hartree-Fock. The Kohn-Sham orbitals give highly accurate electronic density and energy for the ground state. If the problem had been solved for a translationally invariant lattice, the one-particle states will be **Bloch states** indexed by crystal momentum $\mathbf{k}$ and band index n. Nevertheless, these one-particle states cannot be used to build single-particle states that diagonalize the many-body Hamiltonian. More specifically, if we expand the creation-annihilation operators in that basis using the general formulas for one-particle and two-particle parts of the Hamiltonian, it will not be diagonal. Suppose that a material has s and p electrons, for which DFT does a good job. In addition, suppose that there are only a few bands of d character near the Fermi surface. Assuming that the only part of the Hamiltonian that is not diagonal in the DFT basis concerns the states in those d band, it is possible to write a much simpler form of the Hamiltonian. We will see that nevertheless, solving such "model" Hamiltonians is non-trivial, despite their simple-looking form.

After providing a “derivation” the model, we will solve limiting cases that will illustrate one limit where states are extended, and one limit where they are localized, giving a preview of the Mott transition.

Finding an effective Hamiltonian for a few bands near the Fermi level starting from the full electronic structure is a delicate matter that necessitates a much more detailed treatment than the one exposed here. The procedure to find the effective Hamiltonian is called "**downfolding**". This means that one wants to obtain an effective Hamiltonian that focuses on a few bands near the Fermi level. This is in a sense our "model space". These methods, that I will not explain, include **cRPA** [28] where the dielectric constant is computed by using in the bubbles all particle hole-pairs that include at least one of the bands that we do not wish to consider in our model space. The resulting dielectric constant does not screen the Coulomb interaction in the sense of Thomas-Fermi as discussed above. The Coulomb interaction is smaller but still long range. It is only when the model space is metallic that the Coulomb interaction will become truly short-range. For examples of derivations of model Hamiltonians, you can also look at Refs. [29].

35.1 Assumptions behind the Hubbard model

Starting from the general Hamiltonian

$$\begin{aligned}
\hat{K} &= \hat{H} - \mu\hat{N} = \hat{H}_0 + \hat{V} + \hat{V}_n - \mu\hat{N} \\
\hat{H}_0 &= \frac{-1}{2m}\sum_{\sigma_1}\int d\mathbf{x}_1 \psi^\dagger_{\sigma_1}(\mathbf{x}_1)\nabla^2\psi_{\sigma_1}(\mathbf{x}_1) \\
\hat{V} &= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_1)\psi^\dagger_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_2}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_1) \\
\hat{V}_n &= -\sum_{\sigma_1}\int d\mathbf{x}_1\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\psi^\dagger_{\sigma_1}(\mathbf{x}_2)\psi_{\sigma_1}(\mathbf{x}_2)n
\end{aligned} \tag{35.1}$$

The field operators can be expanded in single-particle eigenstates. For the case of interest to us, these would be Bloch states $\phi_{n\mathbf{k}} = \langle\mathbf{r}|\, n\mathbf{k}\rangle$ with band index n and crystal momentum $\mathbf{k}$, so that

$$\begin{aligned}
|\mathbf{r}\rangle &= \sum_{n\mathbf{k}} |n\mathbf{k}\rangle\langle n\mathbf{k}|\,\mathbf{r}\rangle \\
\psi^\dagger(\mathbf{r}) &= \sum_{n\mathbf{k}}\langle n\mathbf{k}|\,\mathbf{r}\rangle c^\dagger_{n\mathbf{k}} = \sum_{n\mathbf{k}}\phi^*_{n\mathbf{k}}(\mathbf{r})c^\dagger_{n\mathbf{k}} \\
\psi(\mathbf{r}) &= \sum_{n\mathbf{k}}\langle\mathbf{r}|\, n\mathbf{k}\rangle c_{n\mathbf{k}} = \sum_{n\mathbf{k}}\phi_{n\mathbf{k}}(\mathbf{r})c_{n\mathbf{k}}
\end{aligned} \tag{35.2}$$

[28] F Aryasetiawan, M Imada, A Georges, G Kotliar, S Biermann, and AI Lichtenstein. Frequency-dependent local interactions and low-energy ef- fective models from electronic structure calculations. Physical Review B, 70(19):195104, 2004.

[29] Kazuma Nakamura, Yoshiro Nohara, Yoshihide Yosimoto, and Yusuke No- mura. Ab initio gw plus cumulant calculation for isolated band systems: Application to organic conductor (TMTSF)2pf6 and transition-metal oxide srvo3. Physical Review B, 93(8):085124, Feb 2016.

Kazuma Nakamura, Yoshihide Yoshimoto, Taichi Kosugi, Ryotaro Arita, and Masatoshi Imada. Ab initio derivation of low-energy model for Œμz-et type organic conductors. Journal of the Physical Society of Japan, 78(8):083710, Aug 2009.

Since screening suggests that in the end we need to consider short range interactions that are better described in a localized basis, we can use the **Wannier basis** $w_n(\mathbf{r}-\mathbf{R}_i)$. In that case, the expansion takes the form,

$$\begin{aligned}
|\mathbf{r}\rangle &= \sum_{n\mathbf{R}_i} |n\mathbf{R}_i\rangle \langle n\mathbf{R}_i|\,\mathbf{r}\rangle \\
\psi^\dagger(\mathbf{r}) &= \sum_{n\mathbf{R}_i} \langle n\mathbf{R}_i|\,\mathbf{r}\rangle c^\dagger_{n\mathbf{R}_i} = \sum_{n\mathbf{R}_i} w^*_n(\mathbf{r}-\mathbf{R}_i) c^\dagger_{n\mathbf{R}_i} \\
\psi(\mathbf{r}) &= \sum_{n\mathbf{R}_i} \langle \mathbf{r}|\,n\mathbf{R}_i\rangle c_{n\mathbf{R}_i} = \sum_{n\mathbf{R}_i} w_n(\mathbf{r}-\mathbf{R}_i) c_{n\mathbf{R}_i}
\end{aligned} \tag{35.3}$$

We can write the kinetic energy and the lattice potential together as

$$\begin{aligned}
&\sum_\sigma \int d^3\mathbf{r} \psi^\dagger_\sigma(\mathbf{r}) \left[\left(-\frac{\nabla^2}{2m}\right) + V_l(\mathbf{r})\right] \psi_\sigma(\mathbf{r}) \\
=&\sum_\sigma \int d^3\mathbf{r} \sum_{m\mathbf{R}'_i} w^*_m(\mathbf{r}-\mathbf{R}'_i) c^\dagger_{m\mathbf{R}'_i} \left[\left(-\frac{\nabla^2}{2m}\right) + V_l(\mathbf{r})\right] \sum_{n\mathbf{R}_i} w_n(\mathbf{r}-\mathbf{R}_i) c_{\sigma n\mathbf{R}_i} \\
=&\sum_\sigma \sum_{m\mathbf{R}_j} \sum_{n\mathbf{R}_i} c^\dagger_{\sigma n\mathbf{R}_i} c_{\sigma m\mathbf{R}_j} \left[\int d^3\mathbf{r} w^*_n(\mathbf{r}-\mathbf{R}_i) \left[\left(-\frac{\nabla^2}{2m}\right) + V_l(\mathbf{r})\right] w_m(\mathbf{r}-\mathbf{R}_j)\right] \\
=&\sum_\sigma \sum_{m\mathbf{R}_j} \sum_{n\mathbf{R}_i} c^\dagger_{\sigma m\mathbf{R}_j} \left\langle n\mathbf{R}_i \left| \hat{T}_{kin} + \hat{V}_\ell \right| m\mathbf{R}_j \right\rangle c_{\sigma n\mathbf{R}_i}
\end{aligned} \tag{35.4}$$

Usually, we define the Wannier function for $\{\phi_{m\mathbf{k}}\}$ in a single band m

$$w_m(\mathbf{r}-\mathbf{R}_j) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j} \phi_{m\mathbf{k}}(\mathbf{r}) \tag{35.5}$$

However, we can also perform a unitary transformation of different bands

$$W_\ell(\mathbf{r}-\mathbf{R}_j) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j} \sum_m U_{\ell m} \phi_{m\mathbf{k}}(\mathbf{r}) \tag{35.6}$$

which give a different set of equally valid orthonormal Wannier orbitals. This has led the group of Vanderbilt to define **maximally localized orbitals**.

In cases where a single band crosses the Fermi level and is far in energy from other bands, we can appeal to perturbation-theory ideas and assume that we can **focus on that single band that crosses the Fermi level**. I then drop the band index and use the short-hand notation $\left\langle n\mathbf{R}_i \left| \widehat{T}_{kin} \right| n\mathbf{R}_j \right\rangle \equiv \left\langle i \left| \widehat{T}_{kin} \right| j \right\rangle$. The Hamiltonian in the presence of the Coulomb interaction then takes the form

$$H = \sum_\sigma \sum_{i,j} c^\dagger_{i\sigma} \left\langle i \left| \widehat{T}_{kin} + \hat{V}_l \right| j \right\rangle c_{j\sigma} + \frac{1}{2} \sum_{\sigma,\sigma'} \sum_{ijkl} \left\langle i \left| \left\langle j \left| \hat{V}_c \right| k \right\rangle \right| l \right\rangle c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{l\sigma'} c_{k\sigma} \tag{35.7}$$

where the first term contains all the one-body parts of the Hamiltonin, namely kinetic energy and lattice potential energy. Remember that $\langle i|$ and $|k\rangle$ belong to the same one-particle Hilbert space as do $\langle j|$ and $|l\rangle$. Here, $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) are creation and annihilation operators for electrons of spin σ in the Wannier orbital centered around site i. A single many-particle state formed by filling orbitals, leading to a Slater determinant as wave function, cannot diagonalize this Hamiltonian because of the interaction part that empties orbitals and fills other ones. The true eigenstates are linear combinations of Slater determinants.

The one-body part by itself is essentially the DFT band structure. In 1964 , Hubbard, Kanamori and Gutzwiller did the most drastic of approximations, hoping to have a model simple enough to solve. They assumed that $\langle i\,|\langle j\,|V_c|\,k\rangle|\,l\rangle$ would be much larger than all other interaction matrix elements when all lattice sites are equal.

Defining $t_{ij} \equiv \langle i|\widehat{T}|j\rangle$ and $U \equiv \left\langle i \left| \left\langle i \left| \hat{V}_c \right| i \right\rangle \right| i \right\rangle$, and using $c_{i\sigma}c_{i\sigma} = 0$ they were left with

$$\begin{aligned} H &= \sum_{\sigma} \sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{\sigma,\sigma'} \sum_{i} U c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma'} c_{i\sigma'} c_{i\sigma} \\ &= \sum_{\sigma} \sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} c_{i\uparrow} \\ &= \sum_{\sigma} \sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} U n_{i\downarrow} n_{i\uparrow}. \end{aligned} \tag{35.8}$$

In this expression, $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the density of spin σ electrons, $t_{ij} = t^{*}_{ji}$ is the hopping amplitude, and U is the screened Coulomb repulsion that acts only on electrons on the same site. Most of the time, one considers hopping only to nearest neighbors. In general, we write $-t, -t', -t''$ respectively for the first-, second- and third-nearest neighbor hopping amplitudes. To go from the first to the second line we used the Pauli exclusion principle $c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma} = 0$.

This last statement is important. To obtain the Hubbard model where up electrons interact only with down, we had to assume that the **Pauli exclusion principle is satisfied exactly**. So approximation methods that do not satisfy this constraint are suspicious.

The model can be solved exactly only in one dimension using the **Bethe ansatz**, and in infinite dimension. The latter solution is the basis for **Dynamical Mean Field Theory** (DMFT) that we will discuss below. Despite the fact that the Hubbard model is the simplest model of interacting electrons, it is far from simple to solve.

Atoms in optical lattices can be used to artificially create a system described by the Hubbard model with parameters that are tunable [101]. A laser interference pattern can be used to create an optical lattice potential using the **AC Stark effect**. One can control tunneling between potential minima as well as the interaction of atoms between them and basically build a physical system that will be described by the Hubbard Hamiltonian. This kind of experimental setup in a sense is an analog computer. The derivation given in the case of solids is phenomenological and the parameters entering the Hamiltonian are not known precisely. In the case of **cold atoms**, one can find conditions where the Hubbard model description is very accurate. By the way, in optical lattices, interesting physics occurs mostly in the nano Kelvin range.

Important physics is contained in the Hubbard model. For example, the interaction piece is diagonal in the localized Wannier basis, while the kinetic energy is diagonal in the momentum basis. Depending on filling and on the strength of U compared with band parameters, the true eigenstates will be localized or extended. The localized solution is called a **Mott insulator**. The Hubbard model can describe ferromagnetism, antiferromagnetism (commensurate and incommensurate) and it is also believed to describe **high-temperature superconductivity**, depending on lattice and range of interaction parameters.

35.2 Where spin fluctuations become important

In deriving the Hubbard model we have used the Pauli exclusion principle. Electrons do not interact with electrons of the same spin since this means they would be in the same state. In other words, we have taken into account the fact that exchange has gotten rid of that type of interactions. This is discussed further from the point of view of diagrams. The consequence of this is that spin now starts to play an important role, contrary to the case of the electron gas. In fact, almost all manifestations of **magnetism** in solids originates from **exchange**, not from direct magnetic-dipole magnetic-dipole interactions. An easy way to see this is to rewrite the Hubbard interaction in terms of density-density interaction $(n_{i\downarrow} + n_{i\uparrow})^2$ and spin-spin interaction $S^z_i S^z_i$ as follows

$$\begin{aligned} U n_{i\downarrow} n_{i\uparrow} &= \frac{U}{4} \left(n_{i\downarrow} + n_{i\uparrow}\right)^2 - \frac{U}{4} \left(n_{i\downarrow} - n_{i\uparrow}\right)^2 \\ &= \frac{U}{4} n_i n_i - \frac{U}{4} S^z_i S^z_i \end{aligned} \tag{35.9}$$

where $n_i \equiv n_{i\downarrow} + n_{i\uparrow}$. The spin operator in Wannier basis is $\mathbf{S}_i = \sum_{\sigma,\sigma'} c^{\dagger}_{i\sigma'} \mathbf{S}_{\sigma'\sigma} c_{i\sigma}$, with $\left(S^i\right)_{\alpha\alpha'} = \frac{1}{2}\left(\sigma^i\right)_{\alpha\alpha'}$. Here $S^z_i = \frac{1}{2}\sum_{\sigma,\sigma'} c^{\dagger}_{i\sigma'} \left(\sigma^z\right)_{\sigma'\sigma} c_{i\sigma} = \frac{1}{2}\left(c^{\dagger}_{i\uparrow} c_{i\uparrow} - c^{\dagger}_{i\downarrow} c_{i\downarrow}\right) = \frac{1}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right)$.

To gain a feeling of the Physics contained in the Hubbard model, let us first discuss two limiting cases where it can be solved exactly.

35.3 The non-interacting limit $U = 0$

As a simple example that comes back often in the context of high-temperature superconductivity, consider a square lattice in two dimensions with nearest-neighbor hopping only. Then, when $U = 0$, we have

$$H_0 = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} \tag{35.10}$$

where t_{ij} is a Hermitian matrix. When there is no magnetic field the one-body states can all be taken real and t_{ij} is symmetric. To take advantage of translational invariance we use our Fourier transforms

$$\begin{aligned} c_{i\sigma} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_i} c_{\mathbf{k}\sigma} \\ c^\dagger_{i\sigma} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}_i} c^\dagger_{\mathbf{k}\sigma} \end{aligned} \tag{35.11}$$

with $\mathbf{r}_i$ the position of site i, and

$$\sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} = N\delta_{\mathbf{k},0} \tag{35.12}$$

Here N is the number of atoms and we take the lattice spacing a to be unity. Defining $\mathbf{r}_j = \mathbf{r}_i + \boldsymbol{\delta}$ and noting that the hopping matrix depends only on the distance to the neighbors $\boldsymbol{\delta}$, we find

$$\begin{aligned} H_0 &= \sum_\sigma \sum_{\mathbf{r}_i,\delta} t_\delta c^\dagger_{r_i,\sigma} c_{r_i+\delta,\sigma} \\ &= \sum_\sigma \sum_{\mathbf{r}_i,\delta} t_\delta \frac{1}{\sqrt{N}} \sum_{\mathbf{k}'} e^{-i\mathbf{k}'\cdot\mathbf{r}_i} c^\dagger_{\mathbf{k}'\sigma} \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_i+\delta)} c_{\mathbf{k}\sigma} \\ &= \frac{1}{N} \sum_\sigma \sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} \sum_\delta e^{i\mathbf{k}\cdot\delta} t_\delta \sum_{\mathbf{r}_i} e^{-i\mathbf{k}'\cdot\mathbf{r}_i} e^{i\mathbf{k}\cdot\mathbf{r}_i} \\ &= \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \end{aligned} \tag{35.13}$$

with $\varepsilon_{\mathbf{k}} \equiv \sum_\delta e^{i\mathbf{k}\cdot\delta} t_\delta$. In the case of nearest-neighbor hopping only, on a two-dimensional square lattice for example where $t_{ij} = -t$ for nearest-neighbor hopping, we have the dispersion relation

$$\varepsilon_{\mathbf{k}} = -2t\,(\cos k_x + \cos k_y) \tag{35.14}$$

where I have assumed that the lattice spacing, or distance δ between nearest neighbors, is equal to unity. Clearly, if the Fermi wave vector is sufficiently small, we can define $t^{-1} = 2m_b$ and approximate the dispersion relation by its quadratic expansion, as in the free electron limit

$$\varepsilon_{\mathbf{k}} = -2t\,(\cos k_x + \cos k_y) \sim C + \frac{k_x^2 + k_y^2}{2m_b} \tag{35.15}$$

35.4 The strongly interacting, atomic, limit $t = 0$

If there are no hoppings and only disconnected atomic sites,

$$K = U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} \tag{35.16}$$

there are two energy levels, correspondig to empty, singly (zero energy) and doubly occupied site (energy U). It is apparently much simpler than the previous problem. But not quite. A simple thing to compute is the partition function. Since each site is independent, $Z = Z_1^N$ where Z_1 is the partition function for one site. We find, since there are four possible states on a site, empty, spin up, spin down and doubly occupied,

$$Z_1 = 1 + e^{\beta\mu} + e^{\beta\mu} + e^{-\beta(U-2\mu)} \tag{35.17}$$

already at this level we see that there are "correlations", since Z_1 cannot be factorized into $(1 + e^{\beta\mu})^2$.

We now consider the dynamics of the system, which is captured by the Green's function

$$\mathcal{G}_\sigma(\tau) = -\left\langle T_\tau \left[c_\sigma(\tau) c_\sigma^\dagger \right] \right\rangle \tag{35.18}$$

we have removed the site index since different sites are not independent and we can factorize the system into that of each site. Imagine using Lehman representation. It is clear that when the time evolution operator acts on the intermediate state, we will need to know if in this intermediate state the system is singly or doubly occupied. We cannot trace only on up electrons without worrying about down electrons. The Lehman representation gives a staightforward way of obtaining the Green function.

We can also proceed with the equation of motion approach, a procedure we will adopt to introduce the concept of **hierarchy of equations** (the analog of the BBGKY hierarchy in classical systems). All that we need is

$$K = U n_\uparrow n_\downarrow - \mu \left(n_\uparrow + n_\downarrow \right) \tag{35.19}$$

$$\frac{\partial c_\sigma}{\partial \tau} = [K, c_\sigma] = [U n_\sigma n_{-\sigma} - \mu n_\sigma, c_\sigma] = -U c_\sigma n_{-\sigma} + \mu c_\sigma \tag{35.20}$$

From this, the equation of motion for the Green function is

$$\begin{aligned} \partial_\tau \mathcal{G}_\sigma(\tau) &= \partial_\tau \left[-\left\langle c_\sigma(\tau) c_\sigma^\dagger \right\rangle \theta(\tau) + \left\langle c_\sigma^\dagger c_\sigma(\tau) \right\rangle \theta(-\tau) \right] \\ &= -\delta(\tau) - \left\langle T_\tau \left\{ [K, c_\sigma](\tau) c_\sigma^\dagger \right\} \right\rangle \\ &= -\delta(\tau) + \mu \mathcal{G}_\sigma(\tau) + U \left\langle T_\tau \left\{ c_\sigma(\tau) n_{-\sigma}(\tau) c_\sigma^\dagger \right\} \right\rangle \end{aligned} \tag{35.21}$$

The structure of the equation of motion is a very general result. One-body Green functions are coupling to higher order correlation functions. Let us write down the equation of motion for that higher order correlation function that we define as follows

$$\mathcal{G}_{2,\sigma}(\tau) = -\left\langle T_\tau \left[c_\sigma(\tau) n_{-\sigma}(\tau) c_\sigma^\dagger \right] \right\rangle \tag{35.22}$$

we then try to find the equation of motion of $\mathcal{G}_{2,\sigma}(\tau)$. Some useful results are

$$\partial_\tau n_{-\sigma} = [K, n_{-\sigma}] = 0 \tag{35.23}$$

$$\begin{aligned} \partial_\tau \mathcal{G}_{2,\sigma}(\tau) &= -\delta(\tau) n_{-\sigma} - \left\langle T_\tau \left[\partial_\tau \left(c_\sigma(\tau) n_{-\sigma}(\tau) \right) c_\sigma^\dagger \right] \right\rangle \\ &= -\delta(\tau) n_{-\sigma} - \left\langle T_\tau \left[\left(-U c_\sigma(\tau) n_{-\sigma}(\tau) + \mu c_\sigma(\tau) \right) n_{-\sigma}(\tau) c_\sigma^\dagger \right] \right\rangle \\ &= -\delta(\tau) n_{-\sigma} + \mu \mathcal{G}_{2,\sigma}(\tau) - U \mathcal{G}_{2,\sigma}(\tau) \end{aligned} \tag{35.24}$$

Instead of generating a higher order correlation function in the term coming from $[K, c_\sigma(\tau)]$, as is usually the case, the system of equations has closed since $n_{-\sigma} n_{-\sigma} = n_{-\sigma}$. This is a very special case. We then have a closed set of equations that is easy to solve in Matsubara frequencies where $\partial_\tau \to -i\omega_n, \qquad \delta(\tau) \to 1$, and the equations are

$$\begin{aligned} \left(i\omega_n + \mu \right) \mathcal{G}_\sigma(i\omega_n) &= 1 + U \mathcal{G}_{2,\sigma}(i\omega_n) \\ \left(i\omega_n + \mu \right) \mathcal{G}_{2,\sigma}(i\omega_n) &= \langle n_{-\sigma} \rangle + U \mathcal{G}_{2,\sigma}(i\omega_n) \end{aligned} \tag{35.25}$$

the solutions are

$$\begin{aligned} \mathcal{G}_{2,\sigma}(i\omega_n) &= \frac{\langle n_{-\sigma} \rangle}{i\omega_n + \mu - U} \\ \mathcal{G}_\sigma(i\omega_n) &= \frac{1 - \langle n_{-\sigma} \rangle}{i\omega_n + \mu} + \frac{\langle n_{-\sigma} \rangle}{i\omega_n + \mu - U} \end{aligned} \tag{35.26}$$

analytic continuation to retarded Green's function, we have

$$\begin{aligned} G_\sigma^R(\omega) &= \frac{1 - \langle n_{-\sigma} \rangle}{\omega + i\eta + \mu} + \frac{\langle n_{-\sigma} \rangle}{\omega + i\eta + \mu - U} \\ A_\sigma(\omega) &= -2 \Im G_\sigma^R(\omega) \\ &= \left(1 - \langle n_{-\sigma} \rangle \right) 2\pi \delta(\omega + \mu) + \langle n_{-\sigma} \rangle \, 2\pi \delta(\omega + \mu - U) \end{aligned} \tag{35.27}$$

The two levels correspond respectively to the **electron afinity** and **ionization potential** of the atom. Physically speaking, if the fraction of sites occupied by down electrons is $\langle n_{-\sigma} \rangle$, then a spin up electron will have an energy $-\mu + U$ a fraction $\langle n_{-\sigma} \rangle$ of the time, and an energy $-\mu$ for a fraction $1 - \langle n_{-\sigma} \rangle$ of the time. And that is independent of the momentum. That is very different from a quasiparticle. There is no pole at $\omega = 0$ unless $\mu = 0$.

The non-interacting limit is not a good starting point for this problem clearly. One expects perturbation theory to breakdown. This is simple to see for example at half filling when $\langle n_{-\sigma}\rangle = 1/2$ and $\mu = U/2$. Then,

$$\begin{aligned} G^R_\sigma(\omega) &= \frac{1}{2}\left(\frac{1}{\omega + i\eta + U/2} + \frac{1}{\omega + i\eta - U/2}\right) \\ &= \frac{(\omega + i\eta)}{(\omega + i\eta)^2 - \left(\frac{U^2}{4}\right)^2} \\ &= \frac{1}{(\omega + i\eta) - \frac{U^2}{4(\omega + i\eta)}} \end{aligned} \tag{35.28}$$

so that clearly, the retarded self-energy $\Sigma^R(\omega) = \frac{U^2}{4(\omega+i\eta)}$ is singular at low frequency, not good news for perturbation theory. It gets rid of the pole that is at $\omega = 0$ when there is no interaction.

If t is not zero but $U \gg 1$, then we have a **Mott insulator**. In a Mott insulator, the two peaks that we just found in the single-particle spectral weight are somewhat broadened, but there is a **gap at zero frequency**. We will leave this concept aside for the moment and discuss the weak coupling case.

36 Diagrammatic Method for the Hubbard Model

In this Chapter, we follow the same steps as the electron gas and derive RPA equations for the response functions. While spin fluctuations did not play a prominent role in the electron gas, they will be dominant in the Hubbard model and we will see why. RPA for the Hubbard model however has a major deficiency: **It does not satisfy the Pauli exclusion principle**, as we will see. This had no major consequence for the electron gas, but in the case of the Hubbard model this is crucial. We will see how to cure this problem and others using the **Two-Particle Self-Consistent Approach** in the next Chapter.

36.1 Single-particle properties

The Hubbard model

$$K = \sum_\sigma \sum_{i,j} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U n_{i\downarrow} n_{i\uparrow} - \mu \sum_{i\sigma} n_{i\sigma} \tag{36.1}$$

Following functional methods of the Schwinger school, we begin, as we have done earlier, with the generating function with source fields ϕ_σ and field destruction operators ψ in the grand canonical ensemble

$$Z[\phi] = \mathrm{Tr}\left(e^{-\beta(H-\mu N)} \mathcal{T}_\tau e^{-\psi^\dagger_{\bar\sigma}(\bar 1)\phi_{\bar\sigma}(\bar 1,\bar 2)\psi_{\bar\sigma}(\bar 2)}\right) \tag{36.2}$$

defining

$$S[\phi] \equiv e^{-\psi^\dagger_{\bar\sigma}(\bar 1)\phi_{\bar\sigma}(\bar 1,\bar 2)\psi_{\bar\sigma}(\bar 2)} \tag{36.3}$$

We adopt the convention that 1 stands for the lattice site position and imaginary time indices $(\mathbf{r}_1, \tau_1)$. We should identify $\psi_\sigma(1) \equiv c_{r_1\sigma}(\tau_1)$. We will also define $\delta(1-2) \equiv \delta(\tau_1 - \tau_2)\delta_{r_1,r_2}$. The over-bar notation means

$$\psi^\dagger_{\bar\sigma}(\bar 1)\phi_{\bar\sigma}(\bar 1,\bar 2)\psi_{\bar\sigma}(\bar 2) \equiv \sum_\sigma \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{r_1,r_2} c^\dagger_{r_1\sigma}(\tau_1)\phi_\sigma(\bar 1,\bar 2)c_{r_2\sigma}(\tau_2) \tag{36.4}$$

The propagator in the presence of the source field is obtained from functional differentiation

$$\mathcal{G}_\sigma(1,2)_\phi = -\left\langle T_\tau \psi_\sigma(1)\psi^\dagger_\sigma(2)\right\rangle_\phi = -\frac{\left\langle T_\tau S[\phi]\psi_\sigma(1)\psi^\dagger_\sigma(2)\right\rangle}{\langle T_\tau S[\phi]\rangle} = -\frac{\delta \ln Z[\phi]}{\delta\phi_\sigma(2,1)} \tag{36.5}$$

define the propagator for creation operator

$$S_1[\phi, \tau_f, \tau_i] = \mathcal{T} \exp\left\{-\int_{\tau_i}^{\tau_f} d\tau_1 \sum_{r_1} c^\dagger_{r_1\bar\sigma}(\tau_1)\phi_{\bar\sigma}(\tau_1, r_1, \bar 2)\psi_{\bar\sigma}(\bar 2)\right\} \tag{36.6}$$

$$\begin{aligned}\partial_{\tau_i} S_1[\phi,\tau_f,\tau_i] &= S_1[\phi,\tau_f,\tau_i]\left\{\sum_{r_1} c^\dagger_{r_1\bar\sigma}(\tau_i)\phi_{\bar\sigma}(\tau_i,r_1,\bar 2)\psi_{\bar\sigma}(\bar 2)\right\}\\ \partial_{\tau_f} S_1[\phi,\tau_f,\tau_i] &= \left\{-\sum_{r_1} c^\dagger_{r_1\bar\sigma}(\tau_f)\phi_{\bar\sigma}(\tau_f,r_1,\bar 2)\psi_{\bar\sigma}(\bar 2)\right\} S_1[\phi,\tau_f,\tau_i]\end{aligned} \tag{36.7}$$

so we have

$$\begin{aligned}&\partial_{\tau_1}\left(S[\phi,\beta,\tau_1]\psi_\sigma(1)S[\phi,\tau_1,0]\right)\\ =&S[\phi,\beta,\tau_1]\left[\sum_{r_i} c^\dagger_{r_i\bar\sigma}(\tau_1)\phi_{\bar\sigma}(\tau_1,r_i,\bar 2)\psi_{\bar\sigma}(\bar 2),\psi_\sigma(1)\right] S[\phi,\tau_1,0]\\ =&-\phi_\sigma(\tau_1,r_1,\bar 2)S[\phi,\beta,\tau_1]\psi_\sigma(\bar 2)S[\phi,\tau_1,0]\end{aligned} \tag{36.8}$$

we now wish to obtain an equation of motion for $\mathcal{G}_\sigma(1,2)$. As before, there are three contributions

$$\begin{aligned}\partial_{\tau_1}\mathcal{G}_\sigma(1,2)_\phi =& -\delta(\tau_1-\tau_2)\delta_{r_1,r_2}\\ &-\left\langle T_\tau\left(\partial_{\tau_1}\psi_\sigma(1)\right)\psi^\dagger_\sigma(2)\right\rangle_\phi\\ &+\phi_\sigma(r_1,\tau_1,\bar 2)\left\langle T_\tau\psi_\sigma(\bar 2)\psi^\dagger_\sigma(2)\right\rangle_\phi\end{aligned} \tag{36.9}$$

To calculate the second part, we use the equation of motion for field operator $\psi_\sigma(1) = c_{i_1\sigma}(\tau_1)$

$$\begin{aligned}\partial_\tau c_{i\sigma}(\tau) &= [K, c_{i\sigma}]\\ &= -\sum_k t_{ik}c_{k\sigma} + \mu c_{i\sigma} - U c_{i\sigma}n_{i,-\sigma}\end{aligned} \tag{36.10}$$

in ψ notation

$$\partial_{\tau_1}\psi_\sigma(r_1,\tau_1) = -\sum_{r_2} t_{12}\psi_\sigma(r_2,\tau_1) + \mu\psi_\sigma(r_1,\tau_1) - U\psi_\sigma(r_1,\tau_1)\psi^\dagger_{-\sigma}(r_1,\tau_1)\psi_{-\sigma}(r_1,\tau_1) \tag{36.11}$$

we then have

$$\begin{aligned}\partial_{\tau_1}\mathcal{G}_\sigma(1,2)_\phi =& -\delta(\tau_1-\tau_2)\delta_{r_1,r_2} - \phi_\sigma(1,\bar 2)\mathcal{G}_\sigma(\bar 2,2)_\phi\\ &-\sum_{r_3} t_{13}\mathcal{G}_\sigma(r_3,\tau_1,2)_\phi + \mu\mathcal{G}_\sigma(1,2)_\phi\\ &+U\left\langle T_\tau\psi_\sigma(1)\psi^\dagger_{-\sigma}(1)\psi_{-\sigma}(1)\psi^\dagger_\sigma(2)\right\rangle_\phi\end{aligned} \tag{36.12}$$

with

$$T_{13} \equiv t_{13}\delta(\tau_1-\tau_3) \tag{36.13}$$

$$\begin{aligned}\left(\delta(1-\bar 3)\left(\partial_{\tau_3}-\mu\right)+T_{1\bar 3}\right)\mathcal{G}_\sigma(\bar 3,2)_\phi =& -\delta(1-2) - \phi_\sigma(1,\bar 2)\mathcal{G}_\sigma(\bar 2,2)_\phi\\ &+U\left\langle T_\tau\psi_\sigma(1)\psi^\dagger_{-\sigma}(1)\psi_{-\sigma}(1)\psi^\dagger_\sigma(2)\right\rangle_\phi\end{aligned} \tag{36.14}$$

Define the non-interacting Green's function by setting $U=\phi=0$

$$\left(\delta(1-\bar 3)\left(\partial_{\tau_{\bar 3}}-\mu\right)+T_{1\bar 3}\right)\mathcal{G}^0_\sigma(\bar 3,2)_\phi = -\delta(1-2) \tag{36.15}$$

schematically, this is $L_{1\bar 3}\mathcal{G}_{\bar 3 2} = -I_{12}$. We have identified the inverse of Green's function

$$\left[\mathcal{G}^0_\sigma(1,3)_\phi\right]^{-1} \equiv -\left(\delta(1-3)\left(\partial_{\tau_3}-\mu\right)+T_{13}\right) \tag{36.16}$$

we can then write the equation of motion for the dressed Green's function as

$$\left(\left[\mathcal{G}^0_\sigma(1,\bar 3)_\phi\right]^{-1} - \phi_\sigma(1,\bar 3)\right)\mathcal{G}_\sigma(\bar 3,2)_\phi = \delta(1-2) - U\left\langle T_\tau\psi_\sigma(1)\psi^\dagger_{-\sigma}(1)\psi_{-\sigma}(1)\psi^\dagger_\sigma(2)\right\rangle_\phi \tag{36.17}$$

by definition, $\left(\mathcal{G}_0^{-1}-\phi\right)\mathcal{G} = 1+\Sigma\mathcal{G}$, so the self energy is given by

$$\begin{aligned}\Sigma_\sigma(1,\bar 1)_\phi\mathcal{G}_\sigma(\bar 1,2)_\phi &= -U\left\langle T_\tau\psi^\dagger_{-\sigma}(1^+)\psi_{-\sigma}(1)\psi_\sigma(1)\psi^\dagger_\sigma(2)\right\rangle_\phi\\ &= -U\left[\frac{\delta\mathcal{G}_\sigma(1,2)_\phi}{\delta\phi_{-\sigma}(1^+,1)} - \mathcal{G}_\sigma(1,2)_\phi\mathcal{G}_{-\sigma}(1,1^+)_\phi\right]\end{aligned} \tag{36.18}$$

where we have used the relation for functional derivative:

$$\frac{\delta \mathcal{G}(1,2)_\phi}{\delta\phi(3,4)} = \left\langle T_\tau \psi(1)\psi^\dagger(2)\psi^\dagger(3)\psi(4)\right\rangle_\phi + \mathcal{G}(1,2)_\phi \mathcal{G}(4,3)_\phi \tag{36.19}$$

As in the electron gas, we now need to know the response function $\frac{\delta \mathcal{G}_\sigma(1,2)_\phi}{\delta\phi_{-\sigma}(1^+,1)}$.

36.2 Response functions

Following the standard approach and using matrix notation to abbreviate the summations and integrations we have,

$$\begin{aligned} \mathcal{G}^{-1}\mathcal{G} &= 1 \\ \frac{\delta\mathcal{G}}{\delta\phi}\mathcal{G}^{-1} + \mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi} &= 0 \\ \frac{\delta\mathcal{G}}{\delta\phi} &= -\mathcal{G}\frac{\delta\mathcal{G}^{-1}}{\delta\phi}\mathcal{G} \end{aligned} \tag{36.20}$$

using Dyson equation $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \phi - \Sigma$ we have

$$\begin{aligned} \frac{\delta\mathcal{G}}{\delta\phi} &= \mathcal{G}\left(\frac{\delta\phi'}{\delta\phi} + \frac{\delta\Sigma'}{\delta\phi}\right)\mathcal{G} \\ &= \mathcal{G}\left(\frac{\delta\phi'}{\delta\phi} + \frac{\delta\Sigma'}{\delta\mathcal{G}''}\frac{\delta\mathcal{G}''}{\delta\phi}\right)\mathcal{G} \\ &= \mathcal{G}\wedge\mathcal{G} + \mathcal{G}\left[\begin{array}{c}\frac{\delta\Sigma}{\delta\mathcal{G}}\\ \frac{\delta\mathcal{G}}{\delta\phi}\end{array}\right]\mathcal{G} \end{aligned} \tag{36.21}$$

where we use $'$ and $''$ to keep track of fields with the same indices. To remind ourselves, the wedge puts the indices of ϕ in the middle, and the column tells us that $\delta\mathcal{G}$ need to be summed over

$$\frac{\delta\mathcal{G}_{12}}{\delta\phi_{34}} = \mathcal{G}_{13}\wedge\mathcal{G}_{42} + \mathcal{G}_{15}\left[\begin{array}{c}\frac{\delta\Sigma_{56}}{\delta\mathcal{G}_{78}}\\ \frac{\delta\mathcal{G}_{78}}{\delta\phi_{34}}\end{array}\right]\mathcal{G}_{62} \tag{36.22}$$

In the Coulomb-gas case, we have solved this equation in the RPA approximation, where only charge fluctuations are involved. Here let us drop any special assumption, other than spin-rotation invariance, concerning the form of the irreducible vertices. We will see that in general, both spin and charge fluctuations influence the self-energy, contrary to the Coulomb gas where only charge fluctuations were involved.

To obtain spin and charge fluctuations from the above formula, we restore spin indices explicitly and represent coordinates with numbers. When the external field is diagonal in spin indices we need only one spin label on $\mathcal{G}$ and ϕ. The response function that can be used then to build both spin and charge fluctuations is

$$\begin{aligned} -\frac{\delta\mathcal{G}_\sigma\left(1,1^+\right)}{\delta\phi_{\sigma'}\left(2^+,2\right)} &= \left\langle T_\tau \psi_\sigma^\dagger\left(1^+\right)\psi_\sigma(1)\psi_{\sigma'}^\dagger\left(2^+\right)\psi_{\sigma'}(2)\right\rangle_\phi - \mathcal{G}_\sigma\left(1,1^+\right)_\phi \mathcal{G}_{\sigma'}\left(2,2^+\right)_\phi \\ &= \left\langle T_\tau n_\sigma(1)n_{\sigma'}(2)\right\rangle_\phi - \left\langle n_\sigma(1)\right\rangle_\phi \left\langle n_{\sigma'}(2)\right\rangle_\phi \end{aligned} \tag{36.23}$$

The charge and spin operators are given by

$$\begin{aligned} n_i &\equiv n_{i\uparrow} + n_{i\downarrow} \\ S_i^z &\equiv n_{i\uparrow} - n_{i\downarrow} \end{aligned} \tag{36.24}$$

Hence, the charge fluctuations are obtained from

$$\begin{aligned} \chi_{ch}(1,2) &= \left\langle T_\tau n(1)n(2)\right\rangle_\phi - \left\langle n(1)\right\rangle_\phi \left\langle n(2)\right\rangle_\phi \\ &= -\sum_{\sigma,\sigma'} \frac{\delta\mathcal{G}_\sigma\left(1,1^+\right)}{\delta\phi_{\sigma'}\left(2^+,2\right)} \end{aligned} \tag{36.25}$$

Notice how this makes sense intuitively, since we are asking $\delta n(1)/\delta\phi(2)$ where $\phi(2)$ couples to $n(2)$.

and the spin fluctuations from

$$\begin{aligned}\chi_{sp}(1,2) &= \langle T_\tau S^z(1)S^z(2)\rangle_\phi - \langle S^z(1)\rangle_\phi \langle S^z(2)\rangle_\phi \\ &= -\sum_{\sigma,\sigma'} \sigma \frac{\delta \mathcal{G}_\sigma\left(1,1^+\right)}{\delta \phi_{\sigma'}\left(2^+,2\right)}\sigma'\end{aligned} \tag{36.26}$$

where $\sigma = \pm 1$. Adding the spin indices,

$$\frac{\delta \mathcal{G}_\sigma}{\delta \phi_{\sigma'}} = \mathcal{G}_\sigma \wedge \mathcal{G}_\sigma \delta_{\sigma\sigma'} + \mathcal{G}_\sigma \left[\begin{array}{c} \frac{\delta \Sigma_\sigma}{\delta \mathcal{G}_{\bar{\sigma}}} \\ \frac{\delta \mathcal{G}_{\bar{\sigma}}}{\delta \phi_{\sigma'}} \end{array} \right] \mathcal{G}_\sigma \tag{36.27}$$

We now wish to find a self-consistent equation for $\chi_{ch}(1,2)$. Assuming rotational invariance, we have that $\mathcal{G}_\sigma$ is independent of σ, $\sum_\sigma \frac{\delta \mathcal{G}_\sigma}{\delta \phi_{\sigma'}}, \sum_\sigma \frac{\delta \Sigma_\sigma}{\delta \phi_{\sigma'}}$ are independent of σ' and $\sum_{\sigma'} \frac{\delta \mathcal{G}_\sigma}{\delta \phi_{\sigma'}}$ is independent of σ.

$$\begin{aligned}\chi_{ch}(1,2) &= -\sum_{\sigma,\sigma'} \frac{\delta \mathcal{G}_\sigma\left(1,1^+\right)}{\delta \phi_{\sigma'}\left(2^+,2\right)} \\ &= -\sum_{\sigma,\sigma'} \left\{ \mathcal{G}_\sigma(1,2^+)\mathcal{G}_\sigma(2,1^+)\delta_{\sigma\sigma'} + \mathcal{G}_\sigma(1,\bar{3}) \frac{\delta \Sigma_\sigma(\bar{3},\bar{4})}{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})} \frac{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})}{\delta \phi_{\sigma'}(2^+,2)} \mathcal{G}_\sigma(\bar{4},1^+) \right\} \\ &= -2\mathcal{G}(1,2^+)\mathcal{G}(2,1^+) - \mathcal{G}(1,\bar{3}) \left[\sum_{\sigma''}\sum_{\sigma} \frac{\delta \Sigma_\sigma(\bar{3},\bar{4})}{\delta \mathcal{G}_{\sigma''}(\bar{5},\bar{6})} \sum_{\sigma'} \frac{\delta \mathcal{G}_{\sigma''}(\bar{5},\bar{6})}{\delta \phi_{\sigma'}(2^+,2)} \right] \mathcal{G}(\bar{4},1^+) \\ &= -2\mathcal{G}(1,2^+)\mathcal{G}(2,1^+) - \mathcal{G}(1,\bar{3}) \left[\sum_{\sigma} \frac{\delta \Sigma_\sigma(\bar{3},\bar{4})}{\delta \mathcal{G}_{\sigma'''}(\bar{5},\bar{6})} \sum_{\sigma''}\sum_{\sigma'} \frac{\delta \mathcal{G}_{\sigma''}(\bar{5},\bar{6})}{\delta \phi_{\sigma'}(2^+,2)} \right] \mathcal{G}(\bar{4},1^+)\end{aligned} \tag{36.28}$$

where σ''' is arbitrary. Define the irreducible charge vertex $U_{ch} = \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\downarrow} + \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\uparrow}$:

$$U_{ch}(3,4,5,6) = \sum_\sigma \frac{\delta \Sigma_\sigma(3,4)}{\delta \mathcal{G}_{\sigma'''}(5,6)} = \frac{\delta \Sigma_\uparrow(3,4)}{\delta \mathcal{G}_\downarrow(5,6)} + \frac{\delta \Sigma_\uparrow(3,4)}{\delta \mathcal{G}_\uparrow(5,6)} \tag{36.29}$$

$$\chi_{ch}(5,6,2) \equiv -\sum_{\sigma''}\sum_{\sigma'} \frac{\delta \mathcal{G}_{\sigma''}(5,6)}{\delta \phi_{\sigma'}(2^+,2)} \tag{36.30}$$

we can then write

$$\chi_{ch}(1,2) = -2\mathcal{G}(1,2^+)\mathcal{G}(2,1^+) + \mathcal{G}(1,\bar{3}) \left[U_{ch}(\bar{3},\bar{4},\bar{5},\bar{6}) \chi_{ch}(\bar{5},\bar{6},2) \right] \mathcal{G}(\bar{4},1^+) \tag{36.31}$$

schematically, we write

$$\chi_{ch} = -2\mathcal{G}\cdot\mathcal{G} + \mathcal{G}\left[\left(\frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\uparrow} + \frac{\delta \Sigma_\downarrow}{\delta \mathcal{G}_\uparrow} \right) \chi_{ch} \right] \mathcal{G} \tag{36.32}$$

notice that we have abused the notation for χ_{ch}, since now there are two different definitions with different number of arguments for χ_{ch}.

Similarly, to find the consistent-equation for χ_{sp},

$$\begin{aligned}\chi_{sp}(1,2) &= -\sum_{\sigma,\sigma'} \sigma \frac{\delta \mathcal{G}_\sigma\left(1,1^+\right)}{\delta \phi_{\sigma'}\left(2^+,2\right)}\sigma' \\ &= -\sum_{\sigma,\sigma'} \sigma \left\{ \mathcal{G}_\sigma(1,2^+)\mathcal{G}_\sigma(2,1^+)\delta_{\sigma\sigma'} + \mathcal{G}_\sigma(1,\bar{3}) \frac{\delta \Sigma_\sigma(\bar{3},\bar{4})}{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})} \frac{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})}{\delta \phi_{\sigma'}(2^+,2)} \mathcal{G}_\sigma(\bar{4},1^+) \right\} \sigma' \\ &= -2\mathcal{G}(1,2^+)\mathcal{G}(2,1^+) - \mathcal{G}(1,\bar{3}) \left[\sum_{\sigma''}\sum_{\sigma} \sigma \frac{\delta \Sigma_\sigma(\bar{3},\bar{4})}{\delta \mathcal{G}_{\sigma''}(\bar{5},\bar{6})} \sigma'' \sum_{\sigma'} \sigma'' \frac{\delta \mathcal{G}_{\sigma''}(\bar{5},\bar{6})}{\delta \phi_{\sigma'}(2^+,2)} \sigma' \right] \mathcal{G}(\bar{4},1^+) \\ &= -2\mathcal{G}(1,2^+)\mathcal{G}(2,1^+) - \mathcal{G}(1,\bar{3}) \left[U_{sp}(\bar{3},\bar{4},\bar{5},\bar{6}) \chi_{sp}(\bar{5},\bar{6},2) \right] \mathcal{G}(\bar{4},1^+)\end{aligned} \tag{36.33}$$

so we have

$$\chi_{sp}(1,2) = -2\mathcal{G}(1,2^+)\mathcal{G}(2,1^+) - \mathcal{G}(1,\bar{3}) \left[U_{sp}(\bar{3},\bar{4},\bar{5},\bar{6}) \chi_{sp}(\bar{5},\bar{6},2) \right] \mathcal{G}(\bar{4},1^+) \tag{36.34}$$

where we define

$$\begin{aligned} U_{sp} &\equiv -\sum_{\sigma} \sigma \frac{\delta \Sigma_{\sigma}}{\delta \mathcal{G}_{\sigma''}} \sigma'' \\ &= -\left(\frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\sigma''}} - \frac{\delta \Sigma_{\downarrow}}{\delta \mathcal{G}_{\sigma''}} \right) \sigma'' \\ &= \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\downarrow}} - \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\uparrow}} \end{aligned} \tag{36.35}$$

$$U_{sp}(3,4,5,6) = \frac{\delta \Sigma_{\uparrow}(3,4)}{\delta \mathcal{G}_{\downarrow}(5,6)} - \frac{\delta \Sigma_{\uparrow}(3,4)}{\delta \mathcal{G}_{\uparrow}(5,6)} \tag{36.36}$$

$$\chi_{sp}(5,6,2) \equiv -\sum_{\sigma'} \sigma'' \frac{\delta \mathcal{G}_{\sigma''}(5,6)}{\delta \phi_{\sigma'}(2^+,2)} \sigma' \tag{36.37}$$

in summary, we define irreducible vertices appropriate for spin and charge responses as follows,

$$\begin{aligned} U_{sp} &= \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\downarrow}} - \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\uparrow}} \\ U_{ch} &= \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\downarrow}} + \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\uparrow}} \end{aligned} \tag{36.38}$$

36.3 Hartree-Fock and RPA

We first write expand the self-energy

$$\begin{aligned} \Sigma_{\sigma}(1,3)_{\phi} &= U \left[\mathcal{G}_{-\sigma}(1,1^+)_{\phi} \mathcal{G}_{\sigma}(1,\bar{2})_{\phi} - \frac{\delta \mathcal{G}_{\sigma}(1,\bar{2})_{\phi}}{\delta \phi_{-\sigma}(1^+,1)} \right] \mathcal{G}^{-1}(\bar{2},3)_{\phi} \\ &= U \left[\mathcal{G}_{-\sigma}(1,1^+)_{\phi} \mathcal{G}_{\sigma}(1,\bar{2})_{\phi} - \mathcal{G}_{\sigma}(1,\bar{3}) \frac{\delta \Sigma_{\sigma}(\bar{3},\bar{4})}{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})} \frac{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})}{\delta \phi_{-\sigma}(1^+,1)} \mathcal{G}_{\sigma}(\bar{4},\bar{2}) \right] \mathcal{G}^{-1}(\bar{2},3)_{\phi} \\ &= U \left[\mathcal{G}_{-\sigma}(1,1^+)_{\phi} \delta(1-3) - \mathcal{G}_{\sigma}(1,\bar{3}) \frac{\delta \Sigma_{\sigma}(\bar{3},\bar{4})}{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})} \frac{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})}{\delta \phi_{-\sigma}(1^+,1)} \mathcal{G}_{\sigma}(3,\bar{2}) \right] \end{aligned} \tag{36.39}$$

We have used the fact that $\delta_{\sigma,-\sigma} = 0$, and

$$\frac{\delta \mathcal{G}_{\sigma}(1,\bar{2})_{\phi}}{\delta \phi_{-\sigma}(1^+,1)} = \mathcal{G}_{\sigma}(1,\bar{3}) \frac{\delta \Sigma_{\sigma}(\bar{3},\bar{4})}{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})} \frac{\delta \mathcal{G}_{\bar{\sigma}}(\bar{5},\bar{6})}{\delta \phi_{-\sigma}(1^+,1)} \mathcal{G}_{\sigma}(\bar{4},\bar{2}) \tag{36.40}$$

the Hartree-Fock approximation corresponds to keeping only the first order term

$$\Sigma^H_{\sigma}(1,2)_{\phi} = U \mathcal{G}_{-\sigma}(1,1^+)_{\phi} \delta(1-2) \tag{36.41}$$

so we have

$$\begin{aligned} \frac{\delta \Sigma^H_{\uparrow}(1,2)}{\delta \mathcal{G}_{\downarrow}(3,4)} &= U \delta(1-3) \delta(1-4) \delta(1-2) \\ \frac{\delta \Sigma^H_{\uparrow}(1,2)}{\delta \mathcal{G}_{\uparrow}(3,4)} &= 0 \end{aligned} \tag{36.42}$$

this means that

$$U_{sp} = U_{ch} = \frac{\delta \Sigma_{\uparrow}}{\delta \mathcal{G}_{\downarrow}} = U \tag{36.43}$$

where we have hidden the delta functions involving the four arguments. We can now substitute this result into the previous self-consistent equations for the susceptibilities, which now takes the form

$$\begin{aligned} \chi^{RPA}_{ch}(1,2) &= \chi^0(1,2) - \frac{1}{2} U \chi^0(1,\bar{3}) \chi^{RPA}_{ch}(\bar{3},2) \\ \chi^{RPA}_{sp}(1,2) &= \chi^0(1,2) + \frac{1}{2} U \chi^0(1,\bar{3}) \chi^{RPA}_{sp}(\bar{3},2) \end{aligned} \tag{36.44}$$

where we have defined $\chi^0(1,2) \equiv -2\mathcal{G}(1,2^+)\mathcal{G}(2,1^+)$. We now Fourier Transform the above equations,

$$\begin{aligned}\chi_{ch}^{RPA}(q) &= \chi^0(q) - \frac{1}{2}U\chi^0(q)\chi_{ch}^{RPA}(q) \\ \chi_{sp}^{RPA}(q) &= \chi^0(q) + \frac{1}{2}U\chi^0(q)\chi_{sp}^{RPA}(q)\end{aligned} \tag{36.45}$$

and we have

$$\begin{aligned}\chi_{ch}^{RPA}(q) &= \frac{\chi^0(q)}{1+\frac{1}{2}U\chi^0(q)} \\ \chi_{sp}^{RPA}(q) &= \frac{\chi^0(q)}{1-\frac{1}{2}U\chi^0(q)}\end{aligned} \tag{36.46}$$

the retarded non-interacting susceptibility is still the Lindhard function

$$\chi^{0R}(\mathbf{q},\omega) = -\frac{2}{N}\sum_{\mathbf{k}} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{\omega + i\eta + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}} \tag{36.47}$$

since the Hamiltonian for the Hubbard model with $U = 0$ can be written as

$$H = \sum_{\mathbf{k}\sigma} \zeta_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \tag{36.48}$$

and the Lindhard function can be calculated directly from this Hamiltonian, as we have done in section 9.2.

36.4 RPA and violation of the Pauli exclusion principle

RPA has a drawback that is particularly important for the Hubbard model. It violates the Pauli exclusion principle that is assumed to be satisfied exactly in its definition where up spins interact only with down spins. To see this requires a bit more thinking. We derive a sum rule that rests on the use of the Pauli exclusion principle and check that it is violated by RPA to second order in U.

First note that if we sum the spin and charge susceptibilities over all wave vectors $\mathbf{q}$ and all Matsubara frequencies iq_n, we obtain local, equal-time correlation functions, namely

$$\begin{aligned}\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n} \chi_{sp}(\mathbf{q}, iq_n) &= \chi_{sp}(\mathbf{r}=0, \tau=0^-) = \left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle - 2\langle n_\uparrow n_\downarrow \rangle \\ \frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n} \chi_{ch}(\mathbf{q}, iq_n) &= \chi_{ch}(\mathbf{r}=0, \tau=0^-) = \left\langle (n_\uparrow + n_\downarrow)^2 \right\rangle - \langle n_\uparrow + n_\downarrow \rangle^2 = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle + 2\langle n_\uparrow n_\downarrow \rangle - n^2\end{aligned} \tag{36.49}$$

where we assume $\langle n_\uparrow \rangle = \langle n_\downarrow \rangle$ due to rotational invariance. On the right-hand side we used the Pauli exclusion principle $n_\sigma^2 = n_\sigma$. We call the first of the above displayed equations the **local spin sum-rule** and the second one the **local charge sum-rule**. For RPA, adding the two sum rules yields

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n} \left(\chi_{sp}(\mathbf{q}, iq_n) + \chi_{ch}(\mathbf{q}, iq_n)\right) = \frac{T}{N}\sum_{q} \left(\frac{\chi_0(q)}{1-\frac{1}{2}U\chi_0(q)} + \frac{\chi_0(q)}{1+\frac{1}{2}U\chi_0(q)}\right) = 2n - n^2 \tag{36.50}$$

expanding in U, we have

$$2n - n^2 = \frac{T}{N}\sum_q 2\chi_0(q)\left[1 + \left(\frac{1}{2}U\chi_0(q)\right)^2 + \left(\frac{1}{2}U\chi_0(q)\right)^4 + ...\right] \tag{36.51}$$

Since the non-interacting susceptibility $\chi_0(q)$ satisfies the sum rule, the equation is satisfied to zeroth order. Higher order terms in U will violate the relation unless they make exactly zero contribution. This is impossible, since we can show higher order terms are always positive, so $\sum_q \chi_0(q)^3, \chi_0(q)^5...$ cannot vanish. To positivity of $\sum_q \chi_0(q)$ can be seen from

$$\begin{aligned}\sum_q \chi_0(q) &= -\frac{2}{N}\sum_{\mathbf{q},\mathbf{k}}\left\{\sum_{iq_n} \frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})}{iq_n + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}}}\right\} \\ &= -\frac{2}{N}\sum_{\mathbf{q},\mathbf{k}}\left\{\sum_{q_n>0} \frac{2\left[f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k}+\mathbf{q}})\right](\zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}})}{q_n^2 + (\zeta_{\mathbf{k}} - \zeta_{\mathbf{k}+\mathbf{q}})^2}\right\} > 0\end{aligned} \tag{36.52}$$

since the function $f(x)$ is monotonically decreasing. To prove this for all odd orders, we need more work, consider

$$\sum_{k=-\infty}^{\infty}\left(\frac{-a}{a+ik}\right)^{2n+1}=\sum_{k=-\infty}^{\infty}\frac{-a^{2n+1}}{(a+ik)^{2n+1}}=a^{2n+1}(-1)^{n+1}i\left[\zeta(2n+1,ia+1)-\zeta(2n+1,-ia)\right] \tag{36.53}$$

where we have rescaled the Matsubara frequency and we defined Hurwitz zeta function

$$\zeta(s,a)=\sum_{n=0}^{\infty}\frac{1}{(n+a)^s}. \tag{36.54}$$

Notice that this function is even in a, so we can focus on $a>0$. We can check

$$\begin{cases}\pi^3\coth(\pi a)\text{csch}^2(\pi a) & n=1\\ \frac{1}{3}\pi^5\left(\coth^3(\pi a)\text{csch}^2(\pi a)+2\coth(\pi a)\text{csch}^4(\pi a)\right) & n=3\\ \ldots & \\ i^{1-2n}\left[\zeta(2n+1,ia+1)-\zeta(2n+1,-ia)\right] & n\end{cases} \tag{36.55}$$

so at least up to order $\mathcal{O}(U^2)$, the summation would be positive and the Pauli-exclusion would be violated. (See Onenote for the diagrammatic explanation)

36.5 RPA, phase transitions and Mermin-Wagner theorem

The RPA predicts that the normal state is sometimes unstable, namely that if we decrease the temperature, spin fluctuations at zero frequency start, in certain cases, to diverge. Below the temperature where that occurs, the spin susceptibility is negative, which is prohibited by thermodynamic stability. This indicates that a paramagnetic ground state is an unstable state. This happens even in two-dimensions with RPA because

$$\begin{aligned}\chi(z)&=\int\frac{d\omega'}{\pi}\frac{\chi''(\omega')}{\omega'-z}\\ \chi_{sp}(q)&=\int\frac{d\omega'}{\pi}\frac{\chi''_{sp}(\mathbf{q},\omega')}{\omega'-iq_n}\\ &=\int\frac{d\omega'}{\pi}\frac{\omega'\chi''_{sp}(\mathbf{q},\omega')}{q_n^2+\omega'^2}>0\end{aligned} \tag{36.56}$$

where we used the oddness and positivity of χ''_{AA}. On the other hand, the expression

$$\chi_{sp}(q)=\frac{\chi_0(q)}{1-\frac{1}{2}U\chi_0(q)} \tag{36.57}$$

is quite likely to become negative if U is large enough.

Why does a negative spin susceptibility at $q_n=0$ signal an **instability**? Because there is a thermodynamic inequality that says that susceptibilities of the form dA/da, where A and a are thermodynamically conjugate variables, are positive since entropy is a maximum at equilibrium. But there is another way to look at this from the thermodynamic sum rule

$$\chi_{sp}(\mathbf{Q},0)=\int\frac{d\omega}{\pi}\frac{\chi''_{sp}(\mathbf{Q},\omega)}{\omega} \tag{36.58}$$

Indeed, if the left-hand side is negative, this means that the imaginary part of the spin susceptibility for positive frequencies has to be negative. This violates the positivity criterion imposed by stability, namely that $\chi''_{sp}(\mathbf{Q},\omega)\omega>0$. Hence the system is unstable.

Such an **instability in two dimensions** at finite temperature is **prohibited** by the **Mermin-Wagner theorem** that says that a continuous symmetry cannot be broken in two dimensions at finite temperature. We will come back on this theorem in a later chapter, but for now the theorem may intuitively be understood as follows.

If there is long-range order in the presence of a continuous symmetry, there will be a term in the free energy that will be proportional to $|\nabla\phi|^2$, where ϕ is the angle representing the deviation of the spins say, from their equilibrium position. The equipartition theorem then says that

$$\mathbf{q}^2\left\langle\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\right\rangle=\frac{T}{2} \tag{36.59}$$

Thus, in two dimensions, the thermal fluctuations of the angle is infinite, proving the theorem by contradiction

$$\left\langle \phi^2 \right\rangle = \int_0^\infty d^2q \left\langle \phi_{\mathbf{q}} \phi_{-\mathbf{q}} \right\rangle = \int_0^\infty \frac{d^2q}{q^2} \frac{T}{2} = \infty \tag{36.60}$$

We may think that the instability will occur only for large enough U so that RPA would still be useful below that threshold. This is not the case. Let us illustrate with a specific example where the instability occurs for infinitesimal U.

We evaluate the Lindhard function at zero frequency in the case where we have only nearest neighbor hopping on a square lattice ($d = 3$), where $\varepsilon_{\mathbf{k}} = -2t\left(\cos k_x + \cos k_y + \cos k_z\right)$. Then, if we take $\mu = 0$, which in this case corresponds to half-filling, and choose the wave vector corresponding to an antiferromagnetic fluctuation, namely $Q = (\pi, \pi)$ that leads to a phase $+1$ or -1 on alternating sites. Notice that $\varepsilon_{\mathbf{k}+\mathbf{Q}} = -\varepsilon_{\mathbf{k}}$, $1 - f(x) = f(-x)$ we find

$$\begin{aligned} \chi^{0R}(\mathbf{Q}, \omega = 0) &= -\frac{2}{N} \sum_{\mathbf{k}} \frac{2f(\beta\varepsilon_{\mathbf{k}}) - 1}{2\varepsilon_{\mathbf{k}}} \\ &= \frac{2}{N} \sum_{\mathbf{k}} \frac{\tanh\left(\beta\varepsilon_{\mathbf{k}}/2\right)}{2\varepsilon_{\mathbf{k}}} \\ &= \frac{2}{n} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\tanh\left(\beta\varepsilon_{\mathbf{k}}/2\right)}{2\varepsilon_{\mathbf{k}}} \\ &= \frac{1}{n} \int d\varepsilon N(\varepsilon) \frac{\tanh\left(\beta\varepsilon/2\right)}{2\varepsilon} \end{aligned} \tag{36.61}$$

at $d = 3$, the density of states at fermi surface $\varepsilon = 0$ remain constant up to some cutoff energy Λ, so we can approximate $N(\varepsilon)$ by $N(0)$ in this range. At the same time, as $T \to 0$, the integrand become more and more concentrated around zero, thus the cutoff is justified. We separate the integral into two parts

$$\begin{aligned} \int_0^\Lambda d\varepsilon \frac{\tanh(\beta\varepsilon/2)}{2\varepsilon} &= \int_0^{\beta\Lambda/2} dx \frac{\tanh(x)}{2x} \\ &= \int_0^1 dx \frac{\tanh(x)}{2x} + \int_1^{\beta\Lambda/2} dx \frac{\tanh(x)}{2x} \\ &\approx I(0,1) + \int_1^{\beta\Lambda/2} dx \frac{1}{2x} \\ &= 0.455... + \frac{1}{2} \ln\left(\frac{\Lambda}{2T}\right) \end{aligned} \tag{36.62}$$

so we have

$$\lim_{T\to 0} \chi^{0R}(\mathbf{Q}, \omega = 0) = \frac{N(0)}{2n} \ln\left(\frac{\Lambda}{2T}\right) = A \ln(\Lambda/T) \tag{36.63}$$

where we used $\lim_{x\to\infty} \tanh(x) = 1$. We see that as $T \to 0$, the upper bound of the integral go to infinity and $\frac{\tanh(x)}{2x} \to 1/2x$, so the integral diverge logarithmically with $1/T$. For T sufficiently small, $\chi^{0R}(\mathbf{Q}, 0)$ diverges, which means that

$$\lim_{T\to 0} \chi_{sp}^{RPA}(\mathbf{Q}) = \frac{A \ln(\Lambda/T)}{1 - \frac{1}{2} UA \ln(\Lambda/T)} \tag{36.64}$$

Even with infinitesimal U, at $T_0 = \Lambda e^{-2/(UA)}$ the denominator will cross zero, and the spin susceptibility will diverge. Below T_0, χ_{sp} is negative, signaling instability. This instability signals a **second-order phase transition** that is physical.

In two dimensions, $N(\varepsilon)$ has a logarithmic divergence at $\varepsilon = 0$ so the above result must be modified. We would obtain a $\ln^2\left(E_F/T\right)$ instead of $\ln\left(E_F/T\right)$. Nevertheless, the qualitative result would be the same. There is an instability even in the presence of an infinitesimal U. However, in two-dimensions, Mermin Wagner theorem states that one cannot have a phase transition that breaks a continuous symmetry at finite temperature. Hence, RPA fails miserably on many grounds in two dimensions: It violates the Pauli exclusion principle and the Mermin-Wagner Theorem. The approach in the next section fixes these two problems and more.

37 The Two-particle Self-Consistent Approach (TPSC)

TPSC is valid from **weak to intermediate coupling**. Hence, on the negative side, it does not describe the Mott transition. Nevertheless, there is a large number of physical phenomena that it allows to study. An important one is **antiferromagnetic fluctuations**. It is extremely important physically that in two dimensions there is a wide range of temperatures where there are huge antiferromagnetic fluctuations in the paramagnetic state, without long-range order, as imposed by the Mermin Wagner theorem. The standard way to treat fluctuations in many-body theory, RPA, misses this and also violates the Pauli exclusion principle. The **composite operator method** (**COM**), by F. Mancini, is another approach that satisfies the Mermin Wagner theorem and the Pauli exclusion principle. The **Fluctuation Exchange Approximation** (**FLEX**), and the self-consistent renormalized theory of Moriya-Lonzarich are other approaches that satisfy the Mermin-Wagner theorem at weak coupling.

In summary, the advantages and disadvantages of TPSC are as follows. Advantages:

1. There are no adjustable parameters.
2. Several exact results are satisfied: Conservation laws for spin and charge, the Mermin-Wagner theorem, the Pauli exclusion principle in the form $\left\langle n_\uparrow^2 \right\rangle = \langle n_\uparrow \rangle$, the local moment and local-charge sum rules and the f sum-rule.
3. Consistency between one and two-particle properties serves as a guide to the domain of validity of the approach. (Double occupancy obtained from sum rules on spin and charge equals that obtained from the self-energy and the Green function).
4. Up to intermediate coupling, TPSC agrees within a few percent with Quantum Monte Carlo (QMC) calculations. Note that QMC calculations can serve as benchmarks since they are exact within statistical accuracy, but they are limited in the range of physical parameter accessible.
5. We do not need to assume that Migdal's theorem applies to be able to obtain the self-energy.

The main successes of TPSC include

1. Understanding the physics of the pseudogap induced by precursors of a long-range ordered phase in two dimensions. For this understanding, one needs a method that satisfies the Mermin-Wagner theorem to create a broad temperature range where the antiferromagnetic correlation length is larger than the thermal de Broglie wavelength. That method must also allow one to compute the self-energy reliably. Only TPSC does both.
2. Explaining the pseudogap in electron-doped cuprate superconductors over a wide range of dopings.
3. Finding estimates of the transition temperature for d-wave superconductivity that were found later in agreement with quantum cluster approaches such as the Dynamical Cluster Approximation.
4. Giving quantitative estimates of the range of temperature where quantum critical behavior can affect the physics.

The drawbacks of this approach, that I explain as we go along, are that

1. It works well in two or more dimensions, not in one dimension
2. It is not valid at strong coupling, except at very high temperature and large U where it recovers the atomic limit
3. It is not valid deep in the renormalized classical regime
4. For models other than the one-band Hubbard model, one usually runs out of sum rules and it is in general not possible to find all parameters self-consistently. With nearest-neighbor repulsion, it has been possible to find a way out.

37.1 First Step: TPSC for first order quantities

To liberate ourselves from diagrams and find results that are valid beyond perturbation theory, we start from the exact expression for the self-energy,

$$\begin{aligned}\Sigma_\sigma(1,\bar{1})_\phi \mathcal{G}_\sigma(\bar{1},2)_\phi &= -U\left\langle T_\tau \psi^\dagger_{-\sigma}\left(1^+\right)\psi_{-\sigma}(1)\psi_\sigma(1)\psi^\dagger_\sigma(2)\right\rangle_\phi \\ &= -U\left[\frac{\delta\mathcal{G}_\sigma(1,2)_\phi}{\delta\phi_{-\sigma}\left(1^+,1\right)} - \mathcal{G}_{-\sigma}\left(1,1^+\right)_\phi \mathcal{G}_\sigma(1,2)_\phi\right]\end{aligned} \tag{37.1}$$

In Hartree-Fock approximation, we have set $\frac{\delta\mathcal{G}_\sigma(1,2)_\phi}{\delta\phi_{-\sigma}(1^+,1)} = 0$ and includes only

$$\Sigma^{HF}_\sigma(1,\bar{1})_\phi \mathcal{G}^{HF}_\sigma(\bar{1},2)_\phi = U\mathcal{G}_{-\sigma}\left(1,1^+\right)_\phi \mathcal{G}_\sigma(1,2)_\phi \tag{37.2}$$

setting $2 \to 1^+$, we have

$$\Sigma^{HF}_\sigma(1,\bar{1})_\phi \mathcal{G}^{HF}_\sigma(\bar{1},1^+)_\phi = U\left\langle n_\uparrow\right\rangle\left\langle n_\downarrow\right\rangle \tag{37.3}$$

however, in the exact expression, if we set $2 \to 1^+$, we obtain

$$\Sigma_\sigma(1,\bar{1})_\phi \mathcal{G}_\sigma(\bar{1},1^+)_\phi = U\left\langle n_\uparrow n_\downarrow\right\rangle \tag{37.4}$$

We see that Hartree-Fock ignores the correlation between $n_\uparrow$ and $n_\downarrow$ and factors $\langle n_\uparrow n_\downarrow\rangle$ exactly. We now insist that the exact relation should be satisfied exactly, and try to determine $\langle n_\uparrow n_\downarrow\rangle$ self-consistently. In the Hubbard model, there are only two local four point functions: $\langle n_\uparrow n_\downarrow\rangle$ and $\left\langle n^2_\uparrow\right\rangle = \left\langle n^2_\downarrow\right\rangle = \langle n_\uparrow\rangle = \langle n_\downarrow\rangle = n/2$. We will consider these quantities as already known and try to find equations to solve for them. The failure of Hartree-Fock at $2 \to 1^+$ is clearly due to the local Hubbard interaction. If 2 is at a distance from 1 (in both space and time), the Hartree factorization should be a more reasonable approximation. Therefore, we still make a Hartree-Fock factorization, but with a different coefficient by postulating that

$$\Sigma^{(1)}_\sigma(1,\bar{1})_\phi \mathcal{G}^{(1)}_\sigma(\bar{1},2)_\phi = A_\phi \mathcal{G}^{(1)}_{-\sigma}\left(1,1^+\right)_\phi \mathcal{G}^{(1)}_\sigma(1,2)_\phi \tag{37.5}$$

where A_ϕ depends on external field and is chosen such that the exact result

$$\Sigma_\sigma(1,\bar{1})_\phi \mathcal{G}_\sigma\left(\bar{1},1^+\right)_\phi = U\left\langle n_\uparrow(1)n_\downarrow(1)\right\rangle_\phi \tag{37.6}$$

is satisfied. It is easy to see that the solution is

$$A_\phi = U\frac{\left\langle n_\uparrow(1)n_\downarrow(1)\right\rangle_\phi}{\left\langle n_\uparrow(1)\right\rangle_\phi\left\langle n_\downarrow(1)\right\rangle_\phi} \tag{37.7}$$

Substituting A_ϕ back into our ansatz, we obtain our first approximation for the self-energy by right-multiplying by $\left(\mathcal{G}^{(1)}_\sigma\right)^{-1}$:

$$\begin{aligned}\Sigma^{(1)}_\sigma(1,2)_\phi &= A_\phi \mathcal{G}^{(1)}_{-\sigma}\left(1,1^+\right)_\phi \delta(1-2) \\ &= U\frac{\left\langle n_\uparrow(1)n_\downarrow(1)\right\rangle_\phi}{\left\langle n_\uparrow(1)\right\rangle_\phi\left\langle n_\downarrow(1)\right\rangle_\phi}\mathcal{G}^{(1)}_{-\sigma}\left(1,1^+\right)_\phi \delta(1-2)\end{aligned} \tag{37.8}$$

Notice that A_ϕ is also dependent on $\mathcal{G}$. This gives

$$\begin{aligned}\frac{\delta\Sigma^{(1)}_\uparrow(1,2)}{\delta\mathcal{G}_\downarrow(3,4)} &= A_\phi\delta(1-3)\delta(1-4)\delta(1-2) + \frac{\delta A_\phi}{\delta\mathcal{G}_\downarrow(3,4)}\mathcal{G}^{(1)}_\downarrow\left(1,1^+\right)_\phi\delta(1-2) \\ \frac{\delta\Sigma^{(1)}_\uparrow(1,2)}{\delta\mathcal{G}_\uparrow(3,4)} &= \frac{\delta A_\phi}{\delta\mathcal{G}_\uparrow(3,4)}\mathcal{G}^{(1)}_\downarrow\left(1,1^+\right)_\phi\delta(1-2)\end{aligned} \tag{37.9}$$

It is in general difficult to calculate $\frac{\delta A_\phi}{\delta\mathcal{G}_\uparrow(3,4)}$, but we do not need to, since rotational invariance demands $\frac{\delta A_\phi}{\delta\mathcal{G}_\uparrow} = \frac{\delta A_\phi}{\delta\mathcal{G}_\downarrow}$, we see that

$$U_{sp}(1,2,3,4) = \frac{\delta\Sigma_\uparrow(1,2)}{\delta\mathcal{G}_\downarrow(3,4)} - \frac{\delta\Sigma_\uparrow(1,2)}{\delta\mathcal{G}_\uparrow(3,4)} = A_{\phi=0}\delta(1-3)\delta(1-4)\delta(1-2) \tag{37.10}$$

is now independent of the complicated factor $\frac{\delta A_\phi}{\delta \mathcal{G}_\uparrow(3,4)}$. If we were to calculate $U_{ch} = \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\downarrow} + \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\uparrow}$ directly, we would still need this factor which involves six-point correlation functions, but this is unnecessary, since we already have enough sum rules to solve for it. We have now a relation

$$U_{sp} = A_{\phi=0} = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle} \tag{37.11}$$

The renormalization of this irreducible vertex may be physically understood as coming from the physics described by **Kanamori and Brueckner** (in the latter case in the context of nuclear physics): The value of the bare interaction is renormalized down by the fact that the two-particle wave function will want to be smaller where U is larger. In the language of perturbation theory, one must sum the Born series to compute how two particles scatter off each other and not work in the first Born approximation. This completes the derivation of the ansatz that is central to TPSC.

In summary, spin and charge fluctuations are obtained from

$$\begin{aligned} \chi_{sp}(q) &= \frac{\chi^{(1)}(q)}{1 - \frac{1}{2} U_{sp} \chi^{(1)}(q)} \\ \chi_{ch}(q) &= \frac{\chi^{(1)}(q)}{1 + \frac{1}{2} U_{ch} \chi^{(1)}(q)} \end{aligned} \tag{37.12}$$

with the irreducible vertices determined from the sum rules and the relation for U_{sp}

$$\begin{aligned} \frac{T}{N} \sum_{\mathbf{q}} \sum_{iq_n} \frac{\chi^{(1)}(q)}{1 - \frac{1}{2} U_{sp} \chi^{(1)}(q)} &= n - 2 \langle n_\uparrow n_\downarrow \rangle \\ \frac{T}{N} \sum_{\mathbf{q}} \sum_{iq_n} \frac{\chi^{(1)}(q)}{1 + \frac{1}{2} U_{ch} \chi^{(1)}(q)} &= n + 2 \langle n_\uparrow n_\downarrow \rangle - n^2. \end{aligned} \tag{37.13}$$

$$U_{sp} = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle} \tag{37.14}$$

37.2 Second Step: TPSC for second order self-energy

The self-energy is sensitive to collective modes since these are important at low frequency. The second step of TPSC is thus to find a better approximation for the self-energy. This is similar in spirit to what is done in the electron gas where plasmons are found with non-interacting particles and then used to compute an improved approximation for the self-energy. This two step process is also analogous to renormalization group calculations where renormalized interactions are evaluated to one-loop order and quasiparticle renormalization in two-loop order.

Starting with relation $(\Sigma, \frac{\delta \mathcal{G}}{\delta \phi})$

$$\Sigma_\sigma(1,\overline{1}) \mathcal{G}_\sigma(\overline{1},2) = U \mathcal{G}_{-\sigma}\left(1,1^+\right)_\phi \mathcal{G}_\sigma(1,2)_\phi - U \left. \frac{\delta \mathcal{G}_\sigma(1,2)_\phi}{\delta \phi_{-\sigma}\left(1^+,1\right)} \right|_{\phi=0} \tag{37.15}$$

the first term is the Hartree-Fock approximation. In the limit $\omega \to \infty$, Hartree-Fock gives the exact result. The $\delta \mathcal{G}/\delta\phi$ term thus gives a contribution at lower frequencies, coming from charge and spin fluctuations.

$$\Sigma^{(2)}_\sigma(1,2) = U \mathcal{G}^{(1)}_{-\sigma}\left(1,1^+\right) \delta(1-2) - U \mathcal{G}^{(1)}_\sigma(1,\overline{3}) \left[\left. \frac{\delta \Sigma^{(1)}_\sigma(\overline{3},2)_\phi}{\delta \mathcal{G}^{(1)}_{\bar{\sigma}}(\overline{4},\overline{5})_\phi} \right|_{\phi=0} \left. \frac{\delta \mathcal{G}^{(1)}_{\bar{\sigma}}(\overline{4},\overline{5})_\phi}{\delta \phi_{-\sigma}\left(1^+,1\right)_\phi} \right|_{\phi=0} \right] \tag{37.16}$$

We can prove that $\frac{\delta \Sigma^{(1)}_\sigma(1,2)}{\delta \mathcal{G}^{(1)}_{\bar{\sigma}}(3,4)} \propto \delta(1-2)(3-4)$:

$$\begin{aligned} \frac{\delta \Sigma^{(1)}_\uparrow(1,2)}{\delta \mathcal{G}_\downarrow(3,4)} &= A_\phi \delta(1-3)\delta(1-4)\delta(1-2) + \frac{\delta A_\phi}{\delta \mathcal{G}_\downarrow(3,4)} \mathcal{G}^{(1)}_\downarrow\left(1,1^+\right)_\phi \delta(1-2) \\ \frac{\delta \Sigma^{(1)}_\uparrow(1,2)}{\delta \mathcal{G}_\uparrow(3,4)} &= \frac{\delta A_\phi}{\delta \mathcal{G}_\uparrow(3,4)} \mathcal{G}^{(1)}_\downarrow\left(1,1^+\right)_\phi \delta(1-2) \end{aligned} \tag{37.17}$$

$$\frac{\delta A_\phi(1)}{\delta \mathcal{G}_\sigma(3,4)} = U \frac{\delta n_\sigma(3)}{\mathcal{G}_\sigma(3,4)} \frac{\delta}{\delta n_\sigma(3)} \frac{\langle n_\uparrow(1) n_\downarrow(1)\rangle_\phi}{\langle n_\uparrow(1)\rangle_\phi \langle n_\downarrow(1)\rangle_\phi} \propto \delta(1-3)\delta(3-4) \tag{37.18}$$

Therefore, U_{sp}, U_{ch} should also all be proportional to $\delta(1-2)\delta(1-3)(1-4)$. So we have

$$\begin{aligned} \frac{\delta \Sigma_\uparrow(1,2)}{\delta \mathcal{G}_\downarrow(3,4)} &= \frac{1}{2}\left(U_{ch}+U_{sp}\right)\delta(1-2)\delta(1-3)(1-4) \\ \frac{\delta \Sigma_\uparrow(1,2)}{\delta \mathcal{G}_\uparrow(3,4)} &= \frac{1}{2}\left(U_{ch}-U_{sp}\right)\delta(1-2)\delta(1-3)(1-4) \end{aligned} \tag{37.19}$$

this allows us to write

$$\begin{aligned} \frac{\delta \Sigma_\sigma^{(1)}(3,2)}{\delta \mathcal{G}_{\bar{\sigma}}^{(1)}(\overline{4},\overline{5})} \frac{\delta \mathcal{G}_{\bar{\sigma}}^{(1)}(\overline{4},\overline{5})}{\delta \phi_{-\sigma}\left(1^+,1\right)} &= \frac{\delta \Sigma_\sigma^{(1)}(3,2)}{\delta \mathcal{G}_\sigma^{(1)}(\overline{4},\overline{5})} \frac{\delta \mathcal{G}_\sigma^{(1)}(\overline{4},\overline{5})}{\delta \phi_{-\sigma}\left(1^+,1\right)} + \frac{\delta \Sigma_\sigma^{(1)}(3,2)}{\delta \mathcal{G}_{-\sigma}^{(1)}(\overline{4},\overline{5})} \frac{\delta \mathcal{G}_{-\sigma}^{(1)}(\overline{4},\overline{5})}{\delta \phi_{-\sigma}\left(1^+,1\right)} \\ &= \frac{1}{2}\left(U_{ch}-U_{sp}\right)\frac{\delta \mathcal{G}_\sigma^{(1)}(2,2^+)}{\delta \phi_{-\sigma}\left(1^+,1\right)}\delta(2-3) + \frac{1}{2}\left(U_{ch}+U_{sp}\right)\frac{\delta \mathcal{G}_{-\sigma}^{(1)}(2,2^+)}{\delta \phi_{-\sigma}\left(1^+,1\right)}\delta(2-3) \\ &= \delta(2-3)\left\{\frac{U_{ch}}{2}\left(\frac{\delta \mathcal{G}_\sigma^{(1)}(2,2^+)}{\delta \phi_{-\sigma}\left(1^+,1\right)} + \frac{\delta \mathcal{G}_{-\sigma}^{(1)}(2,2^+)}{\delta \phi_{-\sigma}\left(1^+,1\right)}\right) - \frac{U_{sp}}{2}\left(\frac{\delta \mathcal{G}_\sigma^{(1)}(2,2^+)}{\delta \phi_{-\sigma}\left(1^+,1\right)} - \frac{\delta \mathcal{G}_{-\sigma}^{(1)}(2,2^+)}{\delta \phi_{-\sigma}\left(1^+,1\right)}\right)\right\} \\ &= \delta(2-3)\left\{-\frac{U_{ch}}{4}\chi_{ch}(2,1) - \frac{U_{sp}}{4}\chi_{sp}(2,1)\right\} \\ &= -\frac{1}{4}\delta(2-3)\left\{U_{ch}\chi_{ch}(2,1) + U_{sp}\chi_{sp}(2,1)\right\} \end{aligned} \tag{37.20}$$

where we used

$$\begin{aligned} U_{sp} &= \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\downarrow} - \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\uparrow} \qquad & \chi_{ch}(1,2) &= -\sum_{\sigma,\sigma'}\frac{\delta \mathcal{G}_\sigma\left(1,1^+\right)}{\delta \phi_{\sigma'}\left(2^+,2\right)} = -2\left(\frac{\delta \mathcal{G}_\uparrow\left(1,1^+\right)}{\delta \phi_\downarrow\left(2^+,2\right)} + \frac{\delta \mathcal{G}_\uparrow\left(1,1^+\right)}{\delta \phi_\uparrow\left(2^+,2\right)}\right) \\ U_{ch} &= \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\downarrow} + \frac{\delta \Sigma_\uparrow}{\delta \mathcal{G}_\uparrow}, \qquad & \chi_{sp}(1,2) &= -\sum_{\sigma,\sigma'}\sigma\frac{\delta \mathcal{G}_\sigma\left(1,1^+\right)}{\delta \phi_{\sigma'}\left(2^+,2\right)}\sigma' = 2\left(\frac{\delta \mathcal{G}_\uparrow\left(1,1^+\right)}{\delta \phi_\downarrow\left(2^+,2\right)} - \frac{\delta \mathcal{G}_\uparrow\left(1,1^+\right)}{\delta \phi_\uparrow\left(2^+,2\right)}\right) \end{aligned} \tag{37.21}$$

finally, the second order self energy is given by

$$\Sigma_\sigma^{(2)}(1,2) = U\mathcal{G}_{-\sigma}^{(1)}\left(1,1^+\right)\delta(1-2) + \frac{U}{4}\mathcal{G}_\sigma^{(1)}(1,2)\left[U_{ch}\chi_{ch}(2,1) + U_{sp}\chi_{sp}(2,1)\right] \tag{37.22}$$

with Fourier Transform, this gives

$$\left[\Sigma_\sigma^{(2)}(k)\right]_{long} = Un_{-\sigma} + \frac{U}{4}\frac{T}{N}\sum_q \mathcal{G}_\sigma^{(1)}(k+q)\left[U_{ch}\chi_{ch}(q) + U_{sp}\chi_{sp}(q)\right] \tag{37.23}$$

There is an ambiguity in obtaining the self-energy formula. If we had replaced the external interaction

$$\sum_\sigma \psi_\sigma^\dagger(\overline{1})\phi_\sigma(\overline{1},\overline{2})\psi_\sigma(\overline{2}) \to \sum_\sigma \psi_\sigma^\dagger(\overline{1})\phi_{\sigma,-\sigma}(\overline{1},\overline{2})\psi_{-\sigma}(\overline{2}) \tag{37.24}$$

we would obtain $\mathcal{G}_{\sigma,-\sigma}$ and $\delta\mathcal{G}_{\sigma,-\sigma}/\delta\phi_{\sigma',-\sigma'}$ would generate the same $\Sigma\mathcal{G} = \mathcal{T}\psi^\dagger\psi^\dagger\psi\psi$ expression. This is called the **transverse channel**. The interaction where $\phi_\sigma = \phi_{\sigma\sigma}$ is called the **longitudinal channel**. In the transverse channel, the result will be changed into

$$\frac{U_{ch}}{4}\chi_{ch} + \frac{U_{sp}}{4}\chi_{sp} \to \frac{U_{sp}}{2}\chi_{sp} \tag{37.25}$$

Taking the average of the longitudinal and transverse channels gives a better approximation

$$\Sigma_\sigma^{(2)}(k) = Un_{-\sigma} + \frac{U}{8}\frac{T}{N}\sum_q \left[3U_{sp}\chi_{sp}(q) + U_{ch}\chi_{ch}(q)\right]\mathcal{G}_\sigma^{(1)}(k+q) \tag{37.26}$$

The superscript (2) reminds us that we are at the second level of approximation. $\mathcal{G}^{(1)}_\sigma$ is the same Green's function as that used to compute the susceptibilities $\chi^{(1)}(q)$. Since the self-energy is constant at that first level of approximation, this means that $\mathcal{G}^{(1)}_\sigma$ is the non-interacting Green's function with the chemical potential that gives the correct filling. That chemical potential $\mu^{(1)}$ is slightly different from the one that we must use in $\left(\mathcal{G}^{(2)}\right)^{-1} = iq_n + \mu^{(2)} - \varepsilon_{\mathbf{k}} - \Sigma^{(2)}$ to obtain the same density.

37.3 Physically motivated approach, spin and charge fluctuations

As basic physical requirements, we would like our approach to satisfy a) conservation laws, b) the Pauli exclusion principle and c) the Mermin Wagner theorem. The standard RPA approach satisfies the first requirement but not the other two. How can we go about curing this violation of the Pauli exclusion principle while not damaging the fact that RPA satisfies conservation laws? The simplest way is to proceed in the spirit of Fermi liquid theory and assume that the effective interaction (irreducible vertex in the jargon) is renormalized. This renormalization has to be different for spin and charge so that

$$\begin{aligned}\chi_{sp}(q) &= \frac{\chi^{(1)}(q)}{1 - \frac{1}{2}U_{sp}\chi^{(1)}(q)} \\ \chi_{ch}(q) &= \frac{\chi^{(1)}(q)}{1 + \frac{1}{2}U_{ch}\chi^{(1)}(q)}\end{aligned} \tag{37.27}$$

In practice $\chi^{(1)}(q)$ is the same as the Lindhard function $\chi_0(q)$ for $U = 0$ but, strictly speaking, there is a constant self-energy term that is absorbed in the definition of μ. We are almost done with the collective modes. Substituting the above expressions for $\chi_{sp}(q)$ and $\chi_{ch}(q)$ in the two sum-rules, local-spin and local-charge, we could determine both U_{sp} and U_{ch} if we knew $\langle n_\uparrow n_\downarrow \rangle$. The following ansatz

$$U_{sp} \langle n_\uparrow \rangle \langle n_\downarrow \rangle = U \langle n_\uparrow n_\downarrow \rangle \tag{37.28}$$

gives us the missing equation. Now notice that U_{sp}, or equivalently $\langle n_\uparrow n_\downarrow \rangle$ depending on which of these variables you want to treat as independent, is determined self-consistently. That explains the name of the approach, "Two-Particle-Self-Consistent". Since the the sum-rules are satisfied exactly, when we add them up the resulting equation, and hence the Pauli exclusion principle, will also be satisfied exactly.

Since U_{sp} and U_{ch} are renormalized with respect to the bare value, one might have expected that one should use the dressed Green's functions in the calculation of $\chi_0(q)$. It is explained in appendix A of Ref.[255] that this would lead to a violation of the results $\chi^R_{sp}(\mathbf{q} = \mathbf{0}, \omega) = 0$ and $\chi^R_{ch}(\mathbf{q} = \mathbf{0}, \omega) = 0$. In the present approach, we use the f-sum rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{A_i A_j}(\omega) = \langle [[A_i(t), H], A_j(0)] \rangle_{t=0} \tag{37.29}$$

$$\begin{aligned} H &= \sum_\sigma \sum_{i,j} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U n_{i\downarrow} n_{i\uparrow} \\ &= \sum_\sigma \sum_{i,j} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{U}{4} \sum_i \left(n_i n_i - S^z_i S^z_i \right) \end{aligned} \tag{37.30}$$

$$\begin{aligned} \int \frac{d\omega}{\pi} \omega \chi''_{ch,sp}(\mathbf{q}, \omega) &= \lim_{\eta \to 0} T \sum_{iq_n} \left(e^{-iq_n \eta} - e^{iq_n \eta} \right) iq_n \chi_{ch,sp}(\mathbf{q}, iq_n) \\ &= \frac{1}{N} \sum_{\mathbf{k}\sigma} \left(\epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}-\mathbf{q}} - 2\epsilon_{\mathbf{k}} \right) n_{\mathbf{k}\sigma} \end{aligned} \tag{37.31}$$

is satisfied with $n_{\mathbf{k}\sigma} = n^{(1)}_{\mathbf{k}\sigma}$, the same as the Fermi function for the non-interacting case since it is computed from $\mathcal{G}^{(1)}$. The right-hand side of the first line above is just the equal-time commutator calculated in imaginary time. The denominators containing U_{sp} or U_{ch} above, will lead to contributions to the sum that are of order $1/\left(iq_n\right)^2$ or higher, so that the convergence factor are not needed which means that they do not contribute. So, then only the contribution $\chi^{(1)}$ from the numerator contributes, which explains the result, which is essentially the non-interacting one where Luttinger's theorem is obviously satisfied.

37.4 Mermin-Wagner, Kanamori-Brueckner

The functional form of the results that we found for spin and charge fluctuations have the RPA form but the renormalized interactions U_{sp} and U_{ch} must be computed from the two sum rules and renormalized U_{sp}

$$\begin{aligned}\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1-\frac{1}{2}U_{sp}\chi^{(1)}(q)} &= n-2\langle n_\uparrow n_\downarrow\rangle \\ \frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\frac{\chi^{(1)}(q)}{1+\frac{1}{2}U_{ch}\chi^{(1)}(q)} &= n+2\langle n_\uparrow n_\downarrow\rangle - n^2.\end{aligned} \tag{37.32}$$

$$U_{sp}\langle n_\uparrow\rangle\langle n_\downarrow\rangle = U\langle n_\uparrow n_\downarrow\rangle \tag{37.33}$$

The first equation is solved with the ansaztz, which gives an expression for the double occupancy $\langle n_\uparrow n_\downarrow\rangle$. We then put this in the second equation to obtain U_{ch}. The fastest way to numerically compute $\chi^{(1)}(q)$ is through FFT[30].

Let us begin with Kanamori-Brueckner renormalization of U. Many years ago, Kanamori in the context of the Hubbard model, and Brueckner in the context of nuclear physics, introduced the notion that the bare U corresponds to computing the scattering of particles in the first Born approximation. In reality, we should use the full scattering cross section and the effective U should be smaller. From Kanamori's point of view, the two-body wave function can minimize the effect of U by becoming smaller to reduce the value of the probability that two electrons are on the same site. The maximum energy that this can cost is the bandwidth since that is the energy difference between a one-body wave function with no nodes and one with the maximum allowed number. Let us see how this physics comes out of our results. Far from phase transitions, we can expand the denominator of the local moment sum-rule equation to obtain

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi^{(1)}(q)\left(1+\frac{1}{2}U_{sp}\chi^{(1)}(q)\right) = n-2\frac{U_{sp}}{U}\langle n_\uparrow\rangle\langle n_\downarrow\rangle \tag{37.34}$$

Without interaction, we have $\chi=\chi^{(0)}$ and $\langle n_\uparrow n_\downarrow\rangle = \langle n_\uparrow\rangle\langle n_\downarrow\rangle$, so

$$\frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi^{(0)}(q) = n-2\langle n_\uparrow\rangle\langle n_\downarrow\rangle \tag{37.35}$$

This allows us to solve for U_{sp}

$$\begin{aligned}U_{sp} &= \frac{U}{1+\Lambda U} \\ \Lambda &\equiv \frac{1}{n^2}\frac{T}{N}\sum_{iq_n}\sum_{\mathbf{q}}\left(\chi^{(1)}\right)^2(\mathbf{q},iq_n)\end{aligned} \tag{37.36}$$

We see that at large U, U_{sp} saturates to $1/\Lambda$, which in practice we find to be of the order of the bandwidth. For those that are familiar with diagrams, note that the Kanamori-Brueckner physics amounts to replacing each of the interactions U in the ladder or bubble sum for diagrams in the particle-hole channel by infinite ladder sums in the particle-particle channel. This is not quite what we obtain here since $\left(\chi^{(1)}\right)^2$ is in the particle-hole channel, but in the end, numerically, the results are close and the Physics seems to be the same. One cannot make strict comparisons between TPSC and diagrams since TPSC is non-perturbative.

Checking Mermin Wagner Theorem While Kanamori-Brueckner renormalization, or screening, is a quantum effect that occurs even far from phase transitions, when we are close we need to worry about the Mermin-Wagner theorem. To satisfy this theorem, approximate theories must prevent $\langle n_\uparrow n_\downarrow\rangle$ from taking unphysical values. This quantity is positive and bounded by its value for $U=\infty$ and its value for non-interacting systems, namely $0 \le \langle n_\uparrow n_\downarrow\rangle \le n^2/4$. Hence, the right-hand side of the local-moment sum-rule: $n-2\langle n_\uparrow n_\downarrow\rangle \in \left[n, n-\frac{1}{2}n^2\right]$. To see how the Mermin-Wagner theorem is satisfied, write the self-consistency condition in the form

$$\frac{T}{N}\sum_{q}\frac{\chi^{(1)}(q)}{1-\frac{1}{2}U\frac{\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}\chi^{(1)}(q)} = n-2\langle n_\uparrow n_\downarrow\rangle \tag{37.37}$$

[30] Dominic Bergeron, Vasyl Hankevych, Bumsoo Kyung, and A.-M. S. Trem- blay. Optical and dc conductivity of the two-dimensional hubbard model in the pseudogap regime and across the antiferromagnetic quantum critical point including vertex corrections. Phys. Rev. B, 84(8):085128, Aug 2011.

suppose we now determine $\langle n_\uparrow n_\downarrow \rangle$ self-consistently, we can prove that the fixed point is stable. Suppose $\langle n_\uparrow n_\downarrow \rangle$ is at equilibrium value, increasing $\langle n_\uparrow n_\downarrow \rangle$ corresponds to increasing LHS, the equation then give a solution $\langle n_\uparrow n_\downarrow \rangle$ which is smaller, so this is a negative feed-back loop and the fixed point is stable. Suppose we increase U, LHS then increases and the solution $\langle n_\uparrow n_\downarrow \rangle$ decreases, the equilibrium $\langle n_\uparrow n_\downarrow \rangle$ is then smaller than before. This keeps the value U_{sp} from increasing indefinitely and make it harder for χ_{sp} to diverge.

This, however, does not prevent the expected phase transition in three dimensions. To see this, we need to look in more details at the phase space for the integral in the sum rule. Spectral representation gives

$$\chi_{ch,sp}\left(\mathbf{q}, iq_n\right) = \int \frac{d\omega'}{\pi} \frac{\chi''_{ch,sp}\left(\mathbf{q}, \omega'\right)}{\omega' - iq_n} = \int \frac{d\omega'}{\pi} \frac{\omega' \chi''_{ch,sp}\left(\mathbf{q}, \omega'\right)}{\left(\omega'\right)^2 + \left(q_n\right)^2} \tag{37.38}$$

the zero Matsubara frequency contribution is always the largest. Therefore, the only quantity which has the potential of becoming infinite is the zeroth order frequency, therefore we focus on $q_n = 0$ mode. There, we find the so-called **Ornstein-Zernicke form** for the susceptibility.

Ornstein-Zernicke form Let us focus on the zero Matsubara frequency contribution and expand the denominator near a local maximum of $\chi^{(1)}$, where $\partial\chi^{(1)}/\partial\mathbf{q} = 0$ at $\mathbf{q} = \mathbf{Q}$, we find that the retarded spin susceptibility can be approximated as

$$\begin{aligned} \chi^R_{sp}(\mathbf{q}+\mathbf{Q}, \omega) &\simeq \left[\frac{\chi^{(1)}}{1 - \frac{1}{2}U_{sp}\chi^{(1)} - \frac{1}{4}U_{sp}\frac{\partial^2\chi^{(1)}}{\partial q^2}q^2 - \frac{1}{2}U_{sp}\frac{\partial\chi^{(1)}}{\partial\omega}\omega} \right]_{\chi^{(1)}(\mathbf{Q},0)} \\ &\sim \frac{\xi^2}{1 + \xi^2 q^2 - i\omega/\omega_{sp}} \\ \chi_{sp}(\mathbf{q}+\mathbf{Q}, iq_n) &\sim \frac{\xi^2}{1 + \xi^2 q^2 + q_n/\omega_{sp}} \end{aligned} \tag{37.39}$$

where

$$\begin{aligned} \xi^2 &\equiv -\frac{1}{4}U_{sp}\frac{\partial^2\chi^{(1)}(\mathbf{Q},0)}{\partial\mathbf{q}^2} \Big/ \left(1 - \frac{1}{2}U_{sp}\chi^{(1)}(\mathbf{Q},0)\right) \\ \omega_{sp}^{-1} &\equiv -i\frac{1}{2}U_{sp}\frac{\partial\chi^{(1)}(\mathbf{Q},0)}{\partial\omega} \Big/ \left(1 - \frac{1}{2}U_{sp}\chi^{(1)}(\mathbf{Q},0)\right) \end{aligned} \tag{37.40}$$

where we have defined ξ, the **correlation length**. This length is determined self-consistently. We will evaluate the sum $\sum_{iq_n}$, finite Matsubara frequency contributions are negligible if even the smallest non-zero contribution satisfies $q_{n=1}/\omega_{sp} = 2\pi T/\omega_{sp} \gg 1$ or $T \gg \omega_{sp}$. Since $\omega_{sp}^{-1} \sim \xi^2$, we can also express this condition as $T\xi^2 \gg 1$. This is the **renormalized classical regime**. The classical regime of a harmonic oscillator occurs when $\omega \ll T$. The regime here is "renormalized" classical because at temperatures above the degeneracy temperature, the system is a free classical gas. As temperature decreases below the Fermi energy, it becomes quantum mechanical, then close to the phase transition, it becomes classical again.

Substituting the Ornstein-Zernicke form for the susceptibility in the self-consistency relation

$$\begin{aligned} n - 2\left\langle n_\uparrow n_\downarrow \right\rangle &= \frac{T}{N}\sum_{\mathbf{q}}\sum_{iq_n}\chi_{sp}(\mathbf{q}+\mathbf{Q}, iq_n) \\ &= \frac{T}{N}\sum_{\mathbf{q}}\frac{\xi^2}{1+\xi^2q^2} + \sum_{iq_n\neq 0}\left[\frac{T}{N}\sum_{\mathbf{q}}\frac{\xi^2}{1+\xi^2q^2}\right] \end{aligned} \tag{37.41}$$

we can rewrite this expression as

$$T\int \frac{d^d\mathbf{q}}{(2\pi)^d}\frac{1}{q^2 + \xi^{-2}} = \tilde{C} \tag{37.42}$$

where $\tilde{C}$ contains non-zero Matsubara frequency contributions as well as $n - 2\left\langle n_\uparrow n_\downarrow \right\rangle$. Suppose we have a phase transition at finite T, at this temperature then we have $1 - \frac{1}{2}U_{sp}\chi^{(1)} = 0$ at the maximum value of $\chi^{(1)}$: $\mathbf{q} = \mathbf{Q}$. This must correspond to the vanishing zero order term in q: $\xi^{-2} \to 0$ or $\xi \to \infty$

$$\chi_{sp}(\mathbf{q}+\mathbf{Q}, iq_n = 0) \sim \frac{1}{\xi^{-2} + q^2} \to \frac{1}{q^2} \tag{37.43}$$

Therefore, the condition is translated into

$$\int \frac{d^d\mathbf{q}}{(2\pi)^d}\frac{1}{q^2} \sim \int_0^\Lambda dq q^{d-3}\frac{\tilde{C}}{T} = \text{const} \tag{37.44}$$

for $d = 1, 2$ this integral has an infrared divergence, but for $d = 3, 4, ...$ the integral is finite. Therefore, the relation is satisfied only when $d > 2$. This is in agreement with the Mermin-Wagner theorem. In general, we can write

$$\int_0^\Lambda dq \frac{q^{d-1}}{q^2+\xi^{-2}} = \frac{(2\pi)^d}{S_{d-1}}\tilde{C}/T \tag{37.45}$$

When $d = 2$, we see that the integral gives a logarithm

$$\ln\left(1+\Lambda^2\xi^2\right) \approx 2\ln\left(\Lambda\xi\right) = 2\frac{(2\pi)^d}{S_{d-1}}\tilde{C}/T \tag{37.46}$$

so the correlation length scales as

$$\xi \sim \Lambda^{-1}\exp\left(C'/T\right) \tag{37.47}$$

where in general, C' can be temperature dependent. When ξ diverges, we will have a phase transition, but this happens only at $T = 0$, so our theory satisfies Mermin Wagner theorem. For finite T in $d = 2$, there is always a finite ξ, which means that the denominator $1 - \frac{1}{2}U_{sp}\chi^{(1)} = 0$ can never turn negative. This is guaranteed by the local moment sum rule which determines U_{sp} self-consistently.

38 Antiferromagnetism close to half-filling and Pseudogap in $d = 2$

We return to the normal state and look at the dominant **instability** in the half filled case $n = \langle n_\uparrow\rangle + \langle n_\downarrow\rangle = 1$. In that case, the **Fermi surface** of the Hubbard model with nearest-neighbor hopping exhibits the phenomenon of **nesting**. For example, the Fermi surface in the two-dimensional case is a diamond. All the points of the flat surfaces are connected by the same wave vector $\mathbf{Q} = (\pi, \pi)$ which leads to a very large susceptibility. Whereas at low filling the maximum susceptibility is at $q = 0$, in the present case it is a local maximum that is smaller than the maximum at $\mathbf{Q}$, as we will see.

Let us compute the spin susceptibility at that nesting wave vector. Given the dispersion relation

$$\zeta_{\mathbf{k}} = -2t\left(\cos k_x + \cos k_y\right) \tag{38.1}$$

Nesting in the present case means that

$$\zeta_{\mathbf{k}+\mathbf{Q}} = -\zeta_{\mathbf{k}} \tag{38.2}$$

Using this result we find that the zero-frequency susceptibility at wave vector $\mathbf{Q}$ is

$$\begin{aligned}
\chi_0^R(\mathbf{Q},\omega=0) &= -\frac{2}{N}\sum_{\mathbf{k}}\frac{f\left(\zeta_{\mathbf{k}}\right)-f\left(\zeta_{\mathbf{k}+\mathbf{Q}}\right)}{\zeta_{\mathbf{k}}-\zeta_{\mathbf{k}+\mathbf{Q}}} \\
&= \frac{2}{N}\sum_{\mathbf{k}}\frac{1-2f(\zeta_{\mathbf{k}})}{2\zeta_{\mathbf{k}}} \\
&= \int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{1-2f(\zeta_{\mathbf{k}})}{\zeta_{\mathbf{k}}} \\
&= \int_{-W}^{W} d\varepsilon\frac{N(\varepsilon)}{2}\frac{\tanh(\beta\varepsilon/2)}{\varepsilon} \\
&= \int_0^W d\varepsilon N(\varepsilon)\frac{\tanh(\beta\varepsilon/2)}{\varepsilon} \\
&\approx N(0)\left\{\int_0^{1/2} dx\frac{\tanh(x)}{x} + \ln(W/T)\right\}
\end{aligned} \tag{38.3}$$

where W is the bandwidth and we have assumed that the density of states is a constant. We obtain a contribution that diverges at low temperature like $\ln(W/T)$. This means that at sufficiently low temperature, the criterion $1 - \frac{U}{2}\chi_0^R(\mathbf{Q}, 0) = 0$ will always be satisfied whatever the value of U and there will be a transition to a state

characterized by the wave vector $\mathbf{Q}$. This is the **antiferromagnetic state** where spins alternate in direction from one site to the other. In two dimensions for example, the chemical potential at $n = 1$ sits right at a **logarithmic van Hove singularity** in $N(\varepsilon)$ so that in fact $\chi_0^R(\mathbf{Q}, 0)$ scales like $\ln^2(W/T)$, which is larger than the single power of ln that one would obtain at $q = 0$.

When there is no nesting, like when the next-nearest neighbor hopping t' contributes, the susceptibility does not diverge at low temperature. In that case, the transition will occur only if U is large enough.

38.1 Pseudogap in the renormalized classical regime

When we compared TPSC with Quantum Monte Carlo simulations and with FLEX in Fig. 58-2 above, perhaps you noticed that at the Fermi surface, the frequency dependent spectral weight has two peaks instead of one. In addition, at zero frequency, it has a minimum instead of a maximum. That is called a **pseudogap**. A cartoon explanation of this pseudogap is given in Fig. 59-1. At high temperature we start from a Fermi liquid, as illustrated in panel I. Now, suppose the ground state has long-range antiferromagnetic order as in panel III, in other words at a filling between half-filling and n_c. In the mean-field approximation we have a gap and the Bogoliubov transformation from fermion creation-annihilation operators to quasi-particles has weight at both positive and negative energies. In two dimensions, because of the Mermin-Wagner theorem, as soon as we raise the temperature above zero, long-range order disappears, but the antiferromagnetic correlation length ξ remains large so we obtain the **pseudogap** illustrated in panel II. As we will explain analytically below, the pseudogap survives as long as ξ is much larger than the thermal de Broglie wave length $\xi_{th} \equiv v_F/(\pi T)$ in our usual units. At the crossover temperature T_X, the relative size of ξ and ξ_{th} changes and we recover the Fermi liquid.

We now proceed to sketch analytically where these results come from starting from finite T. We begin from the TPSC expression for the self-energy

$$\Sigma_\sigma^{(2)}(k) = U n_{-\sigma} + \frac{U}{8}\frac{T}{N}\sum_q \left[3U_{sp}\chi_{sp}(q) + U_{ch}\chi_{ch}(q)\right] \mathcal{G}_\sigma^{(1)}(k+q) \tag{38.4}$$

Normally one has to do the sum over bosonic Matsubara frequencies first, but the zero Matsubara frequency contribution has the correct asymptotic behavior in fermionic frequencies iq_n so that one can once more isolate on the right-hand side the contribution from the zero Matsubara frequency. In the **renormalized classical regime** then, we have

$$\Sigma\left(\mathbf{k}_F, ik_n\right) \propto T \int d^d\mathbf{q} \frac{1}{q^2 + \xi^{-2}} \frac{1}{ik_n - \zeta_{\mathbf{k}_F+\mathbf{Q}+\mathbf{q}}} \tag{38.5}$$

where $\mathbf{Q}$ is the wave vector of the instability. (Remember that in writing $\chi \sim (q^2 + \xi^{-2})^{-1}$, we have expanded q around $\mathbf{Q}$, where χ is most likely to diverge, so we should shift $\mathbf{q} \to \mathbf{q} + \mathbf{Q}$. This integral can be done analytically in two dimensions. But it is more useful to analyze limiting cases. Expanding around the points known as hot spots where $\zeta_{\mathbf{k}_F+\mathbf{Q}} = 0$:

$$\begin{aligned}
\zeta_{\mathbf{k}_F+\mathbf{Q}+\mathbf{q}} &\approx \frac{\partial\zeta}{\partial\mathbf{q}}\Big|_{\mathbf{q}=\mathbf{k}_F+\mathbf{Q}} \cdot \mathbf{q} \\
&= \frac{\partial\zeta}{\partial q}\Big|_{q=|\mathbf{k}_F+\mathbf{Q}|} \left(\frac{\partial q}{\partial\mathbf{q}}\Big|_{\mathbf{q}=\mathbf{k}_F+\mathbf{Q}} \cdot \mathbf{q}\right) \\
&\equiv v'_F \frac{\mathbf{k}_F + \mathbf{Q}}{|\mathbf{k}_F + \mathbf{Q}|} \cdot \mathbf{q} \\
&\equiv v'_F q_\parallel
\end{aligned} \tag{38.6}$$

we find after analytical continuation that the imaginary part of the retarded self-energy at zero frequency takes the form

$$\begin{aligned}
\Sigma''^R\left(\mathbf{k}_F, 0\right) &\propto -\pi T \int d^{d-1}q_\perp dq_\parallel \frac{1}{q_\perp^2 + q_\parallel^2 + \xi^{-2}} \delta\left(v'_F q_\parallel\right) \\
&\propto \pi T \int \frac{d^{d-1}q_\perp}{q_\perp^2 + \xi^{-2}} \\
&\propto \frac{\pi T}{v'_F} \xi^{3-d}
\end{aligned} \tag{38.7}$$

with dimensional analysis. One hidden assumption here is that $\xi \to \infty$ as T decreases, no matter which dimension we are in. This could be understood from the self-consistency relation in the Mermin Wagner section.

The importance of dimension now comes out clearly. In $d = 4$, $\Sigma''(\mathbf{k}_F, 0)$ vanishes as temperature decreases, $d = 3$ is the marginal dimension and in $d = 2$ we have that $\Sigma''(\mathbf{k}_F, 0) \propto \xi/\xi_{th}$ that diverges at zero temperature. In a Fermi liquid the quantity $\Sigma''(\mathbf{k}_F, 0)$ vanishes at zero temperature, hence in three or four dimensions one recovers the Fermi liquid (or close to one in $d = 3$). But in two dimensions, a diverging $\Sigma''(\mathbf{k}_F, 0)$ corresponds to a vanishingly small $A(\mathbf{k}_E, \omega = 0)$ as we can see from

$$A(\mathbf{k}, \omega) = \frac{-2\Sigma''^R(\mathbf{k}_F, \omega)}{\left(\omega - \varepsilon_{\mathbf{k}} - \Sigma'^R(\mathbf{k}_F, \omega)\right)^2 + \Sigma''^R(\mathbf{k}_F, \omega)^2} \tag{38.8}$$

At stronger U the scattering rate is large over a broader region, leading to a depletion of $A(\mathbf{k}, \omega)$ over a broader range of $\mathbf{k}$ values.

To understand the splitting into two peaks seen in Figs. 58-2 and 59-1 consider the singular renormalized contribution coming from the spin fluctuations in Eq. (59.4) at frequencies $\omega \gg v_F \xi^{-1}$. Taking into account that contributions to the integral come mostly from a region $q \leq \xi^{-1}$, one finds

$$\Sigma'(\mathbf{k}_F, \omega) = \left(T \int \frac{d^d\mathbf{q}}{q^2 + \xi^{-2}}\right) \frac{1}{\omega - \zeta_{\mathbf{k}_F + \mathbf{Q}}} \equiv \frac{\Delta^2}{\omega - \zeta_{\mathbf{k}_F + \mathbf{Q}}} \tag{38.9}$$

where we expanded around the hot spot, but now $\zeta_{\mathbf{k}_F + \mathbf{Q}} \neq 0$ in general. The quasiparticle dispersion is given by

$$\omega - \varepsilon_{\mathbf{k}} - \frac{\Delta^2}{\omega - \zeta_{\mathbf{k}_F + \mathbf{Q}}} = 0 \tag{38.10}$$

equivalently, this is where the spectral function has peaks. We can solve for the location of the peaks ω:

$$\omega = \frac{(\zeta_{\mathbf{k}} + \zeta_{\mathbf{k}_F + \mathbf{Q}}) \pm \sqrt{(\zeta_{\mathbf{k}} - \zeta_{\mathbf{k}_F + \mathbf{Q}})^2 + 4\Delta^2}}{2} \tag{38.11}$$

which, at $\omega = 0$, corresponds to the position of the hot spots. At finite frequencies, this turns into the dispersion relation for the antiferromagnet.

It is important to understand that analogous arguments hold for **any fluctuation that becomes soft because of the Mermin-Wagner theorem**, including superconducting ones. The wave vector $\mathbf{Q}$ would be different in each case.

38.2 Pseudogap in electron-doped cuprates

High-temperature superconductors are made of layers of CuO_2 planes. The rest of the structure is commonly considered as providing either electron or hole doping of these planes depending on chemistry. At half-filling, or zero-doping, the ground state is an antiferromagnet. As one dopes the planes, one reaches a doping, so-called **optimal doping**, where the superconducting transition temperature T_c is maximum. Let us start from optimal hole or electron doping and decrease doping towards half-filling. That is the **underdoped regime**. In that regime, one observes a curious phenomenon, the pseudogap. What this means is that as temperature decreases, physical quantities behave **as if the density of states near the Fermi level was decreasing**. Finding an explanation for this phenomenon has been one of the major challenges of the field.

To make progress, we need a microscopic model for high-temperature superconductors. Band structure calculations reveal that a single band crosses the Fermi level. Hence, it is a common assumption that these materials can be modeled by the **one-band Hubbard model**. Whether this is an oversimplification is still a subject of controversy. Indeed, spectroscopic studies show that hole doping occurs on the oxygen atoms. The resulting hole behaves as a copper excitation because of Zhang-Rice singlet formation. In addition, the phase diagram and many properties of the hole-doped cuprates can be described by the one-band Hubbard model. Typically, the band parameters that are used are: nearest-neighbor hopping $t = 350$ to 400meV and next-nearest-neighbor hopping $t' = -0.15$ to $-0.3t$ depending on the compound. Third-nearest-neighbor hopping $t'' = -0.5t'$ is sometimes added to fit finer details of the band structure. The hoppings beyond nearest-neighbor mean that **particle-hole symmetry is lost** even at the band structure level.

In electron-doped cuprates, the doping occurs on the copper, hence there is little doubt that the single-band Hubbard model is even a better starting point in this case. Band parameters are similar to those of hole-doped cuprates. It is sometimes claimed that there is a pseudogap only in the hole-doped cuprates. The origin of the pseudogap is indeed probably different from the hole-doped cuprates. But even though the standard signature of

a pseudogap is absent in nuclear magnetic resonance (NMR) there is definitely a pseudogap in the electron-doped case as well, as can be seen in optical conductivity and in Angle Resolved Photoemission Spectroscopy (ARPES). As we show in the rest of this section, in electron-doped cuprates strong evidence for the origin of the pseudogap is provided by detailed comparisons of TPSC with ARPES as well as by verification with neutron scattering that the TPSC condition for a pseudogap, namely $\xi > \xi_{th}$, is satisfied. The latter length makes sense from weak to intermediate coupling when quasi-particles exist above the pseudogap temperature. In strong coupling, i.e. for values of U larger than that necessary for the Mott transition, there is evidence that there is another mechanism for the formation of a pseudogap. The recent discovery that at sufficiently large U there is a first order transition in the paramagnetic state between two kinds of metals, one of which is highly anomalous, gives a sharper meaning to what is meant by strong-coupling pseudogap.

Let us come back to modeling of electron-doped cuprates. Evidence that these are less strongly coupled than their hole-doped counterparts comes from the fact that a) The value of the optical gap at half-filling, ~ 1.5eV, is smaller than for hole doping, ~ 2.0eV. b) In a simple Thomas-Fermi picture, the screened interaction scales like $\partial\mu/\partial n$. Quantum cluster calculations show that $\partial\mu/\partial n$ is smaller on the electron-doped side(hole-doped side?), hence U should be smaller. c) Mechanisms based on the exchange of antiferromagnetic calculations with U/t at weak to intermediate coupling predict that the superconducting T_c increases with U/t. Hence T_c should decrease with increasing pressure in the simplest model where pressure increases hopping t while leaving U essentially unchanged. The opposite behavior, expected at strong coupling where $J = 4t^2/U$ is relevant, is observed in the hole-doped cuprates. d) Finally and most importantly, there is detailed agreement between TPSC calculations and measurements such as ARPES, optical conductivity and neutron scattering.

To illustrate the last point, consider Fig. 59-2 that compares TPSC calculations with experimental results for ARPES. Apart from a tail in the experimental results, the agreement is striking. In particular, if there was no interaction, the Fermi surface would be a line (red) on the momentum distribution curve (MDC). Instead, it seems to disappear at symmetrical points displaced from $(\pi/2, \pi/2)$. These points, so-called **hot spots**, are linked by the wave vector (π, π) to other points on the Fermi surface. This is where the **antiferromagnetic gap** would open first if there was long-range order. The pull back of the weight from $\omega = 0$ at the hot spots is close to the experimental value: 100meV for the 15% doping shown, and 300meV for 10% doping (not shown). The value of the temperature T^* at which the pseudogap appears is also close to that observed in optical spectroscopy. In addition, the size of the pseudogap is about ten times T^* in the calculation as well as in the experiments. For optical spectroscopy, vertex corrections have to be added to be more quantitative. Experimentally, the value of T^* is about twice the antiferromagnetic transition temperature up to $x = 0.13$. That can be obtained by taking $t_z = 0.03t$ for hopping in the third direction. Recall that in strictly two dimensions, there is no long-range order. Antiferromagnetism appears on a much larger range of dopings for electron-doped than for hole-doped cuprates.

These TPSC calculations have predicted the value of the pseudogap temperature at $x = 0.13$ before it was observed experimentally by a group unaware of the theoretical prediction in Fig.59.2. In addition, the prediction that ξ should scale like ξ_{th} at the pseudogap temperature has been verified in neutron scattering experiments in the range $x = 0.04$ to $x = 0.15$. The range of temperatures and doping explored in that work is shown in Fig. 59.2. Note that the antiferromagnetic phase boundary, that occurs here because of coupling in the third dimension, is at a location different from earlier estimates that appear in Fig. 59.2. However, the location of the pseudogp temperature has not changed. At the doping that corresponds to optimal doping, T^* becomes of the order of 100 K, more than four times lower than at $x = 0.04$. The antiferromagnetic correlation length ξ beyond optimal doping begins to decrease and violate the scaling of ξ with ξ_{th}. In that doping range, T^* and the superconducting transition temperature are close. Hence it is likely that there is interference between the two phenomena, an effect that has not yet been taken into account in TPSC.

An important prediction that one should verify is that inelastic neutron scattering will find over-damped spin fluctuations in the pseudogap regime and that the characteristic spin fluctuation energy will be smaller than k_BT whenever a pseudogap is present. Equality should occur above T^*.

Finally, note that the agreement found in Fig. 59-2 between ARPES and TPSC is for $U \sim 6t$. At smaller values of U the antiferromagnetic correlations are not strong enough to produce a pseudogap in that temperature range. For larger U, the weight near $(\pi/2, \pi/2)$ disappears, in disagreement with experiments. The same value of U is found for the same reasons in strong coupling calculations with Cluster Perturbation Theory (CPT) and with slave boson methods. Recent first principle calculations find essentially the same value of U. In that approach, the value of U is fixed, whereas in TPSC it was necessary to increase U by about 10% moving towards half-filling to get the best agreement with experiment. In any case, it is quite satisfying that weak and strong coupling methods agree on the value of U for electron-doped cuprates. This value of U is very near the critical value for the Mott transition at half-filling. Hence, antiferromagnetic fluctuations at finite doping can be very well described by Slaterlike physics

(nesting) in electron-doped cuprates.

39 Dynamical mean field theory and Mott Transitions

In this Chapter, we will see a physically motivated derivation of dynamical mean- Öeld theory and discuss the results found by this method on the Mott transition.

The band picture of electrons explained very well the occurence of metals, with bands that are unfilled, and insulators, with filled bands. De Boer and Verwey (1937) reported that many transition-metal oxides with a partially filled d-electron band were exceptions. They were often poor conductors and indeed often insulators. N_iO became the prototypical example. following their report, Peierls (1937) pointed out the importance of the electron-electron correlation: According to Mott (1937), Peierls noted

> "It is quite possible that the electrostatic interaction between the electrons prevents them from moving at all. At low temperatures the majority of the electrons are in their proper places in the ions. The minority which have happened to cross the potential barrier find therefore all the other atoms occupied, and in order to get through the lattice have to spend a long time in ions already occupied by other electrons. This needs a considerable addition of energy and so is extremely improbable at low temperatures."

Peierls is explaining that at half-filling, every unit cell is occupied by one carrier in the presence of strong Coulomb repulsion. And the electrons cannot move because of the large Coulomb repulsion it would cost. Later, Slater found another way to obtain an insulator at half-filling even when Coulomb interactions are weak. This is when long-range antiferromagnetic order leads to a doubling of the unit cell. We have already seen in the previous Chapter that perfect nesting could lead to a diverging antiferromagnetic susceptibility, and hence to a phase transition with arbitrarily weak interaction. In that case, the Brillouin zone becomes half the size so the band split in two and the lower band is now full. The Mott insulator and the antiferromagnetic insulator are conceptually very different. One has long-range order while the other does not.

In the 1970's vanadium oxide became an example of a material showing a Mott transition. The phase diagram appears in Fig. 60. The substitution of vanadium by another metal with d-electrons is modeled here as pressure. The accuracy of this hypothesis is confirmed by real pressure experiments that appear on the same plot (see the top and bottom horizontal axis). Pressure increases the overlap between orbitals, hence the kinetic energy and tends to delocalize electrons. We see on this phase diagram a finite temperature first order transition between a metal and an insulator without long-range order. This material has a three-dimensional lattice structure.

Layered organic conductors are quasi two-dimensional materials with a half-filled band. These are soft materials, so one can apply pressure and have a sizable effect on the electronic structure. One observes a frst-order metal-insulator transition at high-temperature that ends at a critical point. For both materials there is an antiferromagnetic phase at low temperature, suggesting the importance of electron-electron interactions.

Simple pictures of the Mott transition have been proposed. In the Brinkman-Rice scenario, the effective mass becomes infinite at the Mott transition. In the Mott picture, at large interaction and half-filling, the non-interacting band splits in two and there is an empty and a filled band, so no conduction. As the interaction strength decreases, a metallic phase occurs when the bands overlap.

The modern view of this transition contains a bit of both of the above ideas. That view emerges from dynamical mean-field theory, that we explain in this Chapter. This theory was discovered after Vollhardt and Metzner proposed and **exact solution for the Hubbard model in infinite dimension**. Georges and Kotliar and independently Jarrell arrived at the same theory. I begin by an example in classical statistical mechanics where mean-field theory is exact. Before the contribution of Metzner and Vollhardt, there was no known limit where a mean field theory for a quantum system becomes exact. The mean-field in that case is a function of frequency, not a single number. We will argue that **in infinite dimension the self-energy depends only on frequency**. This allows a mapping to the co-called Anderson impurity model, where a single site with a Hubbard interaction is connected to a bath of non-interacting electrons. When this model can be solved, dynamical mean-field theory establishes a self-consistency relation with the infinite system.

39.1 A simple example of a model exactly soluble by mean-field theory

Let us forget momentarily about quantum mechanics and consider a simpler problem of classical statistical mechanics. Mean-field theory is often taken as an approximate solution to a model. It can also be formulated as an exact solution of a different model. That helps understand the content of mean-field theory. Consider the following

infinite-range Ising model where mean-field theory is the exact solution

$$H = -\frac{1}{2N}\left(\sum_{i=1}^{N} S_i\right)^2 - h\sum_i S_i \tag{39.1}$$

with $S_i = \pm 1$. We have chosen the exchange $J = 1$. The range of the interaction is extremely weak in the thermodynamic limit. The $1/N$ normalization is necessary to have an energy that is extensive, i.e. $H \propto N$. In the usual Ising model, a given site interacts only with its neighbors so the energy is clearly extensive. To compute the partition function, we use the Hubbard-Stratonovich transformation that represents $e^{-\beta H}$ as a Gaussian integral

$$e^{\left[\frac{\beta}{2N}\left(\sum_{i=1}^{N} S_i\right)^2 + \beta h \sum_i S_i\right]} = \left(\frac{N\beta}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\lambda e^{\left[-\frac{\beta N}{2}\lambda^2 + \beta(\lambda+h)\sum_i S_i\right]} \tag{39.2}$$

The partition function can be computed easily

$$\begin{aligned} Z &= \sum_{\{S_i\}} e^{-\beta H} \\ &= \left(\frac{N\beta}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\lambda e^{-\frac{\beta N}{2}\lambda^2} \sum_{\{S_i\}} e^{\beta(\lambda+h)\sum_i S_i} \\ &= \left(\frac{N\beta}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\lambda e^{-\frac{\beta N}{2}\lambda^2} \prod_i \sum_{S_i} e^{\beta(\lambda+h)S_i} \\ &= \left(\frac{N\beta}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\lambda e^{-\frac{\beta N}{2}\lambda^2} \left[2\cosh\left(\beta(\lambda+h)\right)\right]^N \\ &\equiv \left(\frac{N\beta}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\lambda e^{-N\beta F(\lambda)} \end{aligned} \tag{39.3}$$

$$F(\lambda) \equiv \frac{\lambda^2}{2} - \frac{1}{\beta}\ln\left[2\cosh\left(\beta(\lambda+h)\right)\right] \tag{39.4}$$

Because $N \to \infty$, suppose $F(\lambda)$ take maximum at $\lambda = \lambda_0$, using Laplace's method

$$\begin{aligned} \int_{-\infty}^{\infty} d\lambda e^{-N\beta F(\lambda)} &\sim \int_{\lambda_0-\varepsilon}^{\lambda_0+\varepsilon} d\lambda e^{-N\beta\left[F(\lambda_0)+\frac{1}{2}F''(\lambda_0)\lambda^2\right]} \\ &\sim e^{-N\beta F(\lambda_0)} \int_{-\infty}^{\infty} d\lambda e^{-\frac{1}{2}N\beta F''(\lambda_0)\lambda^2} \\ &\sim e^{-N\beta F(\lambda_0)} \left(\frac{2\pi}{N\beta F''(\lambda_0)}\right)^{1/2} \end{aligned} \tag{39.5}$$

so we have

$$\begin{aligned} Z &\sim \frac{e^{-N\beta F(\lambda_0)}}{\left[F''(\lambda_0)\right]^{1/2}} \\ \ln Z &\approx -N\beta F(\lambda_0) - \frac{1}{2}\ln F''(\lambda_0) \sim -N\beta F(\lambda_0) \\ f &= -\ln Z/(N\beta) \approx F(\lambda_0) \end{aligned} \tag{39.6}$$

where f is the free energy per site.

$$f(h) = \min_{\lambda} F(\lambda) + O\left(\frac{1}{N}\right). \tag{39.7}$$

The value of λ which minimizes F has the meaning of magnetization density. Indeed, $\partial F/\partial\lambda = 0$ leads to

$$\lambda = \tanh\left(\beta(\lambda+h)\right) \tag{39.8}$$

and we know

$$m = \left(\frac{\partial F}{\partial h}\right)_{\lambda} = \tanh[\beta(\lambda+h)] = \lambda \tag{39.9}$$

This is what is found in mean-field theory.

39.2 The self-energy is independent of momentum in infinite dimension

It took a long time to find a variant of the Hubbard model that could be solved by a mean-field theory. That the Hubbard model was exactly soluble in inÖnite di- mension was discovered by Metzner and Vollhardt. The key result is that in infinite dimension, the self-energy depends only on frequency. This is in sharp contrast with the TPSC results where we saw that in two dimensions, the spatial dependence of the self-energy is very important. Hot spots appear along the Fermi surface. We have also seen that the hot spot vanishes for $d > 4$ since $\Sigma''(\mathbf{k}_F, 0) \sim T\xi^{3-d}/v_F$. Since the hot spot disappears, it is likely that the self-energy will be less momentum dependent.

First we need to formulate the Hubbard model in such a way that in infinite dimension it gives a non-trivial and physical result. The possibly troublesome term is the kinetic energy. Consider the value of $\left\langle c^\dagger_{i\sigma} c_{j\sigma} \right\rangle$ for nearest neighbors. In the ground state, that quantity can be interpreted as the matrix element $\langle \psi_{i\sigma} \mid \psi_{j\sigma} \rangle$ where $|\psi_{j\sigma}\rangle$ is the ground state with one less particle at site j and $\langle \psi_{i\sigma}|$ the ground state where we remove a particle at site i (think of $c^\dagger_{i\sigma}$ acting to the left bra). Hence $|\langle \psi_{i\sigma} \mid \psi_{j\sigma} \rangle|^2$ is the probability for a particle to go from j to i. It has to scale like $1/d$ if we want particle-number to be conserved. This means that $\left\langle c^\dagger_{i\sigma} c_{j\sigma} \right\rangle$ scales as $1/\sqrt{d}$ so if we want a finite number for the kinetic energy, we need to multiply t by $\sqrt{d}$. Taking into account that there are Z neighbors, with $Z = 2d$ for a hypercubic lattice, we need an additional factor of $1/d$. The kinetic energy in the end is thus written as

$$E_{kin} = -\left(t^*\sqrt{d}\right)\frac{1}{d}\sum_{\langle i,j\rangle}\left(c^\dagger_{i\sigma}c_{j\sigma} + h.c.\right) \tag{39.10}$$

so we have

$$H = -\left(t^*\sqrt{d}\right)\frac{1}{d}\sum_{\langle i,j\rangle}\left(c^\dagger_{i\sigma}c_{j\sigma} + h.c.\right) + \sum_i U n_{i\uparrow}n_{i\downarrow} \tag{39.11}$$

we can check the magnitude $E_{kin} \sim \sqrt{d}\frac{1}{d}Z\left\langle c^\dagger_{i\sigma}c_{j\sigma}\right\rangle \sim \mathcal{O}(1)$ scales to zeroth order in d. The interaction does not need to be scaled, since it is local. The quantity $t^*/\sqrt{d}$ plays the role of the usual t entering the kinetic energy, with t^* finite in the $d \to \infty$ limit.

Alternatively, we can require the bandwidth to remain finite in the infinite dimensional limit. Consider the single-particle density of states

$$N(\omega) = \int_{-\pi}^{\pi}\frac{dk_1}{2\pi}\int_{-\pi}^{\pi}\frac{dk_2}{2\pi}\ldots\int_{-\pi}^{\pi}\frac{dk_d}{2\pi}\delta\left(\omega - \varepsilon_1 - \varepsilon_2 - \ldots\varepsilon_d\right) \tag{39.12}$$

with $\varepsilon_i = -2t\cos k_i$. This has the structure of a probability density for a variable that is the sum of identically distributed statistically independent variables. One can make the change of variables from $P(k_i) = 1/(2\pi)$ to $P(\varepsilon_i)$ so that

$$N(\omega) = \int d\varepsilon_1 \int d\varepsilon_2 \ldots \int d\varepsilon_d P(\varepsilon_1) P(\varepsilon_2)\ldots P(\varepsilon_d)\,\delta\left(\omega - \varepsilon_1 - \varepsilon_2 - \ldots\varepsilon_d\right) \tag{39.13}$$

This is a convolution of d number of identical independent distributions. Each distribution is characterized by $P(\varepsilon_i)$ defined in interval $[-2t, 2t]$, with mean $\langle\varepsilon\rangle = 0$ and variance $\left\langle\varepsilon^2\right\rangle = 2\pi^2t^2$. By central limit theorem,

$$X_i \sim \mathcal{N}(\mu,\sigma) \qquad \to \frac{X_1 + \cdots + X_n}{n} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right) \tag{39.14}$$

therefore, $N(\omega)$ has mean 0 and variance $2\pi^2dt^2$ and approaches a Gaussian distribution in the limit $d \to \infty$:

$$N(\omega) = \frac{1}{\sqrt{2\pi(2t)^2 d}}\exp\left[-\left(\frac{\omega}{2t\sqrt{d}}\right)^2\right] \tag{39.15}$$

this density of states correspond to a bandwidth of the order $\sqrt{d}t$. If we wish to keep the bandwidth constant when taking the limit $d \to \infty$, we must therefore choose $t \equiv t^*/\sqrt{d}$, such that the bandwidth is now a constant of the order t^*.

The fact that $\left\langle c^\dagger_{i\sigma}c_{j\sigma}\right\rangle$ scales as $1/\sqrt{d}$ in the $d \to \infty$ limit has important consequences on the self energy. Indeed, $\mathcal{G}$ will also scale as $1/\sqrt{d}$. Hence, if we consider the real space expression for Σ_{12} where 1 and 2 are near-neighbor sites, then apart from the Hartree-Fock term that arises in first order perturbation theory, we find from second order that the contribution is proportional to $(\mathcal{G}_{1,2})^3$ which is proportional to $1/d^{3/2}$. There is an additional factor $1/\sqrt{d}$ in the Green's function every time the distance increases by one so Σ_{ij} for more distant ij is even smaller. This can be argued probabilistically also as taking two consecutive steps. In the end, this means that the self-energy depends only on frequency.

39.3 The dynamical mean-field self-consistency relation, derivation 1

Suppose we start from the premise that the self-energy is purely local, namely that it is calculated with diagrams where only the local self-consistent Green's function comes in the calculation. Suppose we can solve this problem, either by summing all diagrams or by some other method. Since we have proven that in infinite dimension the exact self-energy for the lattice has only frequency dependence, we take the **impurity self-energy** as the self-energy for the lattice. In other words, the Green's function on the infinite lattice reads in Fourier-Matsubara space

$$\mathcal{G}\left(\mathbf{k}, ik_n\right) = \frac{1}{ik_n - \left(\varepsilon_{\mathbf{k}} - \mu\right) - \Sigma\left(ik_n\right)} \tag{39.16}$$

It is clear that with the appropriate Fourier transform of the lattice Green's function we obtain the Green's function on a single site:

$$\begin{aligned}
\mathcal{G}_{ii}\left(ik_n\right) &= \int \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{ik_n - \left(\varepsilon_{\mathbf{k}} - \mu\right) - \Sigma\left(ik_n\right)} \\
&= \int \frac{d^d\mathbf{k}}{(2\pi)^d} \int d\varepsilon \delta\left(\varepsilon - \left(\varepsilon_{\mathbf{k}} - \mu\right)\right) \frac{1}{ik_n - \varepsilon - \Sigma\left(ik_n\right)} \\
&= \int d\varepsilon N(\varepsilon) \frac{1}{ik_n - \varepsilon - \Sigma\left(ik_n\right)}
\end{aligned} \tag{39.17}$$

That is the only Green's function that is involved in the calculation of the self-energy. Suppose now that we compute the self-energy with that Green's function. When we substitute that self-energy back into the Green's function for the infinite lattice and project it back on a single site as above, it is possible that we do not find the $\mathcal{G}_{ii}\left(ik_n\right)$ that we started with. This means that we need to modify it until self-consistency is achieved. This is not the way it is done in practice, although new methods exist to obtain the self-energy directly from $\mathcal{G}_{ii}\left(ik_n\right)$, so it could be done in principle.

The question we have not answered, is how, given $\mathcal{G}_{ii}\left(ik_n\right)$, do we find the self-energy if we do not have these recent methods available to us? Suppose we can write the new $\mathcal{G}_{ii}\left(ik_n\right)$ obtained with the self-energy in the following form

$$\mathcal{G}_{ii}^{-1}\left(ik_n\right) = \left(\mathcal{G}_{ii}^0\left(ik_n\right)\right)^{-1} - \Sigma\left(ik_n\right) \tag{39.18}$$

In this form, it is $\mathcal{G}_{ii}^0\left(ik_n\right)$ that we need to modify before starting the next iteration. If we want to use perturbative methods in terms of an unperturbed Green's function, it is $\mathcal{G}_{ii}^0(ik_n)$ that we need. It is not clear at this point that this last equation is correct or that we can do that.

And in practice, how do we do we find the self-energy and how do we do this iteration? The answer is that it suffices to solve a single-impurity Anderson model with the same U as the Hubbard model. That allows us to take advantage of a whole set of methods that have been developed to solve that model. But what is the Anderson impurity model? This is the subject of the next section.

39.4 The Anderson impurity model

The problem of a single site with a Hubbard interaction, connected to a bath of non-interacting electrons is the so-called **Anderson impurity model**. It is a generalization of the static single-impurity problem that we saw in an exercice. Its self-energy depends only on frequency. Since in infinite dimension the self-energy depends only on frequency, this will allow us to find a mapping between the single-impurity Anderson model and the DMFT approximation to the lattice problem. I will only set up the problem of quantum impurities without solving it. The **Numerical Renormalization Group approach** (NRG) **Density Matrix Renormalization Group** and **continuous-time quantum Monte-Carlo** methods are examples of approaches that can be used to solve this problem.

Including the chemical potential, the model is defined by

$$\begin{aligned}
K_I &= H_f + H_c + H_{fc} - \mu N \\
K_f &\equiv \sum_\sigma (\varepsilon - \mu) f_{i\sigma}^\dagger f_{i\sigma} + U\left(f_{i\uparrow}^\dagger f_{i\uparrow}\right)\left(f_{i\downarrow}^\dagger f_{i\downarrow}\right) \\
K_c &\equiv \sum_\sigma \sum_{\mathbf{k}} \left(\varepsilon_{\mathbf{k}} - \mu\right) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \\
H_{fc} &\equiv \sum_\sigma \sum_{\mathbf{k}} \left(V_{\mathbf{k}i} c_{\mathbf{k}\sigma}^\dagger f_{i\sigma} + V_{\mathbf{k}i}^* f_{i\sigma}^\dagger c_{\mathbf{k}\sigma}\right)
\end{aligned} \tag{39.19}$$

To physically motivate this model, think of a single f level on an atom where the on-site interaction is very large. That site is hybridized through $V_{\mathbf{k}i}$ with conduction electrons around it. The sum over $\mathbf{k}$ in the hybridization part of the Hamiltonian H_{fc} basically tells us that it is the local overlap of the conduction band with the impurity that produces the coupling.

Suppose we want to know the properties of the impurity, such as the local density of states. It can be obtained from the Green function

$$\mathcal{G}_{ff}(\tau) = -\left\langle T_\tau f_{i\sigma}(\tau) f_{i\sigma}^\dagger \right\rangle. \tag{39.20}$$

We will proceed with the **equations of motion method**, following steps analogous to those in the exercise on non-interacting impurities. We first write the equations of motion for $c_{\mathbf{k}\sigma}$ and $f_{i\sigma}$

$$\begin{aligned}
\frac{\partial}{\partial\tau} c_{\mathbf{k}\sigma} &= [K_I, c_{\mathbf{k}\sigma}] \\
&= -\left(\varepsilon_{\mathbf{k}} - \mu\right) c_{\mathbf{k}\sigma} - V_{\mathbf{k}i} f_{i\sigma} \\
\frac{\partial}{\partial\tau} f_{i\sigma} &= [K_I, f_{i\sigma}] \\
&= -(\varepsilon - \mu) f_{i\sigma} - U f_{i-\sigma}^\dagger f_{i-\sigma} f_{i\sigma} - \sum_{\mathbf{k}} V_{\mathbf{k}i}^* c_{\mathbf{k}\sigma}
\end{aligned} \tag{39.21}$$

$$\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{G}_{ff}(\tau) =& -\delta(\tau)\left\langle \left\{ f_{i\sigma}(\tau), f_{i\sigma}^\dagger \right\} \right\rangle \\
&- \left\langle T_\tau \left(-(\varepsilon-\mu) f_{i\sigma}(\tau) - U f_{i-\sigma}^\dagger(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) - \sum_{\mathbf{k}} V_{\mathbf{k}i}^* c_{\mathbf{k}\sigma} \right) f_{i\boldsymbol{\sigma}}^\dagger \right\rangle \quad (60.24) \\
=& -\delta(\tau) - (\varepsilon-\mu)\mathcal{G}_{ff}(\tau) + U\left\langle T_\tau f_{i-\sigma}^\dagger(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f_{i\sigma}^\dagger \right\rangle - \sum_{\mathbf{k}} V_{\mathbf{k}i}^* \mathcal{G}_{cf}(\mathbf{k},\tau)
\end{aligned} \tag{39.22}$$

where we defined

$$\mathcal{G}_{cf}(\mathbf{k},\tau) = -\left\langle T_\tau c_{\mathbf{k}\sigma}(\tau) f_{i\boldsymbol{\sigma}}^\dagger \right\rangle \tag{39.23}$$

in Matsubara frequency space, the equation of motion gives

$$\left[ik_n - (\varepsilon-\mu)\right]\mathcal{G}_{ff}(ik_n) - \sum_{\mathbf{k}} V_{\mathbf{k}i}^* \mathcal{G}_{cf}(\mathbf{k}, ik_n) = 1 - U\int_0^\beta d\tau e^{ik_n\tau}\left\langle T_\tau f_{i-\sigma}^\dagger(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f_{i\sigma}^\dagger \right\rangle \tag{39.24}$$

To eliminate this quantity, we write its equations of motion

$$\begin{aligned}
\frac{\partial}{\partial\tau}\mathcal{G}_{cf}(\mathbf{k}, i, \tau) =& -\delta(\tau)\left\langle \left\{ c_{\mathbf{k}\sigma}(\tau), f_{i\sigma}^\dagger \right\} \right\rangle \\
&- \left\langle T_\tau \left(-\left(\varepsilon_{\mathbf{k}} - \mu\right) c_{\mathbf{k}\sigma}(\tau) - V_{\mathbf{k}i} f_{i\sigma}(\tau) \right) f_{i\boldsymbol{\sigma}}^\dagger \right\rangle \\
=& -\left(\varepsilon_{\mathbf{k}} - \mu\right)\mathcal{G}_{cf}(\mathbf{k},\tau) - V_{\mathbf{k}i}\mathcal{G}_{ff}(\tau)
\end{aligned} \tag{39.25}$$

that follows because $\left\{ c_{\mathbf{k}\sigma}, f_{i\sigma}^\dagger \right\} = 0$. It can be solved by going to Matsubara frequencies

$$\mathcal{G}_{cf}\left(\mathbf{k}, i, ik_n\right) = \frac{1}{ik_n - \left(\varepsilon_{\mathbf{k}} - \mu\right)} V_{\mathbf{k}i}\mathcal{G}_{ff}\left(ik_n\right) \tag{39.26}$$

Substituting in the equation for $\mathcal{G}_{ff}(ik_n)$ we obtain

$$\begin{aligned}
&\left[ik_n - (\varepsilon-\mu) - \sum_{\mathbf{k}} V_{\mathbf{k}i}^* \frac{1}{ik_n - \left(\varepsilon_{\mathbf{k}} - \mu\right)} V_{\mathbf{k}i} \right] \mathcal{G}_{ff}\left(ik_n\right) \\
=& 1 - U\int_0^\beta d\tau e^{ik_n\tau}\left\langle T_\tau f_{i-\sigma}^\dagger(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f_{i\sigma}^\dagger \right\rangle.
\end{aligned} \tag{39.27}$$

The last term on the right-hand side is related to the self-energy as usual by

$$\Sigma_{ff}\left(ik_n\right)\mathcal{G}_{ff}\left(ik_n\right) \equiv -U\int_0^\beta d\tau e^{ik_n\tau}\left\langle T_\tau f_{i-\sigma}^\dagger(\tau) f_{i-\sigma}(\tau) f_{i\sigma}(\tau) f_{i\boldsymbol{\sigma}}^\dagger \right\rangle \tag{39.28}$$

Except for the self-energy, the equation to be solved has exactly the same Dyson equation structure as that which we would find for a single impurity,

$$\begin{aligned} \mathcal{G}^0_{ff}\left(ik_n\right)^{-1}\mathcal{G}_{ff}\left(ik_n\right) &= 1+\Sigma_{ff}\left(ik_n\right)\mathcal{G}_{ff}\left(ik_n\right) \\ \mathcal{G}_{ff}\left(ik_n\right) &= \mathcal{G}^0_{ff}\left(ik_n\right)+\mathcal{G}^0_{ff}\left(ik_n\right)\Sigma_{ff}\left(ik_n\right)\mathcal{G}_{ff}\left(ik_n\right) \end{aligned} \tag{39.29}$$

with the "non-interacting" Green's function

$$\begin{aligned} \mathcal{G}^0_{ff}\left(ik_n\right)^{-1} &= ik_n-(\varepsilon-\mu)-\sum_{\mathbf{k}}V^*_{\mathbf{k}i}\frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i} \\ &= ik_n-(\varepsilon-\mu)-\Delta_{ff}\left(ik_n\right) \end{aligned} \tag{39.30}$$

This is in fact exactly the non-interacting Green's function that we would find with $U=0$. The significance of $\Delta_{ff}(ik_n)$ is that over the imaginary-time interval β, it takes into account that one can propagate from the impurity site back to the impurity site by going through the bath. This function $\Delta_{ff}\left(ik_n\right)$, defined by

$$\begin{aligned} \Delta_{ff}\left(ik_n\right) &= \sum_{\mathbf{k}}V^*_{\mathbf{k}i}\frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i} \\ &= \sum_{\mathbf{k}}V^\dagger_{i\mathbf{k}}\frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)}V_{\mathbf{k}i} \end{aligned} \tag{39.31}$$

is called the **hybridization function**.

What is important to remember is that the self-energy affects only the site where there is an interaction U. We can write the two equations of motion for $\mathcal{G}_{ff}\left(ik_n\right)$ and $\mathcal{G}_{cf}\left(\mathbf{k},i,ik_n\right)$ succinctly as

$$\begin{pmatrix} ik_n-(\varepsilon-\mu)-\Sigma_{ff}\left(ik_n\right) & -V^*_{\mathbf{k}i} \\ -V_{\mathbf{k}i} & ik_n-(\varepsilon_{\mathbf{k}}-\mu) \end{pmatrix}\begin{pmatrix} \mathcal{G}_{ff}\left(ik_n\right) \\ \mathcal{G}_{cf}\left(\mathbf{k},i,ik_n\right) \end{pmatrix}=\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{39.32}$$

In this equation, the sum over $\mathbf{k}$ is implicit. This problem is analogous to the one we encountered with the coupled harmonic oscillators. Except that we now have a self-energy to compute. Correspondingly, the column vector has $N+1$ elements if there are N possible values of $\mathbf{k}$. Explicitly, for three values of $\mathbf{k}$, the matrix is that acts on the Green's function column is

$$\begin{pmatrix} ik_n-(\varepsilon-\mu)-\Sigma_{ff}\left(ik_n\right) & -V^*_{\mathbf{k}i} & -V^*_{\mathbf{k}'i} & -V^*_{\mathbf{k}''i} \\ -V_{\mathbf{k}i} & ik_n-(\varepsilon_{\mathbf{k}}-\mu) & 0 & 0 \\ -V_{\mathbf{k}'i} & 0 & ik_n-(\varepsilon_{\mathbf{k}'}-\mu) & 0 \\ -V_{\mathbf{k}''i} & 0 & 0 & ik_n-(\varepsilon_{\mathbf{k}''}-\mu) \end{pmatrix} \tag{39.33}$$

What we have done, is to use the second block of this equation to eliminate $\mathcal{G}_{cf}\left(\mathbf{k},i,ik_n\right)$ i.e. the bath, completely. We are left with a single-site problem where the bath is replaced by a hybridization function. We are left with Dyson's equation for $\mathcal{G}_{ff}$ and and a new $\mathcal{G}^0_{ff}\left(ik_n\right)^{-1}$ which contains the bath as a hybridization function.

The solution to this impurity problem is complicated. The structure in imaginary time is highly non-trivial. Contrary to the atomic limit, the number of electrons on a site is not conserved, i.e. it is time-dependent, and the simplicity of the problem is lost. There is a complicated dynamics where electrons move in and out of the impurity site and what happens at a given time depends on what happened at earlier ones. For example, if there is a down electron on the impurity site, another down electron will not be able to come on the site unless the previous one comes out. This problem, when U is large, contains the rich Physics that goes under the name of **Kondo** and could be the subject of many chapters in this book. It has been the focus of much attention in Condensed Matter Physics for decades. We will not for now expand further on this.

Block Matrix Inverse We can write the above problem as follows,

$$\begin{pmatrix} \mathcal{G}^0_{ff}\left(ik_n\right)^{-1}-\Sigma_{ff} & -V^\dagger \\ -V & \mathcal{G}^0\left(\mathbf{k},ik_n\right)^{-1} \end{pmatrix}\begin{pmatrix} \mathcal{G}_{ff}\left(ik_n\right) \\ \mathcal{G}_{cf}\left(\mathbf{k},ik_n\right) \end{pmatrix}=\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{39.34}$$

similarly, if we calculate the E.O.M for $\mathcal{G}^0_{cc}$, with non-interacting part

$$\mathcal{G}^0_{cc}\left(\mathbf{k},ik_n\right)=\frac{1}{ik_n-(\varepsilon_{\mathbf{k}}-\mu)} \tag{39.35}$$

we'd have a relation between $\mathcal{G}_{cc}$ and $\mathcal{G}_{cf}$. Finally, we would have a full matrix equation

$$\begin{pmatrix} \mathcal{G}^0_{ff}\left(ik_n\right)^{-1} - \Sigma_{ff} & -V^\dagger \\ -V & \mathcal{G}^0_{cc}\left(\mathbf{k}, ik_n\right)^{-1} \end{pmatrix} \begin{pmatrix} \mathcal{G}_{ff}\left(ik_n\right) & \mathcal{G}_{cf}\left(\mathbf{k}, ik_n\right) \\ \mathcal{G}_{fc}\left(\mathbf{k}, ik_n\right) & \mathcal{G}_{cc}\left(ik_n\right) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & \mathcal{I} \end{pmatrix} = I \tag{39.36}$$

the matrix can be inverted. In general, the inverse of a Block matrix is

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix}^{-1} = \begin{bmatrix} \left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1} & -\left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1}\mathbf{B}\mathbf{D}^{-1} \\ -\mathbf{D}^{-1}\mathbf{C}\left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{C}\left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1}\mathbf{B}\mathbf{D}^{-1} \end{bmatrix} \tag{39.37}$$

so we have a new Dyson's equation

$$\begin{aligned} \mathcal{G}_{ff}\left(ik_n\right)^{-1} &= \mathcal{G}^0_{ff}\left(ik_n\right)^{-1} - \Sigma_{ff}(ik_n) - V^\dagger \mathcal{G}^0_{cc}\left(\mathbf{k}, ik_n\right) V \\ &= \mathcal{G}^0_{ff}\left(ik_n\right)^{-1} - \Delta_{ff}(ik_n) - \Sigma_{ff}(ik_n) \end{aligned} \tag{39.38}$$

or we can write

$$\begin{aligned} \mathcal{G}^0_{ff}\left(ik_n\right) &= \frac{1}{\mathcal{G}^0_{ff}\left(ik_n\right)^{-1} - \Sigma_{ff}(ik_n) - V^\dagger \mathcal{G}^0_{cc}\left(\mathbf{k}, ik_n\right) V} \\ &= \frac{1}{ik_n - (\varepsilon - \mu) - \Sigma_{ff}(ik_n) - V^\dagger \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V} \\ &= \frac{1}{ik_n - (\varepsilon - \mu) - \Sigma_{ff}(ik_n) - \sum V^*_{\mathbf{k}} \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu)} V_{\mathbf{k}}} \\ &= \frac{1}{ik_n - (\varepsilon - \mu) - \Sigma_{ff}(ik_n) - \Delta_{ff}(ik_n)} \end{aligned} \tag{39.39}$$

39.5 The dynamical mean-field self-consistency relation, derivation 2

Summing all diagrams of the original problem, but using only the local Green's function $\mathcal{G}_{ff}\left(ik_n\right)$, is equivalent to solving exactly a single-impurity Anderson model. In the next section then, I will show that perturbation theory, or more generally the many-body problem for the Anderson impurity model, has the same structure as the original problem when the self-energy of the original problem is calculated using $\mathcal{G}^{(0)}_{ff}\left(ik_n\right)$ that contains the hybridization function.

For now, suppose we have an **impurity solver** which can solve the Anderson Model and calculate the self-energy $\Sigma_{ff}(ik_n)$. We then have an **impurity solver**. We can then solve DMFT self-consistency problem iteratively. I use the Anderson impurity notation here, but we are really talking about the same objects as before. For example $\mathcal{G}_{ff}\left(ik_n\right) \leftrightarrow \mathcal{G}_{ii}\left(ik_n\right)$. In Anderson model we obtained

$$\begin{aligned} \left[ik_n - (\varepsilon - \mu) - \Delta_{ff}\left(ik_n\right) - \Sigma_{ff}(ik_n)\right] \mathcal{G}_{ff}(ik_n) &= 1 \\ \left[ik_n - (\varepsilon - \mu) - \Delta_{ff}\left(ik_n\right)\right] \mathcal{G}^0_{ff}(ik_n) &= 1 \end{aligned} \tag{39.40}$$

Since we do not know the self-energy from the start, we need to begin with a trial $\Delta^{(n)}_{ff}\left(ik_n\right)$ that can be obtained for example from projecting the lattice Green's function with zero self energy. Then,

1. From $\Delta^{(n)}_{ff}(ik_n)$ obtain $\mathcal{G}^0_{ff}(ik_n)$.
2. Using $\{\mathcal{G}^0_{ff}(ik_n), U\}$, the impurity solver computes $\Sigma^{(n+1)}_{ff}(ik_n)$.
3. With $\Sigma^{(n+1)}_{ff}(ik_n)$ we now know $G^{(n+1)}_{ff}(ik_n)$

$$\mathcal{G}^{(n+1)}_{ff}\left(ik_n\right) = \int \frac{d^d\mathbf{k}}{(2\pi)^d} \frac{1}{ik_n - (\varepsilon_{\mathbf{k}} - \mu) - \Sigma^{(n+1)}\left(ik_n\right)} \tag{39.41}$$

4. Obtain a new hybridization function

$$\Delta^{(n+1)}_{ff}\left(ik_n\right) = ik_n - (\varepsilon - \mu) - \Sigma^{(n+1)}_{ff}(ik_n) - \left[\mathcal{G}^{(n+1)}_{ff}\left(ik_n\right)\right]^{-1} \tag{39.42}$$

5. If $\Delta^{(n)}_{ff}\left(ik_n\right)$ and $\Delta^{(n+1)}_{ff}\left(ik_n\right)$ are not equal, go back to 1 with $\Delta^{(n)}_{ff}\left(ik_n\right) \to \Delta^{(n+1)}_{ff}\left(ik_n\right)$.

39.6 Perturbation theory for the Anderson impurity model

In this section, I want to show that perturbation theory for the impurity site of f electrons has the same structure as the perturbation theory we have done up to now, except that what plays the role of the "unperturbed" Green's function is the Green's function that includes the hybridization function, or if you want

$$\mathcal{G}_{ff}^{0}\left(ik_n\right)^{-1} = ik_n - (\varepsilon - \mu) - \Delta\left(ik_n\right) \tag{39.43}$$

where $\Delta(ik_n)$ is the hybridization function.

There are several possible proofs as usual. I start from the linked-cluster theorem. First we use $K_f + K_c$ as "unperturbed" Hamiltonian in the interaction representation. Since $[K_f, K_c] = 0$, using

$$Z = e^{-\beta\Omega} = \mathrm{Tr}\left(e^{-\beta K}\right) = \mathrm{Tr}\left(e^{-\beta K_0} U_I(\beta, 0)\right) \tag{39.44}$$

$$\begin{aligned} Z &= \mathrm{Tr}_{c,f}\left[e^{-\beta K_f} e^{-\beta K_c} T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right] \\ &= Z_0 \frac{\mathrm{Tr}_f\left\{e^{-\beta K_f}\,\mathrm{Tr}_c\left[e^{-\beta K_c} T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right]\right\}}{\mathrm{Tr}_c\left[e^{-\beta K_c}\right]} \\ &= Z_0\,\mathrm{Tr}_f\left[e^{-\beta K_f}\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_0\right] \end{aligned} \tag{39.45}$$

where $Z_0 \equiv \mathrm{Tr}\left[e^{-\beta K_c}\right]$ and

$$\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_0 \equiv \frac{\mathrm{Tr}_c\left[e^{-\beta K_c} e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right]}{\mathrm{Tr}_c\left[e^{-\beta K_c}\right]} \tag{39.46}$$

Recall the structure for the linked cluster theorem

$$\left\langle e^{-f(\mathbf{x})}\right\rangle = \exp\left[\left\langle e^{-f(\mathbf{x})}\right\rangle_c - 1\right] \tag{39.47}$$

we will use this to express

$$\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_0 = T_\tau \exp\left[\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_{0c} - 1\right] \tag{39.48}$$

The cumulant average is easy to evaluate because the average is over non-interacting electrons. Since in $\left\langle T_\tau\left(-\int_0^\beta H_{fc}(\tau)d\tau\right)\right\rangle_{oc}$ there is a single creation or annihilation operator for the conduction electrons, this first order term vanishes. Only even order terms exist, but higher order terms can always be factored into $\mathcal{O}(H_{fc}^2)$ terms, so the only connected non-zero term is

$$\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_0 = \exp\left[\frac{1}{2}\left\langle T_\tau \int_0^\beta H_{fc}(\tau)d\tau \int_0^\beta H_{fc}\left(\tau'\right)d\tau'\right\rangle_{oc}\right] \tag{39.49}$$

this can be seen from the fact that H_{fc}^2 already produce $f^\dagger f$, which is now independent of $c, c^\dagger$ and thus cannot contract with any other interaction using Wick's theorem. Therefore, any higher order terms must be disconnected

from this term. The interaction is written explicitly as

$$\begin{aligned}
&\frac{1}{2}\left\langle T_\tau \int_0^\beta H_{fc}(\tau)d\tau \int_0^\beta H_{fc}\left(\tau'\right)d\tau' \right\rangle_{oc} \\
=&\frac{1}{2}\sum_{\sigma,\sigma'}\sum_{\mathbf{k},\mathbf{k}'}\int_0^\beta d\tau \int_0^\beta d\tau' \left\langle T_\tau \left(V_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma}(\tau) f_{i\sigma}(\tau) + V^*_{\mathbf{k}} f^\dagger_{i\sigma}(\tau) c_{\mathbf{k}\sigma}(\tau)\right)\left(V_{\mathbf{k}'} c^\dagger_{\mathbf{k}'\sigma'}(\tau') f_{i\sigma'}(\tau') + V^*_{\mathbf{k}'} f^\dagger_{i\sigma'}(\tau') c_{\mathbf{k}'\sigma'}(\tau')\right)\right\rangle_{oc} \\
=&\frac{1}{2}\sum_{\sigma,\sigma'}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2\int_0^\beta d\tau \int_0^\beta d\tau' \left\langle T_\tau \left(f^\dagger_{i\sigma'}(\tau') c_{\mathbf{k}\sigma'}(\tau') c^\dagger_{\mathbf{k}\sigma}(\tau) f_{i\sigma}(\tau) + f^\dagger_{i\sigma}(\tau) c_{\mathbf{k}\sigma}(\tau) c^\dagger_{\mathbf{k}\sigma'}(\tau') f_{i\sigma'}(\tau')\right)\right\rangle_{oc} \\
=&\sum_{\sigma,\sigma'}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2\int_0^\beta d\tau \int_0^\beta d\tau' \left\langle T_\tau \left(f^\dagger_{i\sigma'}(\tau') c_{\mathbf{k}\sigma'}(\tau') c^\dagger_{\mathbf{k}\sigma}(\tau) f_{i\sigma}(\tau)\right)\right\rangle_{oc} \\
=&\mathcal{T}_\tau \sum_{\sigma}\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2\int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau') \left\langle \mathcal{T}_\tau \left(c_{\mathbf{k}\sigma}(\tau') c^\dagger_{\mathbf{k}\sigma}(\tau)\right)\right\rangle_{oc} f_{i\sigma}(\tau) \\
=&-\mathcal{T}_\tau \sum_{\sigma}\int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau')\left(\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2 \mathcal{G}_{\sigma\mathbf{k}}(\tau',\tau)\right) f_{i\sigma}(\tau) \\
\equiv&-\mathcal{T}_\tau \sum_{\sigma}\int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau')\Delta(\tau'-\tau) f_{i\sigma}(\tau)
\end{aligned} \tag{39.50}$$

note here we have used the property that we can add time-ordering inside time ordering freely without changing the value.

$$\mathcal{T}\left(f_1 f_2 f_3 f_4\right) = \mathcal{T}\left(f_1\left(\mathcal{T} f_2 f_3\right) f_4\right) \tag{39.51}$$

we have also defined the hybridization function in imaginary time and note that its Matsubara frequency form is the same as defined in previous sections

$$\begin{aligned}
\Delta(\tau'-\tau) &\equiv \sum_{\mathbf{k}}|V_{\mathbf{k}}|^2 \mathcal{G}_{\sigma\mathbf{k}}(\tau',\tau) \\
\Delta(ik_n) &= \sum_{\mathbf{k}}|V_{\mathbf{k}}|^2 \mathcal{G}_{\sigma\mathbf{k}}(ik_n)
\end{aligned} \tag{39.52}$$

We have, finally

$$\left\langle T_\tau e^{-\int_0^\beta H_{fc}(\tau)d\tau}\right\rangle_0 = \mathcal{T}_\tau \exp\left\{-\sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau')\Delta(\tau'-\tau) f_{i\sigma}(\tau)\right\} \tag{39.53}$$

which we substitute back into the partition function

$$Z = Z_0 \,\mathrm{Tr}_f\left[e^{-\beta K_f}\mathcal{T}_\tau \exp\left\{-\sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau')\Delta(\tau'-\tau) f_{i\sigma}(\tau)\right\}\right] \tag{39.54}$$

This has the same structure as our generating function in the Schwinger formalism, but for a single-site problem that depends only on imaginary time. The imaginary time evolution of the f fermions is through K_f that contains interactions. The equation of motion will be precisely that which we found in the sections before. The perturbation series that can be generated by adding a source term will have precisely the same structure as before, except that the hybridation function will enter in the function that plays the role of the non-interacting Green's function. We can write

$$\begin{aligned}
\beta K_f + \langle H_{cf}\rangle_0 &= \sum_\sigma \beta(\varepsilon-\mu) f^\dagger_{i\sigma} f_{i\sigma} + \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau')\Delta(\tau'-\tau) f_{i\sigma}(\tau) \\
&= \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' \left[(\varepsilon-\mu)\delta(\tau'-\tau) + \Delta(\tau'-\tau)\right] f^\dagger_{i\sigma}(\tau') f_{i\sigma}(\tau)
\end{aligned} \tag{39.55}$$

$$\begin{aligned}
\sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' f^\dagger_{i\sigma}(\tau') F(\tau'-\tau) f_{i\sigma}(\tau) &= \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau' T \sum_{ik'_n} e^{+ik'_n\tau'} f^\dagger_{i\sigma}(\tau') T \sum_{iq_n} e^{-iq_n\tau} F(\tau'-\tau) T \sum_{ik_n} e^{-ik_n\tau} f_{i\sigma}(ik_n) \\
&= \sum_\sigma T \sum_{ik'_n} T \sum_{ip_n} T \sum_{ik_n} f^\dagger_{i\sigma}(ik'_n) F(ip_n) f_{i\sigma}(ik_n) \int_0^\beta d\tau \int_0^\beta d\tau' e^{+ik'_n\tau'} e^{-iq_n(\tau'-\tau)} e^{-ik_n\tau} \\
&= \sum_\sigma T \sum_{ik'_n} \sum_{ip_n} \sum_{ik_n} f^\dagger_{i\sigma}(ik'_n) F(ip_n) f_{i\sigma}(ik_n) \delta_{k'_n q_n} \delta_{k_n q_n} \\
&= \sum_\sigma T \sum_{ik_n} f^\dagger_{i\sigma}(ik_n) F(ik_n) f_{i\sigma}(ik_n)
\end{aligned} \tag{39.56}$$

so we have

$$\beta K_f + \langle H_{cf} \rangle_0 = \sum_\sigma T \sum_{ik_n} f^\dagger_{i\sigma}(ik_n) \left[(\varepsilon - \mu) + \Delta(ik_n) \right] f_{i\sigma}(ik_n) \tag{39.57}$$

We have

$$(\varepsilon - \mu) + \Delta(ik_n) \tag{39.58}$$

$$\begin{aligned}
Z|_{U=0} &= Z_0 \operatorname{Tr}_f \left[\exp \left\{ \sum_\sigma T \sum_{ik_n} f^\dagger_{i\sigma}(ik_n) \left[(\varepsilon - \mu) + \Delta(ik_n) \right] f_{i\sigma}(ik_n) \right\} \right] \\
&= Z_0 \prod_{ik_n,\sigma} \operatorname{Tr}_{f(ik_n)} \exp \left\{ T f^\dagger_{i\sigma}(ik_n) \left[(\varepsilon - \mu) + \Delta(ik_n) \right] f_{i\sigma}(ik_n) \right\} \\
&= Z_0 \prod_{ik_n,\sigma} \left(1 + e^{T[(\varepsilon-\mu)+\Delta(ik_n)]} \right) \\
\ln Z|_{U=0} &= \ln Z_0 + \sum_{ik_n,\sigma} \ln \left(1 + e^{T[(\varepsilon-\mu)+\Delta(ik_n)]} \right)
\end{aligned} \tag{39.59}$$

$$\mathcal{G}^0_{ff}(ik_n) = \frac{T e^{T[(\varepsilon-\mu)+\Delta(ik_n)]}}{1 + e^{T[(\varepsilon-\mu)+\Delta(ik_n)]}} \tag{39.60}$$

so the

$$\mathcal{G}^0_{ff}(ik_n) = \frac{1}{ik_n - (\varepsilon - \mu) + \Delta(ik_n)} \tag{39.61}$$

Another way to think about this result is that if we do perturbation theory for the interaction U, all the diagrams where the Green functions go in the bath can be resummed into the hybridization function.

Part VII
Broken Symmetry

40 Instability of the normal state

40.1 The non-interacting limit and rotational invariance

As a preamble, we recall why it is the connected function that we are interested in

$$\begin{aligned}\left.\frac{\partial \langle S_z\rangle}{\beta\partial h}\right|_{h=0} &= \left.\frac{\partial}{\beta\partial h}\frac{\mathrm{Tr}\left[e^{-\beta(K-hS_z)}S_z\right]}{\mathrm{Tr}\left[e^{-\beta(K-hS_z)}\right]}\right|_{h=0} \\ &= \langle S_z S_z\rangle - \langle S_z\rangle\langle S_z\rangle \equiv \langle S_z S_z\rangle_c\end{aligned} \tag{40.1}$$

The spin susceptibility is obtained from the spin-spin correlation function. Very schematically, consider the connected part of the time-ordered product, which represent spin and charge susceptibility

$$\begin{aligned}\langle T_\tau S_z S_z\rangle_c &= \langle T_\tau\left(n_\uparrow - n_\downarrow\right)\left(n_\uparrow - n_\downarrow\right)\rangle_c \\ &= \langle T_\tau n_\uparrow n_\uparrow\rangle_c + \langle T_\tau n_\downarrow n_\downarrow\rangle_c - \langle T_\tau n_\uparrow n_\downarrow\rangle_c - \langle T_\tau n_\downarrow n_\uparrow\rangle_c\end{aligned} \tag{40.2}$$

$$\begin{aligned}\langle T_\tau \rho\rho\rangle_c &= \langle T_\tau\left(n_\uparrow + n_\downarrow\right)\left(n_\uparrow + n_\downarrow\right)\rangle_c \\ &= \langle T_\tau n_\uparrow n_\uparrow\rangle_c + \langle T_\tau n_\downarrow n_\downarrow\rangle_c + \langle T_\tau n_\uparrow n_\downarrow\rangle_c + \langle T_\tau n_\downarrow n_\uparrow\rangle_c .\end{aligned} \tag{40.3}$$

We have assumed $\hbar/2 = 1$ here for the purposes of this discussion. The first term is $\langle n_\uparrow n_\uparrow\rangle_c = \langle n_\uparrow n_\uparrow\rangle - \langle n_\uparrow\rangle^2 = \langle n_\uparrow\rangle - \langle n_\uparrow\rangle^2$ is non-zero in general, while the third term $\langle T_\tau n_\uparrow n_\downarrow\rangle_c = \langle n_\uparrow n_\downarrow\rangle - \langle n_\uparrow\rangle\langle n_\downarrow\rangle = 0$ for non-interacting systems, where $n_\uparrow$ and $n_\downarrow$ are uncorrelated. So the charge and spin susceptibility are the same, which is the Lindhard function

$$\begin{aligned}\chi_0\left(\mathbf{q}, iq_n\right) &= -\sum_\sigma\sum_k \mathcal{G}_\sigma(k+q)\mathcal{G}_\sigma(k) \\ &= -\frac{1}{N}\sum_{\mathbf{p},\sigma} T\sum_n \mathcal{G}^0_\sigma\left(\mathbf{p}+\mathbf{q}, ip_n + iq_n\right)\mathcal{G}^0_\sigma(\mathbf{p}, ip_n) \\ &= -\frac{2}{N}\sum_{\mathbf{p}}\frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p}+\mathbf{q}})}{iq_n + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}}\end{aligned} \tag{40.4}$$

by rotational symmetry, we can also write the susceptibility as

$$\begin{aligned}\langle T_\tau S_z S_z\rangle_c &= \frac{1}{2}\left(\langle T_\tau S_x S_x\rangle_c + \langle T_\tau S_y S_y\rangle_c\right) \\ &= \frac{1}{4}\langle T_\tau\left(S_x + iS_y\right)\left(S_x - iS_y\right)\rangle_c + \frac{1}{4}\langle T_\tau\left(S_x - iS_y\right)\left(S_x + iS_y\right)\rangle_c \\ &= \left\langle T_\tau S^+ S^-\right\rangle_c + \left\langle T_\tau S^- S^+\right\rangle_c\end{aligned} \tag{40.5}$$

40.2 Effect of interactions for ferromagnetism, the Feynman way

$$\begin{aligned}\left\langle T_\tau S^+ S^-\right\rangle_c &= \frac{\chi_0}{2} + \frac{\chi_0}{2}(-U)\left(-\frac{\chi_0}{2}\right) + \frac{\chi_0}{2}(-U)^2\left(-\frac{\chi_0}{2}\right)^2 + \ldots \\ &= \frac{\chi_0/2}{1 - \frac{U}{2}\chi_0}\end{aligned} \tag{40.6}$$

We thus obtain in Fourier space where the above equation is algebraic,

$$\chi = \left\langle T_\tau S^+ S^-\right\rangle_c + \left\langle T_\tau S^- S^+\right\rangle_c = \langle T_\tau S_z S_z\rangle_c = \frac{\chi_0}{1 - \frac{U}{2}\chi_0}. \tag{40.7}$$

RPA is non-physical when $1 < \frac{U}{2}\chi_0(\mathbf{q}, 0)$, there is a phase transition when the generalized stoner criterion

$$1 = \frac{U}{2}\chi_0(\mathbf{q}, 0) \tag{40.8}$$

is satisfied.

40.3 The thermodynamic Stoner Instability

At finite frequency, a retarded response function can be positive or negative because of resonances. But at zero frequency, we are looking at thermodynamics, hence a **susceptibility must be positive**. One can show that any $\chi(\mathbf{q}, iq_n)$ is positive when $\chi_0''(\mathbf{q},\omega) = -\chi_0''(\mathbf{q},-\omega)$ (T-invariance + Commutator nature), since

$$\chi(\mathbf{q}, iq_n) = \int \frac{d\omega}{\pi} \frac{\chi''(\mathbf{q},\omega)}{\omega - iq_n} = \int \frac{d\omega}{\pi} \frac{\omega\chi''(\mathbf{q},\omega)}{(\omega)^2 + (q_n)^2} \tag{40.9}$$

hence *a fortiori* $\chi(\mathbf{q},0)$ is positive. Hence, the RPA result $\chi = \frac{\chi_0}{1-\frac{U}{2}\chi_0}$ is nonphysical when $1 < \frac{U}{2}\chi_0(\mathbf{q},0)$. There is a phase transition when the generalized Stoner criterion

$$1 = \frac{U}{2}\chi_0(\mathbf{q},0) \tag{40.10}$$

is satisfied. Note that the first wave vector for which the above result is satisfied is the one that becomes unstable. It does not necessarily correspond to a uniform ferromagnet ($\mathbf{q}=0$). It could be an antiferromagnet. In the special case of ferromagnetism, we take the $\mathbf{q}\to 0$ limit of $\chi_0(\mathbf{q},0)$ to get the specific coefficient in the Stoner criterion

$$\lim_{\mathbf{q}\to\mathbf{0}} \chi_0(\mathbf{q},0) = \lim_{\mathbf{q}\to\mathbf{0}} -\frac{2}{N}\sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p}+\mathbf{q}})}{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}} = -\frac{2}{N}\sum_{\mathbf{p}} \frac{\partial f(\zeta_{\mathbf{p}})}{\partial \zeta_{\mathbf{p}}} \to_{T\to 0} 2N(\varepsilon_F) \tag{40.11}$$

which matches the Stoner criterion we will derive through variational principle.

40.4 Magnetic structure factor and paramagnons

The transition to the ferromagnetic state is a **continuous transition** (or **second order transition** in the mean-field language). It is signaled by a diverging susceptibility, as we saw above. The **correlation length** is diverging at the transition point. We can see this by expanding $\chi(\mathbf{q},0)$ near the transition point ($\mathbf{q}=0$) so that it becomes asymptotically equal to

$$\chi(\mathbf{q},0) \approx \frac{\chi_0(\mathbf{0},0)}{1 - \frac{U}{2}\chi_0(\mathbf{q},0) - \frac{1}{2}\left(\frac{U}{2}\right)\frac{\partial^2\chi_0(\mathbf{q},0)}{\partial^2 q^2} q^2} \sim \frac{A}{\xi^{-2} + q^2} \tag{40.12}$$

in real space, this is an exponential decrease with with correlation length $\xi^{-2} \sim 1 - \frac{U}{2}\chi_0(\mathbf{q},0)$. This is agian the **Ornstein Zernicke** functional form. At the transition point, the system becomes "**critical**". The transition point itself is called a **critical point**. The presence of this long correlation length also manifests itself in the existence of "**critical slowing down**". In the present case, we will discover an over-damped collective mode whose typical frequency decreases as we approach the critical point.

Consider for example, the zero temperature transverse magnetic structure factor

$$S_\perp(\mathbf{q},\omega) = \frac{2}{1-e^{-\beta\omega}}\chi_\perp''(\mathbf{q},\omega) = 2\theta(\omega)\chi_\perp''(\mathbf{q},\omega) \tag{40.13}$$

We will then focus on the $\omega > 0$ part, where from RPA result of χ'',

$$\begin{aligned} S_\perp(\mathbf{q},\omega) = 2\Im\left[\frac{\chi_0^R}{1-\frac{U}{2}\chi_0^R}\right] &= \frac{2\chi_0''(\mathbf{q},\omega)\left(1-\frac{U}{2}\chi_0'(\mathbf{q},\omega)\right)}{\left(1-\frac{U}{2}\chi_0'(\mathbf{q},\omega)\right)^2 + \left(\frac{U}{2}\chi_0''(\mathbf{q},\omega)\right)^2} \\ &\approx \left(1-\frac{U}{2}N(\varepsilon_F)\right)\frac{2\chi_0''(\mathbf{q},\omega)}{\left(1-UN(\varepsilon_F)\right)^2 + \left(\frac{U}{2}\chi_0''(\mathbf{q},\omega)\right)^2} \end{aligned} \tag{40.14}$$

where the approximation $\chi_0'(\mathbf{q},\omega) \approx N(\varepsilon_F)$ is made when we consider both $\mathbf{q}$ and ω small.

$$\begin{aligned} \chi_0^R(\mathbf{q},\omega) &= -\frac{2}{N}\sum_{\mathbf{p}} \frac{f(\zeta_{\mathbf{p}}) - f(\zeta_{\mathbf{p}+\mathbf{q}})}{\omega + i\eta + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}} \\ &\approx -\frac{2}{N}\sum_{\mathbf{p}} \frac{\partial f(\zeta_{\mathbf{p}})}{\partial \zeta_{\mathbf{p}}} \frac{\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}}{\omega + i\eta + \zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}}} \end{aligned} \tag{40.15}$$

now, for $q \ll k_F = p_F$, we can approximate

$$\zeta_{\mathbf{p}} - \zeta_{\mathbf{p}+\mathbf{q}} = -\frac{\mathbf{p}\cdot\mathbf{q}}{m} - \frac{q^2}{2m} \approx -\mathbf{v}_F \cdot \mathbf{q} = -v_F q \cos\theta \tag{40.16}$$

where $\theta =< \mathbf{p}, \mathbf{q} >$. With this, we can write

$$\chi_0^R(\mathbf{q},\omega) = 2\int d\varepsilon N(\varepsilon) f'(\varepsilon-\mu) \int_{-1}^{1} \frac{d\cos\theta}{2} \frac{v_F q\cos\theta}{\omega + i\eta - v_F q\cos\theta} \tag{40.17}$$

now take the imaginary part

$$\begin{aligned}
\chi_0''(\mathbf{q},\omega) &= -2\pi \int d\varepsilon N(\varepsilon) f'(\varepsilon-\mu) \int_{-1}^{1} \frac{d\cos\theta}{2} v_F q\cos\theta\, \delta(\omega - v_F q\cos\theta) \\
&= \frac{\pi\omega}{v_F q} \int d\varepsilon N(\varepsilon) \left[-f'(\varepsilon-\mu)\right] \\
&= \pi N(\varepsilon_F) \frac{\omega}{v_F q} \propto \frac{\omega}{v_F q}
\end{aligned} \tag{40.18}$$

this shows that

$$S_\perp(\mathbf{q},\omega) = 2\chi_\perp''(\mathbf{q},\omega) \propto \frac{2C\frac{\omega}{v_F q}}{\left(1 - UN(\varepsilon_F)\right)^2 + \left(C\frac{\omega}{v_F q}\right)^2} \tag{40.19}$$

this function has a peak at $C\frac{\omega}{v_F q} = 1 - UN(\varepsilon_F) \approx \xi^{-2}$, which is a $\omega = \left(\xi^{-2} v_F / C\right) q$ linear dispersion. As the correlation length ξ increases, $1 - UN(\varepsilon_F) \approx \xi^{-2}$ become smaller so the characteristic frequency become smaller.

41 Stoner Ferromagnetism

Consider a quadratic dispersion band which is almost empty. Take U/t small so that we may think a priori that perturbation theory is applicable. Stoner showed using simple arguments that if U is large enough, the system has a tendency to become ferromagnetic. This is easy to understand in the ground state by an energy balance argument. When U is very large, it is energetically favorable to populate the states with only spins with the same orientation, say up. Indeed, there is then no potential energy since $Un_\uparrow n_\downarrow$ then vanishes. This costs kinetic energy since the Fermi energy of the up spins needs to be larger to accommodate more spins than if the spin down band was also occupied. The balance determines whether the symmetry will be broken or not. There is thus a simple energetic argument that tells us why it is preferable to break a symmetry (choose up spins for example). It is often possible to "guess" which symmetry will be broken using that type of arguments, but it is not always possible.

We will look at ferromagnetism from many points of view. And then we will see that so-called Stoner argument has some problems and that ferromagnetism is much harder to find than what Stoner first thought.

41.1 From simple arguments

In Hartree-Fock approximation

$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma^{(1)}(\mathbf{k}) \tag{41.1}$$

In the case of Hubbard model,

$$\Sigma_\sigma^H(1,2)_\phi = U\mathcal{G}_{-\sigma}\left(1,1^+\right)_\phi \delta(1-2) \tag{41.2}$$

we have $\mathcal{G}_{-\sigma}\left(1,1^+\right)_\phi = \langle n_{-\sigma}(1)\rangle = \langle n_{-\sigma}\rangle$ by translational symmetry, so a Fourier Transform results in

$$\Sigma_\sigma^H(k) = U\langle n_{-\sigma}\rangle \tag{41.3}$$

we know that $\langle n_{-\sigma}\rangle = f(\xi_{\mathbf{k}\sigma})$ is dependent only on $\mathbf{k}, \sigma$, so $\Sigma_\sigma^H(k) = \Sigma_\sigma^H(\mathbf{k})$. So we have

$$\tilde{\epsilon}_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}} + U\langle n_{-\sigma}\rangle \tag{41.4}$$

In general, the up band and down band now have different fermi wave-vector k_F and different fermi energy ϵ_F. Notice that ϵ_F is a function of particle density n. Define $\bar{n} \equiv \frac{\langle n_\uparrow \rangle + \langle n_\downarrow \rangle}{2}$

$$\begin{aligned} \epsilon_{F\uparrow} + U \langle n_\downarrow \rangle &= \epsilon_{F\downarrow} + U \langle n_\uparrow \rangle \\ \frac{\partial \epsilon_F(0)}{\partial n} \langle n_\uparrow \rangle + U \langle n_\downarrow \rangle &= \frac{\partial \epsilon_F(0)}{\partial n} \langle n_\downarrow \rangle + U \langle n_\downarrow \rangle \\ \left(\frac{\partial \epsilon_F(0)}{\partial n} - U \right) [\langle n_\uparrow \rangle - \langle n_\downarrow \rangle] &= 0 \end{aligned} \tag{41.5}$$

we have $-\frac{\partial n}{\partial \epsilon}|_{\epsilon=\epsilon_F} = N(\epsilon_F)$ the density of states on the Fermi surface, so either $\langle n_\uparrow \rangle = \langle n_\downarrow \rangle$ or

$$1 = UN(\epsilon_F) \tag{41.6}$$

which is the Stoner criterion for ferromagnetism.

41.2 From variational principle

Using Feynman Variational principle $F \leq F_{\tilde{0}} + \left\langle H - \tilde{H}_0 \right\rangle_{\tilde{0}}$:

$$\begin{aligned} H &= \sum_{\mathbf{k}\sigma} \zeta_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \\ \tilde{H}_0 &= \sum_{\mathbf{k}\sigma} \tilde{\zeta}_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \end{aligned} \tag{41.7}$$

the plan is to find $\tilde{H}_0$ which minimizes the RHS,

$$\begin{aligned} F = -T \ln Z &\leq -T \ln Z_{\tilde{0}} + \left\langle H - \tilde{H}_0 \right\rangle_{\tilde{0}} \\ &= -T \sum_{\mathbf{k}\sigma} \ln \left(1 + e^{-\beta \tilde{\zeta}_{\mathbf{k}\sigma}} \right) + \sum_{\mathbf{k},\sigma} \left(\zeta_{\mathbf{k}} - \tilde{\zeta}_{\mathbf{k}\sigma} \right) \left\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \right\rangle_{\tilde{0}} + U \sum_i \left\langle c^\dagger_{i\uparrow} c_{i\uparrow} \right\rangle_{\tilde{0}} \left\langle c^\dagger_{i\downarrow} c_{i\downarrow} \right\rangle_{\tilde{0}} \end{aligned} \tag{41.8}$$

where the last term can also be written by translational invariance as $UN \langle n_\sigma \rangle_{\tilde{0}} \langle n_{-\sigma} \rangle_{\tilde{0}}$ with, as usual, N the number of sites. To evaluate $\langle H \rangle_{\tilde{0}}$ we have used Wick's theorem since $\tilde{H}_0$ is non-interacting. Our variational parameters are $\tilde{\zeta}_{\mathbf{k}\sigma}$. We thus set to zero the derivative of the above expression with respect to $\tilde{\zeta}_{\mathbf{k}\sigma}$, recalling that the values $\left\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \right\rangle_{\tilde{0}}$ taken with the trial Hamiltonian also depend on $\tilde{\zeta}_{\mathbf{k}\sigma}$. Using translational invariance and the definition of Fourier transforms we have the following equalities

$$N \left\langle c^\dagger_{i\sigma} c_{i\sigma} \right\rangle_{\tilde{0}} = \sum_i \left\langle c^\dagger_{i\sigma} c_{i\sigma} \right\rangle_{\tilde{0}} = \sum_{\mathbf{k},\sigma} \left\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \right\rangle_{\tilde{0}} \tag{41.9}$$

so we can manipulate the third term into

$$U \sum_i \left\langle c^\dagger_{i\sigma} c_{i\sigma} \right\rangle_{\tilde{0}} \left\langle c^\dagger_{i-\sigma} c_{i-\sigma} \right\rangle_{\tilde{0}} = U \left\langle c^\dagger_{-\sigma} c_{-\sigma} \right\rangle_{\tilde{0}} \sum_{\mathbf{k},\sigma} \left\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \right\rangle_{\tilde{0}}. \tag{41.10}$$

$$F \leq -T \sum_{\mathbf{k}\sigma} \ln \left(1 + e^{-\beta \tilde{\zeta}_{\mathbf{k}\sigma}} \right) + \sum_{\mathbf{k},\sigma} \left(\zeta_{\mathbf{k}} - \tilde{\zeta}_{\mathbf{k}\sigma} \right) \langle n_{\mathbf{k}\sigma} \rangle_{\tilde{0}} + U \langle n_{-\sigma} \rangle_{\tilde{0}} \sum_{\mathbf{k},\sigma} \langle n_{\mathbf{k}\sigma} \rangle_{\tilde{0}} \tag{41.11}$$

Differentiating RHS with respect to $\tilde{\zeta}_{\mathbf{k}\sigma}$, and set it equal to zero, we have

$$\begin{aligned} 0 = &- T \frac{e^{-\beta \tilde{\zeta}_{\mathbf{k}\sigma}}}{1 + e^{-\beta \tilde{\zeta}_{\mathbf{k}\sigma}}} (-\beta) - \langle n_{\mathbf{k}\sigma} \rangle_{\tilde{0}} \\ &+ \left(\zeta_{\mathbf{k}\sigma} + U \langle n_{-\sigma} \rangle_{\tilde{0}} - \widetilde{\zeta}_{\mathbf{k}\sigma} \right) \frac{\partial \left\langle c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \right\rangle_{\tilde{0}}}{\partial \widetilde{\zeta}_{\mathbf{k}\sigma}}. \end{aligned} \tag{41.12}$$

where we note that

$$\langle n_{\mathbf{k}} \rangle_{\tilde{0}} = \frac{1}{e^{\beta \tilde{\zeta}_{\mathbf{k}\sigma}} + 1} \tag{41.13}$$

so the first two terms cancel, leaving us with

$$\widetilde{\zeta}_{\mathbf{k}\sigma} = \zeta_{\mathbf{k}} + U \langle n_{-\sigma} \rangle_{\tilde{0}} \tag{41.14}$$

Define

$$\begin{aligned} n &\equiv \langle n_\uparrow \rangle_{\tilde{0}} + \langle n_\downarrow \rangle_{\tilde{0}} \\ m &\equiv \langle n_\uparrow \rangle_{\tilde{0}} - \langle n_\downarrow \rangle_{\tilde{0}} \end{aligned} \tag{41.15}$$

we know n and wish to calculate m. We can write an self consistency equation for m

$$\begin{aligned} m &= \langle n_\uparrow \rangle_{\tilde{0}} - \langle n_\downarrow \rangle_{\tilde{0}} \\ &= \frac{1}{N} \sum_{\mathbf{k}} \left[f(\tilde{\zeta}_{\mathbf{k}\uparrow}) - f(\tilde{\zeta}_{\mathbf{k}\downarrow}) \right] \\ &= \frac{1}{N} \sum_{\mathbf{k}} \left[f(\zeta_{\mathbf{k}} + U \langle n_\downarrow \rangle_{\tilde{0}}) - f(\zeta_{\mathbf{k}} + U \langle n_\uparrow \rangle_{\tilde{0}}) \right] \\ &= \frac{1}{N} \sum_{\mathbf{k}} \left[f(\zeta_{\mathbf{k}} + \frac{Un}{2} - \frac{Um}{2}) - f(\zeta_{\mathbf{k}} + \frac{Un}{2} + U\frac{m}{2}) \right] \\ &= \frac{1}{N} \sum_{\mathbf{k}} \left[-2f'(\zeta_{\mathbf{k}} + \frac{Un}{2}) \left(\frac{Um}{2} \right) - \frac{1}{3} f'''(\zeta_{\mathbf{k}} + \frac{Un}{2}) \left(\frac{Um}{2} \right)^3 + \mathcal{O}(m^5) \right] \\ &\approx (-Um) \left[\frac{1}{N} \sum_{\mathbf{k}} f'(\zeta_{\mathbf{k}} + \frac{Un}{2}) \right] - \frac{1}{3} \left(\frac{Um}{2} \right)^3 \left[\frac{1}{N} \sum_{\mathbf{k}} f'''(\zeta_{\mathbf{k}} + \frac{Un}{2}) \right] \end{aligned} \tag{41.16}$$

Define the overall fermi energy by $\varepsilon_F + U\frac{n}{2} = \mu$, and taking $T \to 0$, we have

$$\begin{aligned} \frac{1}{N} \sum_{\mathbf{k}} f'(\zeta_{\mathbf{k}} + \frac{Un}{2}) &= \frac{1}{N} \sum_{\mathbf{k}} f'(\epsilon_{\mathbf{k}} - \varepsilon_F) \\ &= -\frac{1}{N} \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}} - \varepsilon_F) \\ &= -N(\varepsilon_F) \end{aligned} \tag{41.17}$$

where $N(\varepsilon_F)$ is the density of states for a single species. We will denote

$$\begin{aligned} b &\equiv -\frac{1}{3} \left(\frac{U}{2} \right)^3 \left[\frac{1}{N} \sum_{\mathbf{k}} f'''(\zeta_{\mathbf{k}} + \frac{Un}{2}) \right] \\ &= \frac{N''(\varepsilon_F)}{24} - \frac{(N'(\varepsilon_F))^2}{8N(\varepsilon_F)} \end{aligned} \tag{41.18}$$

after some tedious calculations (which I didn't do), and we can show that b is in general negative. Finally, we have an equation for m:

$$(1 - UN(\varepsilon_F))\, m + (-b)\, m^3 = 0 \tag{41.19}$$

this is the **Landau-Ginzburg equation** for the **magnetization**. This could equivalently come from the minimization of a free energy functional. In any case, we get the Stoner criterion

$$m = \begin{cases} 0 & UN(\varepsilon_F) < 1 \\ \pm\sqrt{\frac{1}{b}\left(1 - UN(\varepsilon_F)\right)} & UN(\varepsilon_F) > 1 \end{cases} \tag{41.20}$$

the second state is a broken symmetry state.

41.3 From Green's function (effective medium)

In effective medium theory, we split the Hamiltonian into three parts

$$H = H_{\tilde{0}} + (H_0 - H_{\tilde{0}}) + V \tag{41.21}$$

and treat both $(H_0 - H_{\tilde{0}}), V$ as interactions. We want to choose the right $H_{\tilde{0}}$ such that the self-energy due to $(H_0 - H_{\tilde{0}})$, and the interaction V up to Hartree-Fock level cancel exactly:

$$\tilde{\Sigma}_\sigma = U \langle n_{-\sigma} \rangle + \varepsilon_{\mathbf{k}} - \widetilde{\varepsilon}_{\mathbf{k}\sigma} = 0 \tag{41.22}$$

we obtain a renormalized Green's function

$$G_\sigma (\mathbf{k}, ik_n) = \frac{1}{ik_n - \widetilde{\varepsilon}_{\mathbf{k}\sigma} + \mu} \tag{41.23}$$

with which we can compute the local density

$$\begin{aligned} \langle n_\sigma \rangle &= T \sum_n e^{ik_n \eta} \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{ik_n - \widetilde{\varepsilon}_{\mathbf{k}\boldsymbol{\sigma}} + \mu} \\ &= \frac{1}{N} \sum_{\mathbf{k}} f \left(\varepsilon_{\mathbf{k}} + U \langle n_{-\sigma} \rangle - \mu \right) \\ &= \frac{1}{N} \sum_{\mathbf{k}} f \left(\zeta_{\mathbf{k}} + U \langle n_{-\sigma} \rangle \right). \end{aligned} \tag{41.24}$$

which will then be equivalent to the two methods above.

42 Goldstone mode

What do the collective modes look like in the ordered state? The minimal energy to excite a particle with an up spin to a state with down spin is $\varepsilon_{k_F\uparrow} - \varepsilon_{k_F\downarrow} = U(\langle n_\uparrow \rangle - \langle n_\downarrow \rangle) = Um$. When $m > 0$, there is a single-particle gap

$$\Delta = Um \tag{42.1}$$

to such single spin flip excitations. This same gap exists for particle-hole excitations in the ordered state that flip a spin. There is thus a gap in the particle-hole continuum for what is called the "**longitudinal susceptibility**". We see in passing that the equation for m is also the equation for the gap Δ. But that is not the whole story. We also need to look at all the collective modes, in particular those of the **transverse spin susceptibility**. It is a general result (Goldstone's theorem) that when there is a continuous symmetry that is broken, such as rotational symmetry, then there is a collective mode whose frequency vanishes at long wave lengths and whose role is to "**restore**" the symmetry. In the case of the ferromagnet, it does not cost any energy to rotate the overall magnetization of the system. This is the mode that restores the symmetry.

42.1 Transverse susceptibility

We already have an expression for the spin susceptibility

$$\langle T_\tau S_z S_z \rangle_c = \left\langle T_\tau S^+ S^- \right\rangle_c + \left\langle T_\tau S^- S^+ \right\rangle_c \tag{42.2}$$

First note that

$$\begin{aligned} \mathbf{S} &= \frac{1}{2} c_\alpha^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_\beta \\ S^+ &= S^x + iS^y = c_\uparrow^\dagger c_\downarrow \\ S^- &= S^x - iS^y = c_\downarrow^\dagger c_\uparrow \end{aligned} \tag{42.3}$$

Define the transverse susceptibility $\chi_\perp^{-+}(i,j,\tau) \equiv \left\langle T_\tau S_i^-(\tau) S_j^+ \right\rangle_c = \left\langle T_\tau c_{i\downarrow}^\dagger(\tau) c_{i\uparrow}(\tau) c_{j\uparrow}^\dagger c_{j\downarrow} \right\rangle_c$. The Fourier Transform is

$$\begin{aligned} \chi_\perp^{-+}(q) &= \sum_{\mathbf{R}_i - \mathbf{R}_j} \int_0^\beta d\tau e^{-i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} e^{iq_n\tau} \chi_\perp^{-+}(i,j,\tau) \\ &= \frac{1}{N} \int_0^\beta d\tau e^{iq_n\tau} \left\langle T_\tau S_{\mathbf{q}}^-(\tau) S_{-\mathbf{q}}^+ \right\rangle_c \end{aligned} \tag{42.4}$$

Consider now RPA of $\chi_\perp^{-+}(i,j,\tau)$, consisting of ladder diagrams, since only opposite spins can interact with each other

$$\sum_i U c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} = \sum_{i,j} U\delta_{i-j} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger c_{j\downarrow} c_{i\uparrow} \tag{42.5}$$

in Fourier space, the interaction is simply a constant

$$U_{\mathbf{q}} = \sum_{\mathbf{R}_i - \mathbf{R}_j} U\delta_{i-j} e^{-i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} = U \tag{42.6}$$

from diagrammatic analysis, let $1 \equiv (i,\tau_1), 2 \equiv (j,\tau_2)$

$$\begin{aligned}
\chi_\perp^{-+}(1,2) &= \left\langle T_\tau c_{i\downarrow}^\dagger(\tau_1) c_{i\uparrow}(\tau_1) c_{j\uparrow}^\dagger(\tau_2) c_{j\downarrow}(\tau_2) \right\rangle_c - \langle n\rangle \langle n\rangle \\
\chi_{0\perp}^{-+}(1,2) &= \left\langle T_\tau c_{i\downarrow}^\dagger(\tau_1) c_{i\uparrow}(\tau_1) c_{j\uparrow}^\dagger(\tau_2) c_{j\downarrow}(\tau_2) \right\rangle_{0c} - \langle n\rangle \langle n\rangle \\
&= -\sum_k \mathcal{G}_\uparrow(k)\mathcal{G}_\downarrow(k+q)
\end{aligned} \tag{42.7}$$

the diagram with one ladder is

$$\left(-\sum_k \mathcal{G}_\uparrow(k)\mathcal{G}_\downarrow(k+q)\right)(-U)\left(\sum_{k'} \mathcal{G}_\uparrow(k')\mathcal{G}_\downarrow(k'+q)\right) = U\left(\chi_{0\perp}^{-+}\right)^2 \tag{42.8}$$

where the minus sign in $-U$ comes from the perturbation order. Similarly, we can

$$\begin{aligned}
\chi_\perp^{-+}(q) &= \chi_{0\perp}^{-+}\left[1 + \left(U\chi_{0\perp}^{-+}\right) + \left(U\chi_{0\perp}^{-+}\right)^2 + ...\right] \\
&= \frac{\chi_{0\perp}^{-+}(q)}{1 - U\chi_{0\perp}^{-+}(q)}
\end{aligned} \tag{42.9}$$

the retarded susceptibility is then

$$\chi_\perp^{R-+}(\mathbf{q},\omega) = \frac{\chi_{0\perp}^{R-+}(\mathbf{q},\omega)}{1 - U\chi_{0\perp}^{R-+}(\mathbf{q},\omega)} \tag{42.10}$$

given the new excitation spectrum (for $\tilde{H}_0$ which breaks the symmetry) of the ordered state, we have a new "non-interacting susceptibility":

$$\chi_{0\perp}^{R-+}(\mathbf{q},\omega) = -\frac{1}{N}\sum_{\mathbf{p}} \frac{f(\widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow}) - f(\widetilde{\zeta}_{\mathbf{p}\downarrow})}{\omega + i\eta + \widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow} - \widetilde{\zeta}_{\mathbf{p}\downarrow}} \tag{42.11}$$

note that $\zeta_{\mathbf{k}\uparrow} \neq \zeta_{\mathbf{k}\downarrow}$ now. To simplify the calculations, we assume that $\Delta << E_F$ so that we can neglect the energy dependence of the density of states and take the Fermi velocities for up and down electrons to be identical. Expanding as before in the small $\mathbf{q}$ limit, we then have, for small wave vector

$$\widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow} - \widetilde{\zeta}_{\mathbf{p}\downarrow} \approx \mathbf{v}_F\cdot\mathbf{q} + U\left(\langle n_\downarrow\rangle - \langle n_\uparrow\rangle\right) = \mathbf{v}_F\cdot\mathbf{q} - \Delta \tag{42.12}$$

for $\mathbf{v}_F\cdot\mathbf{q} \ll \Delta$, we can expand

$$\begin{aligned}
\chi_{0\perp}^{R-+}(\mathbf{q},\omega) \approx& -\frac{1}{N}\sum_{\mathbf{p}} \frac{f(\widetilde{\zeta}_{\mathbf{p}+\mathbf{q}\uparrow}) - f(\widetilde{\zeta}_{\mathbf{p}\downarrow})}{\omega + i\eta - \Delta}\left[1 - \frac{\mathbf{v}_F\cdot\mathbf{q}}{\omega + i\eta - \Delta} + \left(\frac{\mathbf{v}_F\cdot\mathbf{q}}{\omega + i\eta - \Delta}\right)^2 + \cdots\right] \\
\approx& -\frac{1}{N}\sum_{\mathbf{p}} \frac{\partial f}{\partial\tilde{\zeta}}|_{\zeta=0}\frac{\mathbf{v}_F\cdot\mathbf{q} - \Delta}{\omega + i\eta - \Delta}\left[1 - \frac{\mathbf{v}_F\cdot\mathbf{q}}{\omega + i\eta - \Delta} + \left(\frac{\mathbf{v}_F\cdot\mathbf{q}}{\omega + i\eta - \Delta}\right)^2 + \cdots\right] \\
=& N(\varepsilon_F)\int \frac{d\hat{p}}{4\pi}\frac{1}{\omega + i\eta - \Delta}\left[\mathbf{v}_F\cdot\mathbf{q} - \Delta\right]\left[1 - \frac{\mathbf{v}_F\cdot\mathbf{q}}{\omega + i\eta - \Delta} + \left(\frac{\mathbf{v}_F\cdot\mathbf{q}}{\omega + i\eta - \Delta}\right)^2 + \cdots\right] \\
\approx& \frac{-\Delta/U}{\omega + i\eta - \Delta}\left[1 + \frac{C}{\Delta^2}q^2\right]
\end{aligned} \tag{42.13}$$

where we used the gap equation $1 = UN(\varepsilon_F)$. At then end of this section, we prove that $C < 0$, which is necessary for stability as we will show. Note that the above formula immediately gives that at $q = 0$ the imaginary part is vanishing for $\omega < \Delta$, i.e. there is a gap in the particle-hole continuum.

To see the effect of **residual interactions** in the ordered state, in other words the effect of the interactions that are not taken care of by the mean field, we consider the corresponding RPA result in the additional limit $|\omega| < \Delta$

$$\begin{aligned}\chi_\perp^{R-+}(\mathbf{q},\omega) &= \frac{\chi_{0\perp}^{R-+}(\mathbf{q},\omega)}{1 - U\chi_{0\perp}^{R-+}(\mathbf{q},\omega)} \approx \frac{\frac{-\Delta/U}{\omega+i\eta-\Delta}}{1 - \frac{(-\Delta)}{\omega+i\eta-\Delta} - \frac{(-\Delta)C}{(\omega+i\eta-\Delta)\Delta^2}q^2} \\ &\approx \frac{-\Delta/U}{\omega + i\eta - Dq^2},\end{aligned} \tag{42.14}$$

with $D = -C/\Delta > 0$. The complete transverse spin susceptibility is obtained by combining the two results

$$\begin{aligned}\chi_\perp^{R-+}(\mathbf{q},\omega) + \chi_\perp^{R+-}(\mathbf{q},\omega) &= \frac{-\Delta/U}{\omega + i\eta - Dq^2} + \frac{\Delta/U}{\omega + i\eta + Dq^2} \\ &= -\frac{\Delta}{U}\frac{2Dq^2}{(\omega+i\eta)^2 - (Dq^2)^2}\end{aligned} \tag{42.15}$$

In these expressions we have used that the calculation of $\chi_{0\perp}^{R-+}(\mathbf{q},\omega)$ amounts to changing $\Delta \to -\Delta$ as can be seen by repeating the steps above with up and down spins interchanged. Note also that the last form is that of the propagator for a single boson of frequency Dq^2. There is thus a collective mode at $\omega = \pm Dq^2$.

$$\Im\left(\chi_\perp^{R-+}(\mathbf{q},\omega) + \chi_\perp^{R+-}(\mathbf{q},\omega)\right) = \pi\frac{\Delta}{U}\delta\left(\omega - Dq^2\right) - \pi\frac{\Delta}{U}\delta\left(\omega + Dq^2\right) \tag{42.16}$$

It is thus a propagating mode and here it has a **quadratic dispersion relation**, just like we find in the $1/S$ expansion of ferromagnetic spin models. Stability requires that D be positive, otherwise the condition for positivity of dissipation $\Im\left(\chi_\perp^{R-+}(\mathbf{q},\omega) + \chi_\perp^{R+-}(\mathbf{q},\omega)\right)\omega > 0$ is violated.

42.2 Thermodynamics and the Mermin-Wagner theorem

The thermodynamic transverse susceptibility is obtained from the usual thermodynamic sum rule

$$\begin{aligned}\chi_\perp^{R-+}(\mathbf{q},\omega=0) + \chi_\perp^{R+-}(\mathbf{q},\omega=0) &= \int\frac{d\omega'}{\pi}\frac{\Im\left(\chi_\perp^{R-+}(\mathbf{q},\omega') + \chi_\perp^{R+-}(\mathbf{q},\omega')\right)}{\omega'} \\ &= \pi\frac{\Delta}{U}\int\frac{d\omega'}{\pi}\frac{\delta\left(\omega - Dq^2\right) - \delta\left(\omega + Dq^2\right)}{\omega'} \\ &= \frac{2\Delta}{UD}\frac{1}{q^2}\end{aligned} \tag{42.17}$$

the divergence of the susceptibility is physical. It just means that the orientation of the magnetization can be changed at will. Given

$$\chi_\perp^{-+}(\mathbf{q}, iq_n) = \frac{-\Delta/U}{iq_n - Dq^2} \tag{42.18}$$

we can also find the local susceptibility

$$\begin{aligned}\chi_\perp^{-+}(\mathbf{r}=0,\tau=0^+) &= \left\langle\mathcal{T}S_i^-S_i^+\right\rangle = \langle n_{i\downarrow}\rangle - \langle T_\tau n_{i\downarrow}n_{i\uparrow}\rangle \\ &= T\sum_{iq_n}\frac{1}{N}\sum_{\mathbf{q}}e^{iq_n\eta}\frac{-\Delta/U}{iq_n - Dq^2} \\ &\sim \frac{\Delta}{U}\int\frac{d^dq}{(2\pi)^d}T\sum_{iq_n}\frac{e^{iq_n\eta}}{iq_n - Dq^2} \\ &\sim \frac{\Delta}{U}\int\frac{d^dq}{(2\pi)^d}\frac{1}{e^{\beta Dq^2}-1} \\ &\sim \frac{\Delta}{U}\int\frac{d^dq}{(2\pi)^d}\frac{T}{Dq^2}\end{aligned} \tag{42.19}$$

diverge logarithmically in $d = 2$ and finite T. That is a manifestation of the Mermin-Wagner theorem. If we assume that a continuous symmetry is broken at finite temperature, we find that the thermal fluctuations of the Goldstone modes destroy it.

42.3 Kanamori-Bruckner screening: Why Stoner ferromagnetism has problems

Kanamori and Bruckner tells us that instead of the RPA result, we should really use TPSC and renormalize our Hubbard interaction

$$U_{eff}\left(\mathbf{Q}, iQ_n\right) = \frac{U}{1 + U\Lambda\left(\mathbf{Q}, iQ_n\right)} \tag{42.20}$$

usually Ferromagnetism does not occur unless there is a Van Hove singularity where the density of states $N(\varepsilon_F)$diverges

$$1 - UN(\varepsilon_F) = 0 \tag{42.21}$$

43 Electron-phonon interaction in the Jellium model

BCS theory is based on two important concepts, **Cooper pairs** and **broken U (1) symmetry**. Whatever the superconductor, these two emergent properties are always present. Several mechanisms can lead to the same kind of Cooper pair and associated broken symmetry. The one put forward at the beginning by Bardeen, Cooper and Schrieffer was based on electron-phonon interactions. The fact that the transition temperature dependend on the isotopic content of the material had suggested that phonons were important. So we will first discuss these interactions.

43.1 Hamiltonian and matrix elements for interactions in the jellium model

Up to now we have considered a fixed lattice. If we let the lattice have its own dynamics we need to solve the problem of two interspersed jellium models. It is quite amazing that in the end, if we take into account the heavy mass of the ions, this simple model gives us phonons with a linear dispersion relation at long wavelengths along with a retarded electron-phonon interaction that is attractive at low frequencies. This is the basis for the standard electron-phonon theory of superconductivity. We will see in the following sections and chapters why the normal metal is unstable at low temperature in the presence of an effective attraction between electrons.

We want an expression for an effective potential $U(\mathbf{r})$ that takes into account the Coulomb interaction and the retardation effects. In the jellium model, we consider a system of n electrons per cm^3 of mass m and charge $-e$ and ions of mass M and charge $+Ze$. Charge neuterality imposes n/Z ions per cm^3. We only take electrostatic interactions into account and suppose that the ions form a continuous fluid. That model neglects

1. Short range repulsion effects coming from the Pauli exclusion principle.
2. The fact that wave functions must be orthogonal to those of valence electrons.
3. Transverse phonons.

In this simple model, the effective interaction between electrons takes the form,

$$\frac{e^2}{\varepsilon(\mathbf{q}, \omega)q^2} \tag{43.1}$$

Our objective is to compute the dielectric constant. Clearly, there should not be a frequency in a Hamiltonian. It is preferable to think in terms of perturbation theory where there are energy denominators, or to use an action formalism. The calculation of the dielectric constant is as follows:

Consider the poisson equation

$$\nabla \cdot \mathbf{E} = \frac{1}{\varepsilon_0}\rho \tag{43.2}$$

where ρ is the charge density. Using $\mathbf{E} = -\boldsymbol{\nabla}\phi$, the equation for the scalar potential induced by all deviations from electroneutrality is

$$\nabla^2\phi = -\frac{1}{\varepsilon_0}\left(\delta\left\langle\rho_i\right\rangle + \delta\left\langle\rho_e\right\rangle + \rho_{ext}\right) \tag{43.3}$$

where $\delta\langle\rho_i\rangle$ is the fluctuation in the ion density, $\delta\langle\rho_e\rangle$ is the fluctuation in the electronic density, both induced by the electrostatic potential, and ρ_{ext} is an "external" charge that depends on both space and time. The dielectric constant that we are looking for is defined by

$$\nabla^2\phi = -\frac{1}{\varepsilon}\rho_{ext} \tag{43.4}$$

the dielectric constant can be calculated with irreducible susceptibilities

$$q^2\phi(\mathbf{q},\omega) = \frac{1}{\varepsilon_0}\left(-\chi^{irr,R}_{\rho_i\rho_i}(\mathbf{q},\omega)\phi(\mathbf{q},\omega) - \chi^{irr,R}_{\rho_e\rho_e}(\mathbf{q},\omega)\phi(\mathbf{q},\omega) + \rho_{ext}(\mathbf{q},\omega)\right) \tag{43.5}$$

44 Instability of the normal state in the Schwinger formalism

45 BCS theory

Part VIII
Appendix

46 Fourier Transform

We use convention

$$\begin{aligned} f_{\mathbf{q}} &= \int d^3r f(\mathbf{r})\mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}} \\ f(\mathbf{r}) &= \int \frac{d^3q}{(2\pi)^3} f_{\mathbf{q}}\mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}} \\ g_\omega &= \int dt g(t)e^{i\omega t} \\ g(t) &= \int \frac{d\omega}{2\pi} g_\omega e^{-i\omega t} \end{aligned} \tag{46.1}$$

for continuous Fourier Transform. In this version $\int d^3r = (2\pi)^3$ and volume disappears.
In case we need a finite volume version, we have $\int d^3r = \mathcal{V}$.

$$\begin{aligned} f_{\mathbf{q}} &= \int d^3r f(\mathbf{r})\frac{\mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}}}{\sqrt{V}} \\ f(\mathbf{r}) &= \sum_{\mathbf{q}} \frac{\mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}}{\sqrt{V}} f_{\mathbf{q}} \end{aligned} \tag{46.2}$$

or

$$\begin{aligned} f_{\mathbf{q}} &= \int d^3r f(\mathbf{r})\mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}} \\ f(\mathbf{r}) &= \frac{1}{V}\sum_{\mathbf{q}} \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}} f_{\mathbf{q}} \end{aligned} \tag{46.3}$$

For Translation-symmetric functions, one identity is useful:

$$\int d(\mathbf{r}-\mathbf{r}')e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}f(\mathbf{r}-\mathbf{r}') = \frac{1}{\mathcal{V}}\int d\mathbf{r}e^{-i\mathbf{q}\cdot r}\int d\mathbf{r}'e^{+i\mathbf{q}\cdot r'}f(\mathbf{r}-\mathbf{r}') \tag{46.4}$$

$$\chi_{AB}(\mathbf{r}-\mathbf{r}',t-t') = A(\mathbf{r},t)B(\mathbf{r}',t') \tag{46.5}$$

$$\begin{aligned}\chi_{AB}(\mathbf{q},\omega) &= \int d\mathbf{r}dt e^{i\omega t}e^{-i\mathbf{q}\cdot\mathbf{r}}\chi_{AB}(\mathbf{r}-\mathbf{r}',t-t') \\ &= \int d\mathbf{r}d\mathbf{r}'dtdt' e^{i\omega t}e^{-i\mathbf{q}\cdot\mathbf{r}}e^{i\omega' t'}e^{-i\mathbf{q}'\cdot\mathbf{r}'}\chi_{AB}(\mathbf{r}-\mathbf{r}',t-t') \\ &= \frac{1}{V}\frac{1}{T_p}\int \frac{d\mathbf{q}d\mathbf{q}'}{(2\pi)^6}\frac{d\omega d\omega'}{(2\pi)^2}e^{-i\omega t}e^{i\omega t'}e^{i\mathbf{q}\cdot\mathbf{r}}e^{-i\mathbf{q}\cdot\mathbf{r}'}\chi_{AB}(\mathbf{r}-\mathbf{r}',t-t') \\ &= \frac{1}{V}\frac{1}{T_p}A(\mathbf{q},\omega)B(-\mathbf{q},-\omega)\end{aligned} \tag{46.6}$$

46.1 Convolution Theorem

Two

$$(f*g)(x) = \int_{-\infty}^{\infty} dy f(y)g(x-y) \tag{46.7}$$

Convolution theorem states that

$$\mathcal{F}\{f*g\} = \mathcal{F}\{f\}\cdot\mathcal{F}\{g\} \tag{46.8}$$

for three functions

$$(f*g*h)(x) = \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz f(z)g(y-z)h(x-y) \tag{46.9}$$

$$\mathcal{F}\{f*g*h\} = \mathcal{F}\{f\}\cdot\mathcal{F}\{g\}\cdot\mathcal{F}\{h\} \tag{46.10}$$

This is easy to prove,

$$\begin{aligned}\mathcal{F}\{f*g*h\}(k) &= \int dx e^{-ikx}(f*g*h)(x) \\ &= \int dxdydz e^{-ikx}f(z)g(y-z)h(x-y) \\ &= \int dxdydz e^{-ikx}\int \frac{dk_1}{2\pi}e^{ik_1 z}f_{k_1}\int \frac{dk_2}{2\pi}e^{ik_2(y-z)}g_{k_2}\int \frac{dk_3}{2\pi}e^{ik_3(x-y)}h_{k_3} \\ &= \int \frac{dk_1dk_2dk_3}{(2\pi)^3}f_{k_1}g_{k_2}h_{k_3}\int dxdydz e^{-ikx}e^{ik_1z}e^{ik_2(y-z)}e^{ik_3(x-y)} \\ &= \int dk_1dk_2dk_3 f_{k_1}g_{k_2}h_{k_3}\delta(-k+k_3)\delta(k_2-k_3)\delta(k_1-k_2) \\ &= f_k g_k h_k \\ &= \mathcal{F}\{f\}(k)\cdot\mathcal{F}\{g\}(k)\cdot\mathcal{F}\{h\}(k)\end{aligned} \tag{46.11}$$

similarly for any number of convolutions, we can examine

$$\begin{aligned}e^{-ikx}e^{ik_1z}e^{ik_2(y-z)}e^{ik_3(x-y)} &= e^{-ikx}\left(e^{ik_1z}e^{-ik_2z}\right)\left(e^{ik_2y}e^{-ik_3y}\right)e^{ik_3x} \\ &= \left(e^{ik_1z}e^{-ik_2z}\right)\left(e^{ik_2y}e^{-ik_3y}\right)\left(e^{ik_3x}e^{-ikx}\right)\end{aligned} \tag{46.12}$$

this structure is always guaranteed since in the integral $f(z)g(y-z)h(x-y)$ we have $z-z+y-y+x=0$.

46.2 Fourier Transform in d-dim

We have

$$\int \frac{dq}{2\pi}\frac{e^{iqx}}{q^2+r} = \frac{e^{-x\sqrt{r}}}{2\sqrt{r}} \tag{46.13}$$

First, we have the Fourier Transform of Yukawa Potential

$$\int d^3\mathbf{r}\frac{e^{-\lambda r}}{r}e^{-i\mathbf{k}\cdot\mathbf{r}} = \frac{4\pi q^2}{k^2+\lambda^2} \tag{46.14}$$

in the limit $\lambda\to 0$, we have FT of Coulomb potential

$$\int d^3\mathbf{r}\frac{1}{r}e^{-i\mathbf{k}\cdot\mathbf{r}} = \frac{4\pi}{k^2} \tag{46.15}$$

We will evaluate the inverse Fourier transform in d-dim of a Yukawa potential

$$\begin{aligned}
\Gamma_d(\mathbf{x}) &\equiv \int \frac{d^dq}{(2\pi)^d}\frac{e^{i\mathbf{q}\cdot\mathbf{x}}}{q^2+r} \\
&= \int \frac{d^{d-1}p}{(2\pi)^{d-1}}\int\frac{dq_1}{2\pi}\frac{e^{iq_1x}}{q_1^2+p^2+r} \\
&= \int \frac{d^{d-1}p}{(2\pi)^{d-1}}\frac{e^{-x\sqrt{p^2+r}}}{2\sqrt{p^2+r}} \\
&= \frac{S_{d-2}}{(2\pi)^{d-1}}\int dp\left[p^{d-2}\frac{e^{-x\sqrt{p^2+r}}}{2\sqrt{p^2+r}}\right] \\
&= \frac{S_{d-2}}{2(2\pi)^{d-1}}r^{d/2-1}\int_1^\infty dt\left[(t^2-1)^{(d-3)/2}e^{-x\sqrt{r}t}\right] \\
&= \frac{S_{d-2}}{2(2\pi)^{d-1}}r^{d/2-1}\frac{\Gamma(\frac{d-1}{2})}{\pi^{1/2}(\frac{1}{2}x\sqrt{r})^{d/2-1}}K_{d/2-1}(x\sqrt{r}) \\
&= \frac{(\sqrt{r})^{d-2}}{(2\pi)^{d/2}}\left(\sqrt{r}x\right)^{-d/2+1}K_{d/2-1}(\sqrt{r}x)
\end{aligned} \tag{46.16}$$

where we have used $t=\sqrt{p^2/r+1}$, surface area of sphere $S_{d-1}=\frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})}$ and Modified Bessel function

$$K_\nu(z) = \frac{\pi^{\frac{1}{2}}\left(\frac{1}{2}z\right)^\nu}{\Gamma\left(\nu+\frac{1}{2}\right)}\int_1^\infty \mathrm{e}^{-zt}\left(t^2-1\right)^{\nu-\frac{1}{2}}\ \mathrm{d}t \tag{46.17}$$

for $z\to\infty$, $K_\nu(z)\to z^{-1/2}e^{-z}$.
In $d=3$ especially, we have

$$\begin{aligned}
\Gamma_3(\mathbf{x}) &= \frac{(\sqrt{r})}{(2\pi)^{3/2}}\left(\sqrt{r}x\right)^{-1/2}K_{1/2}(\sqrt{r}x) \\
&= \frac{e^{-\sqrt{r}x}}{4\pi x}
\end{aligned} \tag{46.18}$$

for a general $d=3$ spherical function, the Fourier Transform is

$$\begin{aligned}
f(\mathbf{x}) &\equiv \int\frac{d^3q}{(2\pi)^3}e^{i\mathbf{q}\cdot\mathbf{x}}f(q) \\
&= \frac{1}{(2\pi)^2}\int_0^\infty dqq^2f(q)\int_{-1}^{+1}d\cos\theta e^{iqx\cos\theta} \\
&= \frac{1}{2\pi^2}\times\frac{1}{x}\int_0^\infty dq\left[f(q)q\sin(qx)\right]
\end{aligned} \tag{46.19}$$

46.3 Consistency of Fourier Transform

Fourier Transform can take many forms, here we develop a general method to treat different types of Fourier Transforms. We shall not put the real space and momentum space at the same footing, but instead treat all functions of real space as "functions", and functions of k-space as "components".

We will first define an inner produce $(\cdot,\cdot)$ is

$$(f,g) = \int_x f^*(x)g(x) \tag{46.20}$$

then define a set of basis functions $\{\phi_q\}$, which are nor necessarily normalized:

$$(\phi_p,\phi_q) = \mathcal{V}\delta_{pq} \tag{46.21}$$

we then have

$$f = \sum_q \frac{(\phi_q, f)}{(\phi_q, \phi_q)} \phi_q = \frac{1}{\mathcal{V}} \sum_q (\phi_q, f) \phi_q \tag{46.22}$$

we can therefore define

$$\begin{aligned} f &= \frac{1}{\mathcal{V}} \sum_q f_q \phi_q \\ f_q &= (\phi_q, f) \end{aligned} \tag{46.23}$$

alternatively, we can define

$$\begin{aligned} f &= \sum_q f_q \phi_q \\ f_q &= \frac{1}{\mathcal{V}} (\phi_q, f) \end{aligned} \tag{46.24}$$

so there has to be a factor of $1/\mathcal{V}$ in either Fourier Transform or inverse Fourier Transform.

46.3.1 Continuous spatial transform

Take the $(\mathbf{r}, \mathbf{q})$ pair of Fourier Transform

$$\begin{aligned} f_{\mathbf{q}} &= \int d^3 r f(\mathbf{r}) \mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}} \\ f(\mathbf{r}) &= \int \frac{d^3 q}{(2\pi)^3} f_{\mathbf{q}} \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}} \end{aligned} \tag{46.25}$$

to check the validity, we only need to identify $\phi_{\mathbf{q}}(\mathbf{r}) = \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}$ and notice

$$(\phi_{\mathbf{p}}, \phi_{\mathbf{q}}) = \int d^3 r \mathbf{e}^{-i(\mathbf{p}-\mathbf{q})\cdot\mathbf{r}} = (2\pi)^3 \delta(\mathbf{p} - \mathbf{q}) \tag{46.26}$$

so $\mathcal{V} = (2\pi)^3$, and the validity is checked. We have found the F.T. pairs

$$\int d^3 r \leftrightarrow \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \tag{46.27}$$

46.3.2 Discrete spatial transform

Suppose we take another expansion

$$f(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{q}} f_{\mathbf{q}} \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}} \tag{46.28}$$

similarly we set $\phi_{\mathbf{q}}(\mathbf{r}) = \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}$, but now

$$(\phi_{\mathbf{p}}, \phi_{\mathbf{q}}) = \int d^3 r \mathbf{e}^{-i(\mathbf{p}-\mathbf{q})\cdot\mathbf{r}} = V \delta_{\mathbf{p}-\mathbf{q}} \tag{46.29}$$

so we have

$$f_{\mathbf{q}} = (\phi_{\mathbf{q}}, f) = \int d^3 r \mathbf{e}^{-i\mathbf{q}\cdot\mathbf{r}} f(\mathbf{r}) \tag{46.30}$$

we have F.T. pairs

$$\int d^3 r \leftrightarrow \frac{1}{V} \sum_{\mathbf{q}} \tag{46.31}$$

46.3.3 Fourier Transform with spatial PBC

Suppose $f(\mathbf{r})$ satisfy lattice translational symmetry $f(\mathbf{r}+\mathbf{R}) = f(\mathbf{r})$ for lattice vectors $\{\mathbf{R}\}$, suppose we make the following expansion

$$f(\mathbf{r}) = \frac{1}{\Omega}\sum_{\mathbf{G}\in\Lambda^{-1}} f_{\mathbf{G}}\mathbf{e}^{i\mathbf{G}\cdot\mathbf{r}} \tag{46.32}$$

where $\phi_{\mathbf{G}}(\mathbf{r}) = \mathbf{e}^{i\mathbf{G}\cdot\mathbf{r}}$ admit the same lattice symmetry, as can be checked by $\phi_{\mathbf{G}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{G}\cdot\mathbf{R}}\phi_{\mathbf{G}}(\mathbf{r}) = \phi_{\mathbf{G}}(\mathbf{r})$. We have also defined the reciprocal space Λ^{-1}. The inner product is now defined as

$$(f,g) = \int_{\text{unit cell}} d^3\mathbf{r} f^*(x)g(x) \tag{46.33}$$

for the basis, we have

$$(\phi_{\mathbf{G}_1},\phi_{\mathbf{G_2}}) = \int_{\text{unit cell}} d^3r\mathbf{e}^{-i(\mathbf{G}_1-\mathbf{G}_2)\cdot\mathbf{r}} = \Omega\delta_{\mathbf{G}_1,\mathbf{G}_2} \tag{46.34}$$

where Ω is the volume of unit cell. We can use this to define

$$f_{\mathbf{G}} \equiv (\phi_{\mathbf{G}},f) = \int_{\text{unit cell}} d^3re^{-i\mathbf{G}\cdot\mathbf{r}}f(\mathbf{r}) \tag{46.35}$$

we have

$$\int_{\text{unit cell}} d^3r \leftrightarrow \frac{1}{\Omega}\sum_{\mathbf{G}\in\Lambda^{-1}} \tag{46.36}$$

46.3.4 Lattice Fourier Transform

Suppose $f(\mathbf{R})$ take as argument only discrete lattice points $\{\mathbf{R}\}$, $\mathbf{R} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3$, suppose also that there are N points in total with N very large, we can expand $f(\mathbf{R})$ as

$$f(\mathbf{R}) = \frac{1}{N}\sum_{\mathbf{q}\in 1^{st}BZ} f_{\mathbf{q}}\mathbf{e}^{i\mathbf{q}\cdot\mathbf{R}} \tag{46.37}$$

where $\phi_{\mathbf{q}}(\mathbf{R}) = \mathbf{e}^{i\mathbf{q}\cdot\mathbf{R}}$. Notice that $\phi_{\mathbf{q}+\mathbf{G}}(\mathbf{R}) = \phi_{\mathbf{q}}(\mathbf{R})$, so we need only $\mathbf{q}\in 1^{st}BZ$.

$$(f,g) = \sum_{\mathbf{R}} f^*(\mathbf{R})g(\mathbf{R}) \tag{46.38}$$

$$(\phi_{\mathbf{p}},\phi_{\mathbf{q}}) = \sum_{\mathbf{R}} \mathbf{e}^{-i(\mathbf{p}-\mathbf{q})\cdot\mathbf{R}} = N\delta_{\mathbf{p},\mathbf{q}} \tag{46.39}$$

$$f_{\mathbf{q}} \equiv (\phi_{\mathbf{q}},f) = \sum_{\mathbf{R}} e^{-i\mathbf{q}\cdot\mathbf{r}}f(\mathbf{R}) \tag{46.40}$$

we have

$$\sum_{\mathbf{R}} \leftrightarrow \frac{1}{N}\sum_{\mathbf{q}\in 1^{st}BZ} \tag{46.41}$$

46.3.5 Four-momentum Fourier Transform

Suppose we have, with $x = (\mathbf{x},\tau)$, $q = (\mathbf{q}, iq_n)$ with inner product

$$(f,q) = \int dx f(x)g(x) = \int d\mathbf{x}\int_0^\beta d\tau f(x)g(x) \tag{46.42}$$

take $\phi_q(x) \equiv e^{iqx} = e^{i\mathbf{q}\cdot\mathbf{x}}e^{-iq_n\tau}$, we have

$$\begin{aligned}(\phi_p,\phi_q) &= \int dx e^{-i(p-q)x} = \int d\mathbf{x}\int_0^\beta d\tau e^{-i(\mathbf{p}-\mathbf{q})\cdot\mathbf{x}}e^{i(p_n-q_n)\tau} \\ &= (2\pi)^3\delta(\mathbf{p}-\mathbf{q})\beta\delta_{p_nq_n}\end{aligned} \tag{46.43}$$

so $\mathcal{V} = (2\pi)^3\beta$, we have

$$f(x) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} T \sum_{iq_n} f_q e^{i\mathbf{q}\cdot\mathbf{x}} e^{-iq_n\tau} \tag{46.44}$$

$$f_q = \int d^3\mathbf{x} \int_0^\beta d\tau e^{-i\mathbf{q}\cdot\mathbf{x}} e^{iq_n\tau} f(x) \tag{46.45}$$

we have the F.T. pairs

$$\int d\mathbf{x} \int_0^\beta d\tau \leftrightarrow \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{ik_n} \tag{46.46}$$

46.4 Matsubare Fourier Transform

We usually adopt the following conventions

$$\begin{aligned}
\int_1 &\equiv \int d\mathbf{x}_1 \int_0^\beta d\tau_1 \\
\sum_k &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{ik_n} \\
k &= (\mathbf{k}, -ik_n)\,, \quad \text{fermionic} \\
q &= (\mathbf{q}, -iq_n)\,, \quad \text{bosonic} \\
x &= (\mathbf{x}, \tau) \\
\delta(q) &= (2\pi)^3 \delta(\mathbf{q}) \beta \delta_{q_n} \\
\delta(x) &= \delta(\mathbf{x})\delta(\tau) \\
\frac{1}{V}\sum_{\mathbf{k}} &\leftrightarrow \int \frac{d^3\mathbf{k}}{(2\pi)^3}, \quad \text{discrete-to-continuous} \\
e^{-ikx} &= e^{-i\mathbf{k}\cdot\mathbf{x}} e^{ik_n\tau}
\end{aligned} \tag{46.47}$$

$$\begin{aligned}
\mathcal{F} &= \int_x e^{-ikx} \\
\mathcal{F}^{-1} &= \sum_k e^{ikx} \\
\mathcal{G}(x) &= \sum_k e^{ikx} \mathcal{G}(k) \\
\mathcal{G}(\mathbf{r},\tau) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} T \sum_{ik_n} e^{i\mathbf{k}\cdot\mathbf{x}} e^{-ik_n\tau} \mathcal{G}(\mathbf{k}, ik_n)
\end{aligned} \tag{46.48}$$

$$\begin{aligned}
\mathcal{G}(k) &= \int_x e^{-ikx} \mathcal{G}(x) \\
\mathcal{G}(\mathbf{k}, ik_n) &= \int d\mathbf{x}_1 \int_0^\beta d\tau_1 e^{-i\mathbf{k}\cdot\mathbf{x}} e^{ik_n\tau} \mathcal{G}(\mathbf{r},\tau)
\end{aligned} \tag{46.49}$$

47 Peierls Substitution

Suppose we have tight-binding bands of atomic or Wannier orbitals. That problem arises for example when we focus on a few correlated bands near the Fermi level. It is in general necessary to go a localized basis where short-range interactions, Hubbard or Hund's for example, are easiest to write. In this Chapter, I try to answer the question: How do I write the interaction with the electromagnetic field when we take into account only a finite number of bands?

In the presence of the electromagnetic field, we still have the usual intra-atomic transitions, say electric-dipole transitions. But there are extra contributions coming from hopping between atoms. We know, for example, that the vector potential for a uniform electric field couples to the uniform current operator. There is a contribution to that current that is just the gradient of the dispersion relation $\boldsymbol{\nabla}_{\mathbf{k}}\varepsilon_{\mathbf{k}}$. The gauge-invariant current also has an

additional term. In linear response, this later contribution gave the diamagnetic term that depended inversely on the mass. So, intuitively, we expect that the velocity and inverse mass tensor must come in. To derive everything in the most general way with a finite basis in a tight-binding model, our best guide is gauge invariance. In fact, without gauge invariance as a guide, we may be inclined to think that if there are several bands labeled by n then the current operator is $\boldsymbol{\nabla}_{\mathbf{k}}\varepsilon_{\mathbf{k}n}$. This is incorrect for general response functions, as I will show. So, here we go.

Under a guage transformation, one-particle wavefunctions transform as

$$\psi(\mathbf{r},t) \to e^{ie\Lambda(\mathbf{r},t)}\psi(\mathbf{r},t) \tag{47.1}$$

or, in Dirac notation

$$\langle \mathbf{r} \mid \psi(t)\rangle \to e^{ie\Lambda(\mathbf{r},t)}\langle \mathbf{r} \mid \psi(t)\rangle \tag{47.2}$$

we can write it as

$$\left\langle \mathbf{r} \mid e^{-iHt}|\psi\right\rangle \to \langle \mathbf{r} \mid e^{ie\Lambda(\mathbf{r},t)}e^{-iHt}|\psi(t)\rangle \tag{47.3}$$

this provides an alternative transformation, we can fix $|\psi\rangle$ and transform $|\mathbf{r}\rangle$:

$$e^{iHt}\,|\mathbf{r}\rangle \to e^{-ie\Lambda(\mathbf{r},t)}e^{iHt}\,|\mathbf{r}\rangle \tag{47.4}$$

we can write it as

$$\psi^\dagger(\mathbf{r},t)e^{iHt}\,|0\rangle \to e^{-ie\Lambda(\mathbf{r},t)}\psi^\dagger(\mathbf{r},t)e^{iHt}\,|0\rangle \tag{47.5}$$

this tells us how to transform the field operators in Heisenberg picture

$$\begin{aligned}\psi^\dagger(\mathbf{r},t) &\to e^{-ie\Lambda(\mathbf{r},t)}\psi^\dagger(\mathbf{r},t)\\ \psi(\mathbf{r},t) &\to e^{ie\Lambda(\mathbf{r},t)}\psi(\mathbf{r},t)\end{aligned} \tag{47.6}$$

Suppose that $\psi(\mathbf{r},t)$ is expanded in a finite set of Wannier orbitals (or some other local orbitals) as

$$\psi(\mathbf{r},t) = \sum_{n\mathbf{R}_i+\mathbf{r}_\mu} w_n(\mathbf{r}-\mathbf{R}_i-\mathbf{r}_\mu)c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t) \tag{47.7}$$

where n is a band index in the simplest case, or more generally an orbital index (Recall the ambiguity in the definition of the Wannier functions). Here I have generalized the Wannier expansion by allowing **several atoms** that are located at position $\mathbf{r}_\mu$ with respect to the unit cell that is itself located at $\mathbf{R}_i$. Under a gauge transformation, we already know $\psi(\mathbf{r},t)$ will generate a factor $e^{ie\Lambda(\mathbf{r},t)}$. On the RHS, both $w_n(\mathbf{r}-\mathbf{R}_i-\mathbf{r}_\mu)$ and $c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t)$ are position-dependent, so both of them should transform in order to give the same factor $e^{ie\Lambda(\mathbf{r},t)}$, we already know how a wavefunction transforms

$$w_n(\mathbf{r}-\mathbf{R}_i-\mathbf{r}_\mu) \to e^{ie\Lambda(\mathbf{r}-\mathbf{R}_i-\mathbf{r}_\mu,t)}w_n(\mathbf{r}-\mathbf{R}_i-\mathbf{r}_\mu) \tag{47.8}$$

therefore, we must have

$$c'_{n\mathbf{R}_i+\mathbf{r}_\mu}(t) = e^{ie\Lambda(\mathbf{R}_i+\mathbf{r}_\mu,t)}c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t) \tag{47.9}$$

such that the right handside

$$\begin{aligned}RHS \to &\sum_{n\mathbf{R}_i+\mathbf{r}_\mu} w_n(\mathbf{r}-\mathbf{R}_i-\mathbf{r}_\mu)e^{ie\Lambda(\mathbf{r}-\mathbf{R}_i-\mathbf{r}_\mu,t)}e^{ie\Lambda(\mathbf{R}_i+\mathbf{r}_\mu,t)}c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t)\\ &= e^{ie\Lambda(\mathbf{r},t)}RHS\end{aligned} \tag{47.10}$$

and analogously for the creation operators. The finite basis means that for hopping between different atoms, we do not have arbitrary spatial resolution since our basis is finite. So we have no choice but to consider only electromagnetic fields that vary on a scale that is larger than the inter-atomic distance. In all the usual condensed-matter experiments, this is the case.

Since gauge transformation is only position-dependent, the local interaction term in Hubbard model is automatically gauge-invariant. The kinetic term, on the other hand, generate a factor

$$c^\dagger_{m\mathbf{R}_j+\mathbf{r}_\nu}(t)c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t) \to e^{-ie[\Lambda(\mathbf{R}_j+\mathbf{r}_\nu,t)-\Lambda(\mathbf{R}_i+\mathbf{r}_\mu,t)]}c^\dagger_{m\mathbf{R}_j+\mathbf{r}_\nu}(t)c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t) \tag{47.11}$$

the kinetic term must be modified to cancel exactly this factor, the right factor to include is

$$e^{ie\int_{\mathbf{R}_i+\mathbf{r}_\mu}^{\mathbf{R}_j+\mathbf{r}_\nu}\mathbf{A}(\mathbf{r},t)\cdot d\mathbf{r}}c^\dagger_{m\mathbf{R}_j+\mathbf{r}_\nu}(t)c_{n\mathbf{R}_i+\mathbf{r}_\mu}(t) \tag{47.12}$$

which generates exactly the inverse factor under $\mathbf{A}\to\mathbf{A}+\nabla\Lambda$. The above assumes that the integral is taken along the straight line connecting $\mathbf{R}_i+\mathbf{r}_\mu$ and $\mathbf{R}_j+\mathbf{r}_\nu$ and that $\mathbf{A}(\mathbf{r},t)$ does not vary much over the path of integration, or that it can be replaced by its value in the mid point. In other words, the phase in the above exponential is

$$e\int_{\mathbf{R}_i+\mathbf{r}_\mu}^{\mathbf{R}_j+\mathbf{r}_\nu}\mathbf{A}(\mathbf{r},t)\cdot d\mathbf{r}=\mathbf{A}\left(\frac{\mathbf{R}_j+\mathbf{r}_\nu+\mathbf{R}_i+\mathbf{r}_\mu}{2}\right)\cdot(\mathbf{R}_j+\mathbf{r}_\nu-\mathbf{R}_i-\mathbf{r}_\mu) \tag{47.13}$$

The effect of the magnetic induction will come from the part of the vector potential that cannot be represented by a gradient. The flux of this field thus depends on the path chosen to go from one site to the other.

The current operator on the lattice is obtained from

$$\mathbf{j}=-\frac{\delta H}{\delta\mathbf{A}} \tag{47.14}$$

48 Second Quantization

Given a one-particle operator in $\mathcal{F}^N$, we can promote it to the second quantized form:

$$\hat{O}_1=\sum_{n=1}^N\hat{o}_n\to\sum_{\mu\nu}\langle\mu|\,\hat{o}\,|\nu\rangle\,a^\dagger_\mu a_\nu \tag{48.1}$$

where $\hat{o}_n$ acts on the nth particle coordinates $\mathbf{r}_n$ only. $\hat{o}$ acts on $\mathbf{r}$. $\{|\mu\rangle\}$ is a basis in the configuration space.

Given a two-particle operator in $\mathcal{F}^N$, similarly

$$\hat{O}_2=\sum_{n,m}^N\hat{o}_{n,m}\to\sum_{\mu\nu'\lambda\lambda'}\langle\mu,\mu'|\,\hat{o}\,|\lambda,\lambda'\rangle\,a^\dagger_\mu a^\dagger_{\mu'}a_{\lambda'}a_\lambda \tag{48.2}$$

notice that here the convention for turning a ket into bra is $|\mu,\mu'\rangle\to\langle\mu,\mu'|$.

48.1 Field operator representation

If we choose the basis $|\mathbf{r}\rangle$ in the configuration space, we have

$$\hat{O}_1=\sum_{n=1}^N\hat{o}(\mathbf{r}_n)\to\sum_{\sigma,\sigma'}\int d^3\mathbf{r}d^3\mathbf{r}'\hat{o}(\mathbf{r}')\,\langle\mathbf{r}'\sigma'|\,\mathbf{r}\sigma\rangle\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \tag{48.3}$$

notice that $\hat{o}(\mathbf{r}_n)$ includes $\frac{\partial}{\partial\mathbf{r}_n}$ and spin of nth particle.

$$\hat{O}_2=\sum_{n,m}^N\hat{o}(\mathbf{r}_n,\mathbf{r}_m)\to\sum_{\sigma,\sigma',\sigma'',\sigma'''}\int d^3\mathbf{r}d^3\mathbf{r}'d^3\mathbf{r}''d^3\mathbf{r}'''\hat{o}(\mathbf{r}',\mathbf{r}')\,\langle\mathbf{r}\sigma,\mathbf{r}'\sigma'|\,\mathbf{r}''\sigma'',\mathbf{r}'''\sigma'''\rangle\psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_{\sigma'''}(\mathbf{r}'')\psi_{\sigma''}(\mathbf{r}''') \tag{48.4}$$

48.2 Examples

Before we go into the calculation, notice that $\langle\mathbf{r}|\,\mathbf{p}\,|\psi\rangle=-i\nabla\,\langle\mathbf{r}|\,\psi\rangle$, so when we pull out momentum operators, they act on the left bracket. Therefore, for brevity we will write $\langle\mathbf{r}|\,\nabla\,|\psi\rangle=\nabla\,\langle\mathbf{r}|\,\psi\rangle$. In particular, $\langle\mathbf{r}|\,\nabla\,|\mathbf{r}'\rangle=\nabla\,\langle\mathbf{r}|\,\mathbf{r}'\rangle$ acts on the left. For ∇^2 it doesn't matter where we put it, since $\langle\mathbf{r}|\,\nabla^2\,|\mathbf{r}'\rangle=\nabla^2\delta(\mathbf{r}-\mathbf{r}')=\nabla'^2\delta(\mathbf{r}-\mathbf{r}')$.

$$\begin{aligned}
\rho(\mathbf{r}) = \sum_{n=1}^{N} \delta(\hat{\mathbf{r}}_n - \mathbf{r}) &\to \sum_{\sigma,\sigma'} \int d^3\mathbf{r}'' d^3\mathbf{r}' \left\langle \mathbf{r}'\sigma' \right| \delta(\mathbf{r}'' - \mathbf{r}) \left| \mathbf{r}''\sigma \right\rangle \psi^\dagger_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}'') \\
&= \sum_{\sigma} \int d^3\mathbf{r}'' d^3\mathbf{r}' \left\langle \mathbf{r}' \right| \delta(\mathbf{r}'' - \mathbf{r}) \left| \mathbf{r}'' \right\rangle \psi^\dagger_{\sigma}(\mathbf{r}')\psi_\sigma(\mathbf{r}'') \\
&= \sum_{\sigma} \int d^3\mathbf{r}'' d^3\mathbf{r}' \delta(\mathbf{r}'' - \mathbf{r})\delta(\mathbf{r}'' - \mathbf{r}')\psi^\dagger_{\sigma}(\mathbf{r}')\psi_\sigma(\mathbf{r}'') \\
&= \sum_{\sigma} \psi^\dagger_{\sigma}(\mathbf{r})\psi_\sigma(\mathbf{r})
\end{aligned} \tag{48.5}$$

$$\begin{aligned}
\mathbf{P}(\mathbf{r}) = \sum_{n=1}^{N} -i\nabla_n &\to \sum_{\sigma,\sigma'} \int d^3\mathbf{r} d^3\mathbf{r}' \left\langle \mathbf{r}'\sigma' \right| -i\nabla' \left| \mathbf{r}\sigma \right\rangle \psi^\dagger_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \\
&= \sum_{\sigma} \int d^3\mathbf{r} d^3\mathbf{r}' \left(-i\nabla'\right) \delta(\mathbf{r} - \mathbf{r}')\psi^\dagger_{\sigma}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \\
&= \sum_{\sigma} \int d^3\mathbf{r} d^3\mathbf{r}' \left(i\nabla\right) \delta(\mathbf{r} - \mathbf{r}')\psi^\dagger_{\sigma}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \\
&= \sum_{\sigma} \int d^3\mathbf{r} \psi^\dagger_{\sigma}(\mathbf{r}) \left(-i\nabla\right) \psi_\sigma(\mathbf{r})
\end{aligned} \tag{48.6}$$

$$\begin{aligned}
H_0 = \sum_{n=1}^{N} \left(\frac{-\nabla_n^2}{2m} + V(\mathbf{r}_n) \right) &\to \sum_{\sigma} \int d^3\mathbf{r} d^3\mathbf{r}' \left\langle \mathbf{r}' \right| \frac{-\nabla'^2}{2m} + V(\mathbf{r}') \left| \mathbf{r} \right\rangle \psi^\dagger_{\sigma}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \\
&= \sum_{\sigma} \int d^3\mathbf{r} d^3\mathbf{r}' \left(\frac{-\nabla'^2}{2m} + V(\mathbf{r}') \right) \delta(\mathbf{r} - \mathbf{r}')\psi^\dagger_{\sigma}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \\
&= \sum_{\sigma} \int d^3\mathbf{r} d^3\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}')\psi^\dagger_{\sigma}(\mathbf{r}') \left(\frac{-\nabla^2}{2m} + V(\mathbf{r}) \right) \psi_\sigma(\mathbf{r}) \\
&= \sum_{\sigma} \int d^3\mathbf{r} \psi^\dagger_{\sigma}(\mathbf{r}) \left(\frac{-\nabla^2}{2m} + V(\mathbf{r}) \right) \psi_\sigma(\mathbf{r})
\end{aligned} \tag{48.7}$$

$$\begin{aligned}
\hat{\mathbf{S}} = \sum_{n=1}^{N} \hat{\mathbf{S}}_n &\to \sum_{\sigma,\sigma'} \int d^3\mathbf{r} d^3\mathbf{r}' \left\langle \mathbf{r}'\sigma' \right| \hat{\mathbf{S}} \left| \mathbf{r}\sigma \right\rangle \psi^\dagger_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \\
&= \int d^3\mathbf{r} \sum_{\sigma,\sigma'} \mathbf{S}_{\sigma'\sigma} \psi^\dagger_{\sigma'}(\mathbf{r})\psi_\sigma(\mathbf{r})
\end{aligned} \tag{48.8}$$

where $\left(S^i\right)_{\alpha\alpha'} = \frac{1}{2}\left(\sigma^i\right)_{\alpha\alpha'}$.

$$\begin{aligned}
\mathbf{J}(\mathbf{x}) &= \frac{1}{2} \sum_{n=1}^{N} \left[\mathbf{v}_n \delta(\mathbf{x} - \mathbf{r}_n) + \delta(\mathbf{x} - \mathbf{r}_n)\mathbf{v}_n \right] \\
&= \frac{1}{2m} \sum_{n=1}^{N} \left[\mathbf{p}_n \delta(\mathbf{x} - \mathbf{r}_n) + \delta(\mathbf{x} - \mathbf{r}_n)\mathbf{p}_n \right] \\
&\to \frac{1}{2m} \sum_{\sigma,\sigma'} \int d^3\mathbf{r} d^3\mathbf{r}' \left((-i\nabla')\delta(\mathbf{x} - \mathbf{r}') + \delta(\mathbf{x} - \mathbf{r}')(-i\nabla') \right) \left\langle \mathbf{r}'\sigma' \right| \mathbf{r}\sigma \rangle \psi^\dagger_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}) \\
&= \frac{1}{2m} \sum_{\sigma} \int d^3\mathbf{r} d^3\mathbf{r}' \left(\delta(\mathbf{x} - \mathbf{r}')\delta(\mathbf{r} - \mathbf{r}')(i\nabla')\psi^\dagger_{\sigma}(\mathbf{r}')\psi_\sigma(\mathbf{r}) + \delta(\mathbf{x} - \mathbf{r}')\delta(\mathbf{r} - \mathbf{r}')\psi^\dagger_{\sigma}(\mathbf{r}')(-i\nabla)\psi_\sigma(\mathbf{r}) \right) \\
&= \frac{1}{2mi} \left(\psi^\dagger_{\sigma}(\mathbf{x})\nabla\psi_\sigma(\mathbf{x}) - \psi_\sigma(\mathbf{x})\nabla\psi^\dagger_{\sigma}(\mathbf{x}) \right)
\end{aligned} \tag{48.9}$$

$$
\begin{aligned}
V &= \frac{1}{2}\sum_{n,m=1}^{N} V(\mathbf{r}_n,\mathbf{r}_m) \\
&\to \frac{1}{2}\sum_{\sigma,\sigma',\sigma'',\sigma'''}\int d^3\mathbf{r}d^3\mathbf{r}'d^3\mathbf{r}''d^3\mathbf{r}''' \left\langle \mathbf{r}\sigma,\mathbf{r}'\sigma'\right| V(\mathbf{r}'',\mathbf{r}''') \left|\mathbf{r}''\sigma'',\mathbf{r}'''\sigma'''\right\rangle \psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_{\sigma'''}(\mathbf{r}''')\psi_{\sigma''}(\mathbf{r}'') \\
&= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3\mathbf{r}d^3\mathbf{r}'d^3\mathbf{r}''d^3\mathbf{r}''' \left\langle \mathbf{r},\mathbf{r}'\right| V(\mathbf{r}'',\mathbf{r}''') \left|\mathbf{r}'',\mathbf{r}'''\right\rangle \psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_{\sigma'}(\mathbf{r}''')\psi_{\sigma}(\mathbf{r}'') \\
&= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3\mathbf{r}d^3\mathbf{r}'d^3\mathbf{r}''d^3\mathbf{r}'''V(\mathbf{r}'',\mathbf{r}''')\delta(\mathbf{r}-\mathbf{r}'')\delta(\mathbf{r}'-\mathbf{r}''')\psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_{\sigma'}(\mathbf{r}''')\psi_{\sigma}(\mathbf{r}'') \\
&= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3\mathbf{r}d^3\mathbf{r}'V(\mathbf{r},\mathbf{r}')\psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_{\sigma'}(\mathbf{r}')\psi_{\sigma}(\mathbf{r})
\end{aligned}
\tag{48.10}
$$

$$
\begin{aligned}
H_{Ising} &= \sum_{n,m=1}^{N} J(\mathbf{r}_n,\mathbf{r}_m)\mathbf{S}_n\cdot\mathbf{S}_m \\
&\to \sum_{\sigma,\sigma',\sigma'',\sigma'''}\int d^3\mathbf{r}d^3\mathbf{r}'d^3\mathbf{r}''d^3\mathbf{r}''' \left\langle \mathbf{r}\sigma,\mathbf{r}'\sigma'\right| J(\mathbf{r}'',\mathbf{r}''')\mathbf{S}_{\prime\prime}\cdot\mathbf{S}_{\prime\prime\prime} \left|\mathbf{r}''\sigma'',\mathbf{r}'''\sigma'''\right\rangle \psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_{\sigma'''}(\mathbf{r}''')\psi_{\sigma''}(\mathbf{r}'') \\
&= \sum_{\sigma,\sigma',\sigma'',\sigma'''}\int d^3\mathbf{r}d^3\mathbf{r}'d^3\mathbf{r}''d^3\mathbf{r}'''J(\mathbf{r}'',\mathbf{r}''')\delta(\mathbf{r}-\mathbf{r}'')\delta(\mathbf{r}'-\mathbf{r}''') \left\langle \sigma,\sigma'\right| \mathbf{S}_{\prime\prime}\cdot\mathbf{S}_{\prime\prime\prime} \left|\sigma'',\sigma'''\right\rangle \psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_{\sigma'''}(\mathbf{r}''')\psi_{\sigma''}(\mathbf{r}'') \\
&= \sum_{\sigma,\sigma',\sigma'',\sigma'''}\int d^3\mathbf{r}d^3\mathbf{r}'J(\mathbf{r},\mathbf{r}') \left\langle \sigma,\sigma'\right| \mathbf{S}_{\prime\prime}\cdot\mathbf{S}_{\prime\prime\prime} \left|\sigma'',\sigma'''\right\rangle \psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_{\sigma'''}(\mathbf{r}')\psi_{\sigma''}(\mathbf{r}) \\
&= \sum_{\sigma,\sigma',\sigma'',\sigma'''}\int d^3\mathbf{r}d^3\mathbf{r}'J(\mathbf{r},\mathbf{r}') \left(\mathbf{S}_{\sigma\sigma''}\cdot\mathbf{S}_{\sigma'\sigma'''}\right) \psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}')\psi_{\sigma'''}(\mathbf{r}')\psi_{\sigma''}(\mathbf{r})
\end{aligned}
\tag{48.11}
$$

48.3 Coordinate Transformations

Suppose we have basis $\{|\lambda\rangle\}$ and $\{|\lambda'\rangle\}$ in the configuration space,

$$
\left|\tilde{\lambda}\right\rangle = \sum_{\lambda} |\lambda\rangle \langle\lambda|\,\tilde{\lambda}\rangle \tag{48.12}
$$

we can directly promote this to the second quantized creation operator transformation

$$
a^\dagger_{\tilde{\lambda}} = \sum_{\lambda} a^\dagger_\lambda \langle\lambda|\,\tilde{\lambda}\rangle \tag{48.13}
$$

acoordingly, we can dagger both sides

$$
a_{\tilde{\lambda}} = \sum_{\lambda} a_\lambda \left\langle\tilde{\lambda}\right|\lambda\rangle \tag{48.14}
$$

as an example, we have

$$
|\mathbf{p}\rangle = \int d^3x \langle\mathbf{r}|\mathbf{p}\rangle |\mathbf{r}\rangle = \int d^3x \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}} |\mathbf{r}\rangle \tag{48.15}
$$

where we have chosen the convention

$$
\langle\mathbf{r}|\mathbf{p}\rangle \equiv \frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}} \tag{48.16}
$$

and $|\mathbf{p}\rangle$ is normalized. We then have

$$
\begin{aligned}
a^\dagger_{\mathbf{p}} &= \int d^3r \frac{e^{+i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}}\psi^\dagger(\mathbf{r}) \qquad & \psi^\dagger(\mathbf{r}) &= \sum_{\mathbf{p}} \frac{e^{-i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}} a^\dagger_{\mathbf{p}} \\
a_{\mathbf{p}} &= \int d^3r \frac{e^{-i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}}\psi(\mathbf{r}) & \psi(\mathbf{r}) &= \sum_{\mathbf{p}} \frac{e^{+i\mathbf{p}\cdot\mathbf{r}}}{\sqrt{V}} a_{\mathbf{p}}
\end{aligned}
\tag{48.17}
$$

48.4 Commutation relations

$$[a_i, a_j^\dagger]_\zeta = \delta_{ij}, \quad [a_i, a_j]_\zeta = [a_i^\dagger, a_j^\dagger]_\zeta = 0 \tag{48.18}$$

where $\zeta = \pm 1$ for boson/fermion operators, and $[]_+ = []$, $[]_- = \{\}$.

49 BCH formula

Define iterated commutator

$$[^n X, Y] \equiv \underbrace{[X, \cdots [X, [X}_{n \text{ times}}, Y]] \cdots] \tag{49.1}$$

we have identity

$$\begin{aligned} e^X Y e^{-X} &= e^{[X}, Y] \\ &= \sum_{n=0}^{\infty} \frac{[^n X, Y]}{n!} \end{aligned} \tag{49.2}$$

Suppose we have and "eigenvalue relation"

$$[X, Y] = xY \tag{49.3}$$

then the iterated commutator is simple

$$[^n X, Y] = x^n Y \tag{49.4}$$

and

$$e^X Y e^{-X} = \sum_{n=0}^{\infty} \frac{x^n}{n!} Y = e^x Y \tag{49.5}$$

Example Suppose

$$H = \sum_k \omega_k a_k^\dagger a_k \tag{49.6}$$

and we wish to evaluate $e^{iHt} a_p e^{-iHt}$, now notice

$$[iHt, a_p] = (-it\omega_p)\, a_p \tag{49.7}$$

therefore $x = -it\omega_p$, and we have the answer directly

$$e^{iHt} a_p e^{-iHt} = e^{-it\omega_p} a_p \tag{49.8}$$

50 Wannier Functions

For a given Hamiltonian with lattice translation symmetry,

$$[H, T_R] = 0 \tag{50.1}$$

the Bloch function is defined as

$$\Psi_{n\mathbf{k}}(\boldsymbol{r}) = u_{n\mathbf{k}}(\boldsymbol{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \tag{50.2}$$

where $u_{n\mathbf{k}}(\mathbf{r})$ has the same periodicity as the electric potential, $\mathbf{r}$ is the location in real space, $\mathbf{k}$ is the wave vector in the Brillouin zone, n is the band number and $e^{i\mathbf{kr}}$ is called a envelope function (Marzari, Vanderbilt (2012) p. 1421). The states $|\Psi_{n\mathbf{k}}\rangle$ is defined for every n so that $|\Psi_{n\mathbf{k}}\rangle$ is the eigenstates of the Hamiltonian.

50.1 Continuous form

Define Wannier functions in band n by superimposing Bloch functions $|\Psi_{n\boldsymbol{k}}\rangle$ in band n

$$\begin{aligned} |\boldsymbol{R}n\rangle = |w_{n\boldsymbol{R}}\rangle &= \frac{V}{(2\pi)^3}\int_{BZ} |\Psi_{n\boldsymbol{k}}\rangle\, e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} d\boldsymbol{k} \\ w_{n\boldsymbol{R}}(\mathbf{r}) &= \frac{V}{(2\pi)^3}\int_{BZ} \Psi_{n\boldsymbol{k}}(\boldsymbol{r}) e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} d\boldsymbol{k} \end{aligned} \tag{50.3}$$

since Bloch functions are orthogonal,

$$\langle \Psi_{n\mathbf{k}} \mid \Psi_{m\mathbf{k}'}\rangle \overset{\text{def}}{=} \int_{\text{Space}} d\mathbf{r}\Psi_{n\mathbf{k}}(\mathbf{r})\Psi_{m\mathbf{k}'}(\mathbf{r}) = \frac{(2\pi)^3}{V}\delta_{nm}\delta^3(\mathbf{k}-\mathbf{k}') \tag{50.4}$$

$$\int_{BZ} d\boldsymbol{k} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\mathbf{R}')} = \frac{(2\pi)^3}{V}\delta_{\mathbf{R},\mathbf{R}'} \tag{50.5}$$

we can show that Wannier functions defined in such a way are orthonormal

$$\begin{aligned} \langle \mathbf{R}, n|\, \mathbf{R}'m\rangle &= \left(\frac{V}{(2\pi)^3}\int_{BZ} d\boldsymbol{k}\, \langle \Psi_{n\boldsymbol{k}}|\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\right)\left(\frac{V}{(2\pi)^3}\int_{BZ} |\Psi_{m\boldsymbol{k}'}\rangle\, e^{-i\boldsymbol{k}'\boldsymbol{R}'} d\boldsymbol{k}'\right) \\ &= \delta_{nm}\frac{V}{(2\pi)^3}\int_{BZ} d\boldsymbol{k} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\mathbf{R}')} \\ &= \delta_{nm}\delta_{\mathbf{R},\mathbf{R}'} \end{aligned} \tag{50.6}$$

the inverse transformation is given by

$$|\Psi_{n\boldsymbol{k}}\rangle = \int_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} |\boldsymbol{R}n\rangle d\boldsymbol{R} \tag{50.7}$$

50.2 Discrete real space form

In the discrete version of Wannier function, define

$$|\Psi_{n\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |\mathbf{R}n\rangle \tag{50.8}$$

Note here that there is a gauge freedom in how to choose the Bloch functions

$$\begin{aligned} \left|\tilde{\Psi}_{n\mathbf{k}}\right\rangle = e^{i\varphi}|\Psi_{n\mathbf{k}}\rangle \Rightarrow |\tilde{u}_{n\mathbf{k}}\rangle = e^{i\varphi}|u_{n\mathbf{k}}\rangle \\ \tilde{\Psi}_{n\mathbf{k}}(\mathbf{r}) = e^{i\varphi(\mathbf{r})}\Psi_{n\mathbf{k}}(\mathbf{r}) \Rightarrow \tilde{u}_{n\mathbf{k}}(\mathbf{r}) = e^{i\varphi(\mathbf{r})}u_{n\mathbf{k}}(\mathbf{r}) \end{aligned} \tag{50.9}$$

where $\varphi(\mathbf{r})$ is a real function that has the same periodicity as the Hamiltonian. This gauge freedom does not change the physics of the system. By choosing a convenient gauge the Bloch function can be made to be smooth so that it is partially differentiable in every point, that is, $\nabla_{\mathbf{k}}|\tilde{u}_{n\mathbf{k}}\rangle$ is defined at every point. This will change the Wannier functions into

$$|\boldsymbol{R}n\rangle = \frac{V}{(2\pi)^3}\int_{BZ} |\Psi_{n\boldsymbol{k}}\rangle\, e^{i\varphi} e^{-i\mathbf{k}\cdot\boldsymbol{R}} d\mathbf{k} \tag{50.10}$$

which will not be the same function even though it is still a valid Wannier function. The above Wannier function is given for a single band n on the Bloch functions. We can also form Wannier functions using several bands

$$|\boldsymbol{R}n\rangle = \sum_{l=1}^{J}\frac{V}{(2\pi)^3}\int_{BZ} U_{ln}^{(\boldsymbol{k})}\, |\Psi_{l\boldsymbol{k}}\rangle\, e^{i\varphi} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} d\boldsymbol{k} \tag{50.11}$$

Here we have taken $l = 1, ..., J$ bands of Bloch functions to form the Wannier function in band n. $U_{mn}^{(\boldsymbol{k})}$ is a square matrix of size J with the periodicity of the Hamiltonian. This is equivalent to defining a linear combination of $\mathbf{k}$ modes with different band indices

$$\left|\tilde{\Psi}_{l\mathbf{k}}\right\rangle = U_{ln}^{(\mathbf{k})}\, |\Psi_{n\mathbf{k}}\rangle \tag{50.12}$$

and if we require $\left|\tilde{\Psi}\right\rangle$ to follow the same orthogonality condition, in the same way as $|\Psi\rangle$, we must have

$$\begin{aligned}\left\langle\tilde{\Psi}_{n\mathbf{k}}|\tilde{\Psi}_{m\mathbf{k}'}\right\rangle &= \langle\Psi_{l\mathbf{k}}|\, U_{ln}^{(\mathbf{k})*}U_{qm}^{(\mathbf{k}')}\,|\Psi_{q\mathbf{k}'}\rangle \\ &= U_{ln}^{(\mathbf{k})*}U_{qm}^{(\mathbf{k}')}\delta_{lq}\delta_{\mathbf{k}\mathbf{k}'} \\ &= U_{ln}^{(\mathbf{k})*}U_{lm}^{(\mathbf{k})}\delta_{\mathbf{k}\mathbf{k}'} \\ &= \left[U^{(\mathbf{k})\dagger}U^{(\mathbf{k})}\right]_{nm}\delta_{\mathbf{k}\mathbf{k}'} \\ &\equiv \delta_{mn}\delta_{\mathbf{k}\mathbf{k}'}\end{aligned} \tag{50.13}$$

so $U^{(\mathbf{k})}$ must be a unitary matrix.

50.3 Discrete real + discrete k-space form

The Wannier function can also be defined as

$$|\Psi_{n\boldsymbol{k}}\rangle = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}|\boldsymbol{R}n\rangle \Leftrightarrow |\boldsymbol{R}n\rangle = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}\,|\Psi_{n\boldsymbol{k}}\rangle \tag{50.14}$$

In accordance with the fact that

$$(e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}, e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}}) = \sum_{\mathbf{R}} e^{i(\boldsymbol{k}-\mathbf{k}')\cdot\boldsymbol{R}} = N\delta_{\mathbf{k}\mathbf{k}'} \tag{50.15}$$

so $\mathcal{V} = N$ here. We have distributed $\mathcal{V}$ into two $\sqrt{N}$.
Now, we have

$$\langle\Psi_{n\boldsymbol{k}}\,|\Psi_{m\boldsymbol{k}'}\rangle = \delta_{mn}\delta_{\mathbf{k}\mathbf{k}'} \tag{50.16}$$

$$\langle\mathbf{R}n|\,\mathbf{R}'m\rangle = \delta_{mn}\frac{1}{N}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} = \delta_{mn}\delta_{\mathbf{R},\mathbf{R}'} \tag{50.17}$$

We can also obtain the normalization for $|u_{n\mathbf{k}}\rangle$

$$\langle u_{n\boldsymbol{k}}\,|u_{m\boldsymbol{k}'}\rangle = \int d\mathbf{r}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\langle\Psi_{n\boldsymbol{k}}\,|\Psi_{m\boldsymbol{k}'}\rangle = \delta_{mn}\int d\mathbf{r}e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\langle\Psi_{n\boldsymbol{k}}\,|\Psi_{m\boldsymbol{k}'}\rangle \tag{50.18}$$

51 Local Analysis

51.1 Laplace's method

Laplace's method is a very general technique for obtaining the asymptotic behavior as $x \to +\infty$ of integrals in which the large parameter x appears in an exponential:

$$I(x) = \int_a^b f(t)e^{x\phi(t)}dt \tag{51.1}$$

Here, we assume that $f(t)$ and $\phi(t)$ are real continuous functions. Integrals of this form are called Laplace integrals.

Laplace's method rests on an important idea involved in many standard techniques of asymptotic analysis of integrals, such as the **methods of stationary phase** and **steepest descents**. The idea is this: if the real continuous function $\phi(t)$ has its maximum on the interval $a \le t \le b$ at $t = c$ and if $f(c) \neq 0$, then it is only the immediate neighborhood of $t = c$ that contributes to the full asymptotic expansion of $I(x)$ for large x. That is, we may approximate the integral $I(x)$ by $I(x;\varepsilon)$, where

$$I(x;\varepsilon) = \begin{cases}\int_{c-\varepsilon}^{c+\varepsilon} f(t)e^{x\phi(t)}dt & \max \text{ at } t = c \in [a,b] \\ \int_a^{a+\varepsilon} f(t)e^{x\phi(t)}dt & \max \text{ at } t = a \\ I(x;\varepsilon) = \int_{b-\varepsilon}^{b} f(t)e^{x\phi(t)}dt & \max \text{ at } t = b\end{cases} \tag{51.2}$$

Here ε may be chosen to be an arbitrary positive number. It is crucial that the full asymptotic expansion of $I(x;\varepsilon)$

1. Does not depend on ε
2. Is identical to the full asymptotic expansion of $I(x)$ as $x \to \infty$

Both of these surprising results are true because the remainder (when $c \in [a, b]$)

$$\left| \int_a^{c-\varepsilon} f(t) e^{x\phi(t)} dt \right| + \left| \int_{c+\varepsilon}^{b} f(t) e^{x\phi(t)} dt \right| \tag{51.3}$$

is subdominant (exponentially small) with respect to $I(x)$ as $x \to \infty$. This is because $e^{x\phi(t)}$ for all t outside our maximum interval are exponentially smaller than $e^{x\phi(c)}$as $x \to \infty$.

It is helpful to approximate $I(x)$ by $I(x;\varepsilon)$ because $\varepsilon > 0$ may be chosen so small that it is valid to replace $f(t)$ and $\phi(t)$ by their Taylor or asymptotic series expansions around $t = c$.

Example 1 We analyze and integral

$$I(x) = \int_0^{10} dt(1+t)^{-1} e^{-xt} \tag{51.4}$$

First, the leading order

$$\begin{aligned} I(x) &= \int_0^{10} dt(1+t)^{-1} e^{-xt} \\ &\sim \int_0^{\varepsilon} dt(1+t)^{-1} e^{-xt} \\ &\sim \int_0^{\varepsilon} dt e^{-xt} \\ &= \frac{1 - e^{-x\varepsilon}}{x} \\ &\sim \frac{1}{x} \qquad , x \to \infty \end{aligned} \tag{51.5}$$

Now, the full asymptotic expansion

$$I(x;\varepsilon) = \int_0^{\varepsilon} (1+t)^{-1} e^{-xt} dt = \sum_{n=0}^{\infty} \int_0^{\varepsilon} (-t)^n e^{-xt} dt \tag{51.6}$$

we again use the subdominant argument to approximate

$$\int_0^{\varepsilon} (-t)^n e^{-xt} dt \sim \int_0^{\infty} (-t)^n e^{-xt} dt = (-1)^n n! x^{-n-1} \tag{51.7}$$

we can check the subdominant argument through integration by parts

$$\begin{aligned} \int_{\varepsilon}^{\infty} (-t)^n e^{-xt} dt &= (-\varepsilon)^n e^{-x\varepsilon}/x + \frac{1}{x} \int_{\varepsilon}^{\infty} d\left[(-t)^n\right] e^{-xt} \\ &\sim (-\varepsilon)^n e^{-\varepsilon x}/x, \quad x \to +\infty \end{aligned} \tag{51.8}$$

which is exponentially smaller than the $[0, \varepsilon]$ contribution. Finally, we have

$$\begin{aligned} I(x) &= \int_0^{10} dt(1+t)^{-1} e^{-xt} \\ &\sim \sum_{n=0}^{\infty} (-1)^n n! x^{-n-1} \end{aligned} \tag{51.9}$$

Let us pause a moment to review the procedure we have just used. There are three steps involved in Laplace's method applied to an integral $I(x)$. First, we approximate $I(x)$ by $I(x;\varepsilon)$ by restricting the original integration region to a narrow region surrounding the maximum of $\phi(t)$. Second, we expand the functions $f(t)$ and $\phi(t)$ in series which are valid near the location of the maximum of $\phi(t)$. This allows us to expand $I(x;\varepsilon)$ into a series of integrals.

Finally, the most convenient way to evaluate the integrals in the series for $I(x;\varepsilon)$ is to extend the integration region in each integral to infinity. It is this third step that is hardest to grasp. It may seem foolish to first replace the finite number 10 in Example 1 (revisited) by ε and then to replace ε by ∞! However, we must choose ε to be small in order to expand the integrand of $I(x;\varepsilon)$ and thereby obtain a series. We then let the integration region become infinite in order to evaluate the terms in the series. Each time we change the limits of integration, we introduce only exponentially small errors. Note that had we not replaced the integration limit 10 by $\varepsilon < 1$, we could not have used the Taylor expansion for $(1+t)^{-1}$, which is only valid for $|t| < 1$.