Short Lectures on Responses and Correlations

LECTURE 1: [90'] path-integral representation for propagator (sum over paths); Lagrange equation; classical action; importance of quantum fluctuation factor; Gaussian integrations (1D and multi-dimensional); stationary-phase approximation; energy level and wave functions from propagator could be left as exercises;
whole of Sec. A

LECTURE 2: [90'] density matrix and ensembles; correlations in off-diagonal elements in density matrix (if possible, introduce the concept of off-diagonal long-range order); low- and high-temperature limit of density matrix of a harmonic oscillator and thermal wavelength; imaginary time $\beta \leftrightarrow it/\hbar$ and the periodic boundary conditions; briefly mention the path-integral simulations;
whole of Sec. C + first two paragraphs of Sec. D

LECTURE 3: [90'] use Hooke's force to introduce the concept of linear response; "dipole interaction+dipole momentum+susceptibility" for harmonic oscillator to emphasize linear response could be calculated from theory; introduce response function via time-dependent perturbation theory; retarded characteristic should be emphasized; fluctuation–dissipation theorem (damped harmonic oscillator); Kramers–Kronig relation (analyticity/causality); fluctuation–dissipation theorem between correlations and responses (thermal/quantum contribution); importance of $i0^+$ (physically/mathematically);
main part of Sec. F

LECTURE 4: [90'] general definitions of Green's functions; time-ordered nature and Wick's theorem (using example to emphasize); spectral function; example–free particles (detailed calculations to emphasize basic concepts); boundary conditions+Fourier transform to introduce the concept of Matsubara frequency; discontinuity of G gives the spectral function A; path-integral/Wick theorem/diagrams for time-ordered correlations but not for response functions; relations between responses and correlations (in ω space) for imaginary- and real-parts; scheme of determining $D(\omega)$: $\mathrm{Im}\, G(\omega) \to \mathrm{Im}\, D(\omega) \to D(\omega)$;
main part of Sec. G

LECTURE 5: [90'] Fermionic fluctuation–dissipation theorem (relations between A and G); example–relation between spectral function and single-particle momentum distribution $n_{\mathbf{k}}$ (use nucleon); emphasize the difficulties of determining spectral function A theoretically; importance of connecting experimental data (cross section) with spectral function A (spectroscopy); high-momentum tail in $n_{\mathbf{k}}$; Migdal–Luttinger theorem;
main part of Sec. H; Fig. M and Fig. N

LECTURE 6: if possible or necessary: why Green's functions defined on real times are necessary (far from equilibrium problems and no concept of local temperature); analytical continuation techniques for real-time G from imaginary-time G; importance of conservation laws; conventional Boltzmann equations; Kadanoff–Baym equations and why they are complicated; relativistic energy spectrum and the Schwinger–Keldysh contour; Green's functions defined on a close-time-path (CTPGFs); — ALL BRIEF/CONCEPTUAL —
introductory parts of Sec. I to Sec. L

Propagators, Responses, Correlations and Green's Functions

Bao-Jun Cai, 3/12/2024

These notes develop the theories of Green's functions at an elementary level. Section A introduces the method of path integral (sum over all paths) via the propagators for a system of free particles and the harmonic oscillator. In Section B, we give an extra example on using the sum rule method combined with the Green's function to estimate the ground state energy of a 2D harmonic oscillator. Section C is devoted to the density matrix and in Section D we give the first application of using imaginary-time formalism, i.e., simulating the path integral and estimating the ground state energy of a given system. Section E discusses the second example of imaginary-time formalism, namely the thermal effects on a scalar field. Section F introduces the basis of the response functions, correlation functions as well as their inner-connection, the fluctuation–dissipation theorem, here the importance of the retarded response function is emphasized. Section G is on the general theories of (equilibrium) Green's functions, and the spectral function is discussed in some details. In Section H we introduce the concept of spectroscopy which is strongly related to the spectral function, the nucleon momentum distribution in finite nuclei and nuclear matter is also discussed. The last four sections introduce the very basis of non-equilibrium real-time Green's functions (no concept of temperature), their relations with the imaginary-time formalism by analytical continuation, and the closely-related transport equations (conceptual). Exercises and examples are scattered through the notes to help understand the material. A few sections with "$*$" could be omitted without influencing the main development (however, certain important concepts do appear in such sections such as the imaginary-time and the Matsubara frequency). [Draft]

A Propagators: Free Particle and Harmonic Oscillator

Relevant References:

- R. Feynman, *Quantum Mechanics and Path Integrals*, Dover Press, 2010, Chapters 2 and 3.
- A. Zee, *Quantum Field Theory in a Nutshell*, 2nd Edition, Princeton University Press, 2010, Part I.

By using the path integral formulation, one can do relevant quantum mechanical calculations classically. The double-slit experiment tells that the probability amplitude at the detector D is

$$\text{Amplitude}(D) = \sum_{j=1,2} \text{Amplitude}(S \to A_j \to D). \tag{1.1}$$

If there are two walls with one having two slits A_j and the other three slits B_k, then the probability amplitude observed at D is

$$\text{Amplitude}(D) = \sum_{j,k} \text{Amplitude}(S \to A_j \to B_k \to D). \tag{1.2}$$

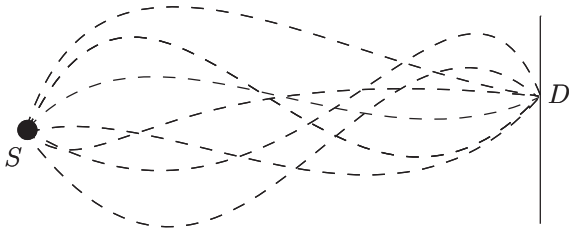

Fig. A: Infinite paths from S to D.

A natural question is: If the number of the walls approaches to infinity and in the meanwhile each wall has an infinite number of slits, what is the probability amplitude? In fact, this corresponds to the situation that there is no slits and walls between the source S and the detector D, and the probability amplitude is given by

$$\boxed{\text{Amplitude}(D) = \sum_{\text{all paths } (S \to D)} \text{Amplitude}(S \to \cdots \to D),} \tag{1.3}$$

see FIG. A. Our task is to compute the sum of these terms.

Assume that the initial and final coordinates of the system are q_i and q_f, respectively, and the propagation time is T, then the sum of the probability amplitude is given by

$$\langle q_\mathrm{f}|e^{-iHT/\hbar}|q_\mathrm{i}\rangle, \tag{1.4}$$

here $\langle q_\mathrm{f}|e^{-iHT/\hbar}$ represents the time evolution of$\langle q_\mathrm{f}|$, and when inner-multiplied with $|q_\mathrm{i}\rangle = |q_\mathrm{i}\rangle(t=0)$, one obtains the transition probability (propagator or its Green function). Decomposing the time as $\delta = T/N$, then

$$\langle q_\mathrm{f}|e^{-iHT/\hbar}|q_\mathrm{i}\rangle = \langle q_\mathrm{f}|\underbrace{e^{-iH\delta t/\hbar}e^{-iH\delta t/\hbar}\cdots e^{-iH\delta t/\hbar}}_{N\text{ times}}|q_\mathrm{i}\rangle. \tag{1.5}$$

Using the complete relation of the coordinate namely $\int \mathrm{d}q|q\rangle\langle q| = 1$, one can rewrite the probability amplitude as

$$\langle q_\mathrm{f}|e^{-iHT/\hbar}|q_\mathrm{i}\rangle = \left(\prod_{j=1}^{N-1}\int \mathrm{d}q_j\right)\langle q_\mathrm{f}|e^{-iH\delta t/\hbar}|q_{N-1}\rangle\cdots\langle q_2|e^{-iH\delta t/\hbar}|q_1\rangle\langle q_1|e^{-iH\delta t/\hbar}|q_\mathrm{i}\rangle. \tag{1.6}$$

The task is to compute the scattering element $\langle q_{j+1}|e^{-iH\delta t/\hbar}|q_j\rangle$. For the free particle, the energy is given by $H = p^2/2m$, and the eigenvalue equation for the momentum operator p is $p|p\rangle = p|p\rangle$, with the eigenvector in the coordinate representation given by $\langle p|q\rangle = (2\pi\hbar)^{-1/2}e^{-ipq/\hbar}$. Thus $\langle q|p\rangle = (2\pi\hbar)^{-1/2}e^{ipq/\hbar}$, then according to the complete relation $\int \mathrm{d}p|p\rangle\langle p| = 1$, one obtains,

$$\langle q_{j+1}|e^{-iH\delta t/\hbar}|q_j\rangle = \int \mathrm{d}p\langle q_{j+1}|\exp\left(-\frac{ip^2\delta t}{2m\hbar}\right)|p\rangle\langle p|q_j\rangle = \frac{1}{2\pi\hbar}\sqrt{\frac{-i2\pi m\hbar}{\delta t}}\exp\left[\frac{i\delta t m}{2\hbar}\left(\frac{q_{j+1}-q_j}{\delta t}\right)^2\right]. \tag{1.7}$$

Multiplying all these elements gives

$$\langle q_\mathrm{f}|e^{-iHT/\hbar}|q_\mathrm{i}\rangle = \left(\frac{m}{2\pi\hbar i\delta t}\right)^{N/2}\times\prod_{j=1}^{N-1}\int \mathrm{d}q_j\exp\left[\frac{im\delta t}{2\hbar}\sum_{j=1}^{N-1}\left(\frac{q_{j+1}-q_j}{\delta t}\right)^2\right], \tag{1.8}$$

where $q_0 = q_\mathrm{i}, q_N = q_\mathrm{f}$. Since,

$$\left[\frac{q_{j+1}-q_j}{\delta t}\right]^2 \to \dot{q}^2,\quad \sum_{j=1}^{N-1}\to\int_0^T \mathrm{d}t,\quad \int\mathcal{D}q = \lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\delta t}\right)^{N/2}\prod_{j=1}^{N-1}\int \mathrm{d}q_j, \tag{1.9}$$

we can rewrite the amplitude in the form,

$$\boxed{\langle q_\mathrm{f}|e^{-iHT/\hbar}|q_\mathrm{i}\rangle = \int\mathcal{D}q\exp\left(\frac{i}{\hbar}\int_0^T \mathrm{d}t\frac{1}{2}m\dot{q}^2\right),} \tag{1.10}$$

which is the path integral representation of the amplitude for free particle. For system with potential(s), the path integral is generalized to

$$\boxed{\langle q_\mathrm{f}|e^{-iHT/\hbar}|q_\mathrm{i}\rangle = \int\mathcal{D}q\exp\left[\frac{i}{\hbar}\int_0^T \mathrm{d}t\left[\frac{1}{2}m\dot{q}^2 - U(q)\right]\right].} \tag{1.11}$$

EXERCISE 1: Finish the Gaussian integration in (1.7).
EXERCISE 2: Prove the relation (1.11).
EXERCISE 3: Derive the classical action for harmonic oscillator.

Slightly rewriting (1.10), one obtains the amplitude for free particle as

$$\boxed{\langle q_\mathrm{f}|e^{-iHT/\hbar}|q_\mathrm{i}\rangle = \sqrt{\frac{m}{2\pi\hbar iT}}\times\exp\left[\frac{i}{\hbar}\frac{m(q_\mathrm{f}-q_\mathrm{i})^2}{2T}\right].} \tag{1.12}$$

The quantity appearing in the exponential is the classical action $iS_\mathrm{cl}/\hbar$ with $S_\mathrm{cl} = \int_{t_1}^{t_2}L(q,\dot{q},t)\mathrm{d}t$. Consider a quadratic Lagrange function, $L(t,q,\dot{q}) = \alpha(t)\dot{q}^2(t)+\beta(t)q(t)\dot{q}(t)+\gamma(t)q^2(t)+\delta(t)\dot{q}(t)+\chi(t)q(t)+\varphi(t)$, where $\alpha(t) = m(t)/2$ is positive. In order to use path integral to deal with the quadratic Lagrange function, one could treat the integration path is formed by fluctuations around the classical path $q_\mathrm{cl}(t)$ determined by the Lagrange equation. Let $\delta q(t)$ be the perturbation around the classical path, and is called the quantum fluctuation about the classical path. Furthermore, the values of $q(t)$ at the two boundaries $t_\mathrm{i}, t_\mathrm{f}$ are fixed and denoted as $q_\mathrm{i}, q_\mathrm{f}$. If the quantum fluctuation is not strong enough, the action could be decomposed into two parts, namely the classical action $S[q_\mathrm{cl}(t)]$ and the quadratic fluctuation part $S_\mathrm{f}[\delta q(t)]$. Keeping

terms up to second order, and considering the equation for $q_{\rm cl}(t)$, we have

$$S[q(t)] = \underbrace{\int_{t_{\rm i}}^{t_{\rm f}} {\rm d}t L(t, q_{\rm cl}, \dot{q}_{\rm cl})}_{S[q_{\rm cl}(t)]} + S_{\rm f}[\delta q(t)], \tag{1.13}$$

where the fluctuation part is given by

$$S_{\rm f}[\delta q(t)] = \int_{t_{\rm i}}^{t_{\rm f}} {\rm d}t \left[\alpha(t)\delta\dot{q}^2 + \beta(t)\delta q\delta\dot{q} + \gamma(t)\delta q^2\right]. \tag{1.14}$$

We call (1.14) the fluctuating action, which is originated from the fluctuation about the classical path, see Fig. B. The above approximation is called the stationary-phase scheme. Under the stationary-phase approximation, then

$$iG(q_{\rm f}, t_{\rm f}; q_{\rm i}, t_{\rm i}) = \langle q_{\rm f}|e^{-iH(t_{\rm f}-t_{\rm i})/\hbar}|q_{\rm i}\rangle = \int \mathcal{D}q(t) e^{iS[q(t)]/\hbar} = \mathscr{F}(t_{\rm f}, t_{\rm i}) e^{iS_{\rm cl}/\hbar}, \tag{1.15}$$

$$\mathscr{F}(t_{\rm f}, t_{\rm i}) = \int \mathcal{D}[\delta q(t)] \times \exp\left[\frac{i}{\hbar}\int_{t_{\rm i}}^{t_{\rm f}} {\rm d}t \left[\alpha(t)\delta\dot{q}^2 + \beta(t)\delta q\delta\dot{q} + \gamma(t)\delta q^2\right]\right]. \tag{1.16}$$

Here, $\mathscr{F}(t_{\rm f}, t_{\rm i})$ is the quantum fluctuation factor. If the system is time-translational invariant, the quantum fluctuation factor could be simplified as $\mathscr{F}(t_{\rm f}, t_{\rm i}) = \mathscr{F}(t_{\rm f} - t_{\rm i}) = \mathscr{F}(T)$. The calculation of the quantum fluctuation is extremely important. It also should be pointed out if there exist higher order terms in coordinates or velocities, the stationary-phase approximation will essentially break down.

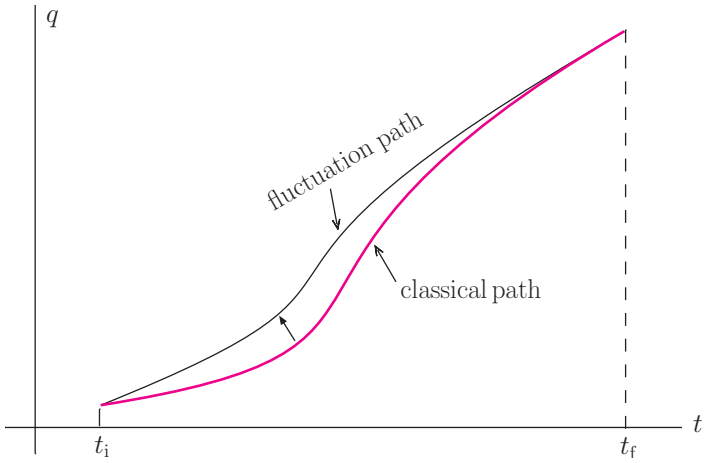

Fig. B: Fluctuation around the classical path.

EXERCISE 4: When the stationary-phase approximation breaks down, we should consider high order corrections to the propagator. Prove the following relation:

$$\int e^{n\phi(x)}{\rm d}x \approx e^{n\phi_{\rm max}} \sqrt{\frac{2\pi}{n|\phi''_{\rm max}|}} \times \left[1 + \frac{1}{24n}\left(\frac{3\phi''''_{\rm max}}{\phi''^{,2}_{\rm max}} + \frac{5\phi'''^{,2}_{\rm max}}{\phi''^{,3}_{\rm max}}\right) + \mathcal{O}\left(\frac{1}{n^2}\right)\right]. \tag{1.17}$$

The propagator is then given by in this case (where $\mathcal{N}$ is a constant),

$$iG(q_{\rm f}, t_{\rm f}; q_{\rm i}, t_{\rm i}) \approx \mathcal{N} e^{iS_{\rm cl}/\hbar} \Big/ \det\left(\frac{1}{\hbar}\frac{\delta^2 S[q_{\rm cl}(t)]}{\delta q_{\rm cl}(t)\delta q_{\rm cl}(t')}\right) \times [1 + \mathcal{O}(\hbar)]. \tag{1.18}$$

As an example, we calculate the path integral for the harmonic oscillator in details. The Lagrange function of the harmonic oscillator is given by $L = 2^{-1}m\dot{q}^2 - 2^{-1}m\omega q^2$. The quantum fluctuation is then,

$$\begin{aligned}\mathscr{F}(t_{\rm f} - t_{\rm i}) &= \int \mathcal{D}[\delta q(t)] \exp\left[\frac{i}{2\hbar}\int_{t_{\rm i}}^{t_{\rm f}} {\rm d}t \left(m\delta\dot{q}\delta\dot{q} - m\omega^2\delta q\delta q\right)\right] \\ &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\delta t}\right)^{N/2}\prod_{j=1}^{N-1}\int {\rm d}\delta q_j \exp\left\{\frac{i\delta t m}{2\hbar}\sum_{j=1}^{N}\left[\left(\frac{\delta q_j - \delta q_{j-1}}{\delta t^2}\right)^2 - \frac{\omega^2(\delta q_j + \delta q_{j-1})^2}{4}\right]\right\}.\end{aligned} \tag{1.19}$$

According to the boundary condition $\delta q(t_\mathrm{i}) = 0 = \delta q(t_\mathrm{f})$, we can set $\delta q_0 = \delta q_N = 0$. By denoting $Q_j = [m/2\hbar\delta t]^{1/2}\delta q_j$,

$$\mathscr{F}(t_\mathrm{f}-t_\mathrm{i}) = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\delta t}\right)^{N/2}\left(\frac{2\hbar\delta t}{m}\right)^{(N-1)/2}\int \mathrm{d}\mathbf{Q}\exp\left(i\mathbf{Q}^\mathrm{T}\vec{\Phi}\mathbf{Q}\right), \tag{1.20}$$

where $\mathbf{Q} = (Q_1,\cdots,Q_{N-1})^\mathrm{T}$. The integration could be done by standard transformation method, and the result is

$$\int \mathrm{d}\mathbf{Q}\exp\left(i\mathbf{Q}^\mathrm{T}\vec{\Phi}\mathbf{Q}\right) = \frac{(i\pi)^{(N-1)/2}}{\sqrt{\det\vec{\Phi}}}. \tag{1.21}$$

The next task is to calculate $\det\vec{\Phi}$. After a long and straightforward derivation, we have

$$\delta t\det\vec{\Phi} = \lim_{N\to\infty}\delta t\det\vec{\Phi}_N = \frac{\sin\omega(t_\mathrm{f}-t_\mathrm{i})}{\omega}, \tag{1.22}$$

leading to the quantum fluctuation as

$$\boxed{\mathscr{F}(t_\mathrm{f}-t_\mathrm{i}) = \left(\frac{m\omega}{2\pi i\hbar\sin\omega(t_\mathrm{f}-t_\mathrm{i})}\right)^{1/2}.} \tag{1.23}$$

On the other hand, the classical action of the oscillator is not hard to calculate,

$$\boxed{S[q_\mathrm{cl}(t)] = \frac{m}{2}\frac{\omega}{\sin\omega(t_\mathrm{f}-t_\mathrm{i})}\left[\left(q_\mathrm{f}^2+q_\mathrm{i}^2\right)\cos\omega(t_\mathrm{f}-t_\mathrm{i}) - 2q_\mathrm{f}q_\mathrm{i}\right],} \tag{1.24}$$

see **EXERCISE 3**. Combining the quantum fluctuation and the classical action gives the final expression for the propagator for the harmonic oscillator,

$$\boxed{\langle q_\mathrm{f}|e^{-iH(t_\mathrm{f}-t_\mathrm{i})/\hbar}|q_\mathrm{i}\rangle = \left(\frac{m\omega}{2\pi i\hbar\sin\omega(t_\mathrm{f}-t_\mathrm{i})}\right)^{1/2}\times\exp\left[\frac{i}{\hbar}\frac{m\omega}{2\sin\omega(t_\mathrm{f}-t_\mathrm{i})}\left[\left(q_\mathrm{f}^2+q_\mathrm{i}^2\right)\cos\omega(t_\mathrm{f}-t_\mathrm{i}) - 2q_\mathrm{f}q_\mathrm{i}\right]\right].} \tag{1.25}$$

Since the harmonic oscillator is time-translation invariant, we could rewrite the above expression as

$$\boxed{iG = \langle q_\mathrm{f}|e^{-iHT/\hbar}|q_\mathrm{i}\rangle = \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2}\times\exp\left[\frac{i}{\hbar}\frac{m\omega}{2\sin\omega T}\left[\left(q_\mathrm{f}^2+q_\mathrm{i}^2\right)\cos\omega T - 2q_\mathrm{f}q_\mathrm{i}\right]\right].} \tag{1.26}$$

The limit of this with $\omega\to 0$ is the corresponding propagator for free particles. In fact the propagator for the oscillator can also include an overall phase factor $e^{i\phi(t)}$, where $\phi(t)$ is a function of time.

EXERCISE 5: Show that the limit $\omega\to 0$ corresponds to the free case.

EXERCISE 6: Prove the identity (1.22).

Based on the result (1.26), one could calculate several relevant quantities for harmonic oscillator. The propagator has the boundary condition $iG(q_\mathrm{f},T;q_\mathrm{i},T) = \delta(q_\mathrm{f}-q_\mathrm{i})$. By calculating the trace of the propagator, we have

$$\begin{aligned}\int \mathrm{d}q\, iG(q,T;q,0) \equiv \mathrm{tr}\left(e^{-iHT/\hbar}\right) &= \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2}\int \mathrm{d}q\exp\left[\frac{i}{\hbar}\frac{m\omega[\cos\omega T-1]q^2}{\sin\omega T}\right]\\ &= \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2}\left(\frac{i\pi\hbar\sin\omega T}{m\omega[\cos\omega T-1]}\right)^{1/2} = \frac{1}{2i\sin(\omega T/2)}\\ &= \frac{1}{e^{i\omega T/2}-e^{-i\omega T/2}} = \frac{e^{-i\omega T/2}}{1-e^{-i\omega T}} = \sum_{n=0}^{\infty}\exp\left[-i\left(n+\frac{1}{2}\right)\omega T\right],\end{aligned} \tag{1.27}$$

from which one immediately obtains the energy level of the oscillator,

$$\boxed{E_n = \left(n+\frac{1}{2}\right)\hbar\omega.} \tag{1.28}$$

Inserting the identity matrix $\mathbf{1}$ gives the propagator in the following form (in the energy representation)

$$\boxed{iG(q_\mathrm{f},t_\mathrm{f};q_\mathrm{i},t_\mathrm{i}) = \sum_n e^{-(i/\hbar)E_n(t_\mathrm{f}-t_\mathrm{i})}\phi_n(q_\mathrm{f})\phi_n^*(q_\mathrm{i}).} \tag{1.29}$$

Setting $\tau = e^{-i\omega t}$ leads to $2i\sin\omega t = (1-\tau^2)/\tau, 2\cos\omega t = (1+\tau^2)/\tau$, then

$$\begin{aligned} iG(q,t;Q,0) &= \left(\frac{m\omega}{2\pi i\hbar\sin\omega t}\right)^{1/2}\exp\left[\frac{i}{\hbar}\frac{m\omega[(q^2+Q^2)\cos\omega t - 2qQ]}{2\sin\omega t}\right] \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\left(\frac{1-\tau^2}{\tau}\right)^{-1/2}\times\exp\left[-\frac{m\omega}{\hbar}\frac{\tau}{1-\tau^2}\frac{(q^2+Q^2)(1+\tau^2)}{2\tau-2qQ}\right] \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\exp\left[-\frac{m\omega(q^2+Q^2)}{2\hbar}\tau^{1/2}(1-\tau^2)^{-1/2}\right]\times\exp\left[\frac{m\omega}{\hbar}\frac{2qQ\tau-(q^2+Q^2)\tau^2}{1-\tau^2}\right]. \end{aligned} \tag{1.30}$$

Compare the results with following formula involving Hermite polynomial $H_n(q)$,

$$\sum_{n=0}^{\infty}\frac{(t/2)^n}{n!}H_n(q)H_n(Q) = (1-t^2)^{-1/2}\exp\left(\frac{2qQt-(q^2+Q^2)t^2}{1-t^2}\right), \tag{1.31}$$

the result is

$$iG(q,t;Q,0) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\exp\left(-\frac{m\omega(q^2+Q^2)}{2\hbar}\right)\times\sum_{n=0}^{\infty}\frac{1}{n!2^n}H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}Q\right)\exp\left[-\frac{i}{\hbar}\left(n+\frac{1}{2}\right)\hbar\omega t\right]. \tag{1.32}$$

The wave function for the harmonic oscillator is thus given by

$$\boxed{\phi_n(q) = 2^{-n/2}(n!)^{-1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega q^2}{2\hbar}\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right).} \tag{1.33}$$

EXERCISE 7: Discuss the classical and quantum probabilities for harmonic oscillator near the equilibrium position.
EXERCISE 8: Determine the probability distribution of the various values of the momentum for an oscillator.
EXERCISE 9: Find the wave function of the states of a linear oscillator that minimize the uncertainty relation, i.e., which the standard deviation of the coordinate and momentum in the wave packet are related by $\delta p\delta x = \hbar/2$, this is the coherent state.
EXERCISE 10: For the forced particle under the constant force f, show its path integral for the propagator is given by

$$iG(q_f,t;q_i,0) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\times\exp\left[\frac{i}{\hbar}\left[\frac{m(q_f-q_i)^2}{2t}+\frac{1}{2}ft(q_f+q_i)-\frac{f^2t^3}{24m}\right]\right]. \tag{1.34}$$

B *Green's Function: Sum Rules for a 2D Harmonic Oscillator

RELEVANT REFERENCES:

- The method of QCD sum rules was developed in the following papers: M. Shifman, A. Vainshtein, and V. Zakharov, *QCD and Resonance Physics. Theoretical Foundations*, Nucl. Phys. **B147**, 385 (1979); *ibid*, *QCD and Resonance Physics. Applications*, Nucl. Phys. **B147**, 448 (1979). This section relies on the introductory material from T. Cohen et al., *QCD Sum Rules and Applications to Nuclear Physics*, Prog. Part. Nucl. Phys. **35**, 221 (1995).
- For a full calculation on equation of state of nuclear matter using QCD sum rules is provided in: B.J. Cai and L.W. Chen, *Relativistic Self-energy Decomposition of Nuclear Symmetry Energy and Equation of State of Neutron Matter within QCD Sum Rules*, Phys. Rev. C **100**, 024303 (2019).

The energy level of the 2-dimensional harmonic oscillator is $E_n = (n_x+n_y+1)\hbar\omega = (2n+1)\omega$ (by setting $\hbar = 1$). We develop algorithm to estimate the ground state energy $B \equiv E_0 = \omega$, the method is the sum rule equation.

The Hamiltonian for the two dimensional harmonic oscillator is given by $H(\mathbf{p},\mathbf{q}) = \mathbf{p}^2/2m + 2^{-1}m\omega^2\mathbf{q}^2$, where $\mathbf{p}^2 = p_x^2+p_y^2, \mathbf{q}^2 = x^2+y^2$. The wave function of the ground state is $\phi_0(\mathbf{q}) = (\alpha/\pi)^{1/2}e^{-\alpha\mathbf{q}^2/2}$ with $\alpha = m\omega$ under $\hbar = 1$. At the origin we have $|\phi_0(\mathbf{0})|^2 = m\omega/\pi$, which holds for any order wave functions. The Green's function of the harmonic oscillator is defined as the weighted average of the energy level, i.e.,

$$G(\mathbf{q}_1t_1;\mathbf{q}_2t_2) = \sum_{n=0}^{\infty}\phi_n^*(\mathbf{q}_2)\phi_n(\mathbf{q}_1)e^{-iE_n(t_2-t_1)}, \tag{2.1}$$

see Eq. (1.29). One main ingredient of all types of sum rule approaches is to weaken the contributions from high excited states. In order to do that in the harmonic oscillator, one can introduce the function,

$$\mathscr{U}(\Omega) = \sum_{n=0}^{\infty}|\phi_n(\mathbf{0})|^2e^{-E_n/\Omega}, \tag{2.2}$$

where Ω is a constant larger than all E_n's, then at the limit $\Omega \to \infty$, only ground state contributes to to $\mathscr{U}(\Omega)$. The function $\mathscr{U}$ is related to G through the analytical continuation, i.e., $\mathscr{U}(\Omega) = G(\mathbf{q}_1 = \mathbf{0}, t_1 = 0; \mathbf{q}_2 = \mathbf{0}, t_2 = 1/i\Omega)$, thus Ω can be treated as the imaginary time. We have many opportunities to discuss the imaginary time in the following sections. For the harmonic oscillator, we have

$$\mathscr{U}_{\text{osci}}(\Omega) = \sum_n^{\infty} \frac{m\omega}{\pi} e^{-(2n+1)\omega/\Omega} = \frac{m\omega}{2\pi \sinh(\omega/\Omega)}. \tag{2.3}$$

In the large Ω limit,

$$\mathscr{U}_{\text{osci}} \approx \frac{m\Omega}{2\pi} \times \left[1 - \frac{1}{6}\left(\frac{\omega}{\Omega}\right)^2 + \frac{7}{360}\left(\frac{\omega}{\Omega}\right)^4 - \frac{31}{15120}\left(\frac{\omega}{\Omega}\right)^6 + \cdots\right]. \tag{2.4}$$

The first term in this expression is the corresponding $\mathscr{U}$ for a free particle, i.e., $\mathscr{U}_{\text{free}}(\Omega) = m\Omega/2\pi$. The terms in the parentheses in Eq. (2.4) are high order corrections originated from the small quantity ω/Ω. On the other hand, the function $\mathscr{U}_{\text{free}}(\Omega)$ can be written as the sum of energy level of the free particle,

$$\mathscr{U}_{\text{free}}(\Omega) = \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} e^{-E_{\mathbf{k}}/\Omega} = \frac{m}{2\pi}\int_0^{\infty} e^{-E/\Omega}\mathrm{d}E = \frac{1}{\pi}\int_{-\infty}^{\infty} e^{-E/\Omega}\rho_{\text{free}}(E)\mathrm{d}E, \tag{2.5}$$

where $E_{\mathbf{k}} = \mathbf{k}^2/2m$ is the free particle energy, and $\rho_{\text{free}} = 2^{-1}m\Theta(E)$ is the corresponding density of the energy level, Θ is the standard step function.

Similarly, the density of the energy level of the oscillator could be given by $\rho_{\text{osci}}(E) = m\omega\sum_{n=0}^{\infty}\delta(E-(2n+1)\omega)$. Then a series of results can be obtained

$$\boxed{\begin{aligned} \frac{1}{m}\int_0^{2\omega}[\rho_{\text{free}}(E) - \rho_{\text{osci}}(E)]\mathrm{d}E &= 0, \qquad (2.6)\\ \frac{1}{m}\int_{2n\omega}^{(2n+1)\omega}[\rho_{\text{free}}(E) - \rho_{\text{osci}}(E)]\mathrm{d}E &= 0, \qquad (2.7)\\ \frac{1}{m}\int_{2n\omega}^{(2n+1)\omega}[\rho_{\text{free}}(E) - \rho_{\text{osci}}(E)]E\mathrm{d}E &= 0, \qquad (2.8) \end{aligned}}$$

etc., which are called dual relations between the free particle and the oscillator. Furthermore,

$$\boxed{\frac{1}{\pi}\int_0^{\infty}[\rho_{\text{osci}}(E) - \rho_{\text{free}}(E)]e^{-E/\Omega}\mathrm{d}E = \sum_{n=1}\frac{A_n}{\Omega^n},} \tag{2.9}$$

the right hand side of which are the high order effects, which should become smaller and smaller as Ω increases. It is also obvious that

$$\boxed{\frac{1}{\pi}\int_0^{\infty}[\rho_{\text{osci}}(E) - \rho_{\text{free}}(E)]\mathrm{d}E = 0,} \tag{2.10}$$

which is another dual relation.

The dual relations indicate that although the structures of the energy level and the wave functions are very different for the free particle and the oscillator, they share large similarities under integrals. Accordingly, we obtain the sum rule equation for the harmonic oscillator through Eq. (2.2) and Eq. (2.4),

$$|\phi_0(\mathbf{0})|^2 e^{-B/\Omega} + \text{“high states”} = \frac{m\Omega}{2\pi} \times \left[1 - \frac{1}{6}\left(\frac{\omega}{\Omega}\right)^2 + \frac{7}{360}\left(\frac{\omega}{\Omega}\right)^4 - \frac{31}{15120}\left(\frac{\omega}{\Omega}\right)^6 + \cdots\right], \tag{2.11}$$

where different “high states” generate different physical consequences. There are no special considerations to define these “high states”, and the only requirement is that when Ω approaches to infinity, effects of the “high states” approach to zero. For instance, if we model the high states like $(m/\pi)e^{-s/\Omega}$ with s the threshold parameter above which the high states contributions become relevant, we then have

$$|\tilde{\phi}_0(\mathbf{0})|^2 e^{-B/\Omega} \approx \frac{\Omega}{2}\left(1 - e^{-s/\Omega}\right) - \frac{\omega^2}{12\Omega} + \frac{7}{720}\frac{\omega^4}{\Omega^3} - \frac{31}{30240}\frac{\omega^6}{\Omega^5} \quad |\tilde{\phi}_0(\mathbf{0})|^2 = (\pi/m)|\phi_0(\mathbf{0})|^2. \tag{2.12}$$

After calculating the derivative of Eq. (2.12) with respect to “$-\Omega^{-1}$”, we obtain,

$$|\tilde{\phi}_0(\mathbf{0})|^2 B e^{-B/\Omega} \approx \frac{\Omega^2}{2} - \frac{\Omega^2}{2}e^{-s/\Omega}\left(1 + \frac{s}{\Omega}\right) - \frac{\omega^2}{12} + \frac{7}{240}\frac{\omega^4}{\Omega^2} - \frac{31}{6048}\frac{\omega^6}{\Omega^4}. \tag{2.13}$$

Dividing Eq. (2.12) by Eq. (2.13) gives the formula for the ground state energy B,

$$\boxed{B/\omega \approx \frac{1-(1+\nu)e^{-\nu}+1/12-7/240\mathrm{x}^2+31/6048\mathrm{x}^4}{1-e^{-\nu}-1/12\mathrm{x}+7/720\mathrm{x}^3-31/30240\mathrm{x}^5},} \tag{2.14}$$

with $\mathrm{x}=\Omega/\omega, f=s/\omega, \nu=f/\mathrm{x}$, this is the sum rule equation for the harmonic oscillator in two dimensions. Several ingredients related to the above method are necessary to be pointed out:

(a) The result for B depends on the approximation of the high states, and in the above example, the approximation is modeled as $e^{-s/\Omega}$.

(b) For a fixed approximation for the high states, the result for B depends on s and Ω. One hopes that at a certain range of Ω, the result for B is insensitive to Ω. This range is often called the smooth region (window) which is of course related to the value of s (or f).

(c) If the approximation for the high states is selected unreasonable, there may not exist the smooth region.

If Eq. (2.12) is truncated, e.g., at order ω^2, one then obtains

$$\boxed{B/\omega \approx \frac{1-(1+\nu)e^{-\nu}+1/12}{1-e^{-\nu}-1/12\mathrm{x}}.} \tag{2.15}$$

From either Eq. (2.15) or Eq. (2.14), we have approximately $B/\omega \approx 1$.

EXERCISE 11: Estimate the ground state energy B using Eq. (2.14) and (2.15) and do the sensitive analysis.

EXERCISE 12: Adopt the "high states" via $\exp[-(s/\Omega)^n]$, do the similar sum rule calculations.

Comments. This very simple example on estimating the ground state energy of the 2D harmonic oscillator shares many similarities of the sum rule (SR) equations used in quantum chromodynamics (QCD): (a) The Ω in the sum rule equations for the harmonic oscillator is very similar as the Borel mass $\mathscr{M}$ in QCDSR, e.g., the smooth region (QCDSR window) of $\mathscr{M}^2$ is found to be about $0.8\,\mathrm{GeV}^2 \lesssim \mathscr{M}^2 \lesssim 1.4\,\mathrm{GeV}^2$; (b) Similarly in QCDSR, the nucleon correlation functions should be constructed by the Lorentz structure of the nucleon self-energies, and they also contain relevant information on the high states effects. Moreover, the high states effects on the physical quantities are weakened (even to be removed) by the Borel transformation, which plays a central role in QCDSR; (c) On the other hand, quark/gluon correlation functions (or more precisely, the quark/gluon condensates) are constructed via the operator product expansion (OPE) method, which is similar to the expansion of the weighted average sum of energy level, i.e., $\mathscr{U}_{\rm osci}$, on the small parameter ω/Ω. The OPE coefficients, called Wilson's coefficients, are determined by standard perturbative methods in quantum field theories; and (d) in QCDSR, the quark/gluon condensates such as $\langle\overline{q}q\rangle$ and $\langle G^2\rangle$ with q and G the quark and gluon fields are determined by experimental analysis or microscopic calculations.

C Density Matrix (Elementary Introduction)

RELEVANT REFERENCE:

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Density matrix is the straightforward generalization of the wave function. Consider an ensemble consisting of N systems, where $N \gg 1$. The state of the system is characterized by the vector $|K\rangle, K=1,2,\cdots,N$. By introducing the orthogonal and normalized basis $|n\rangle$ and writing the state in terms of the basis as $|K\rangle=\sum_n\langle n|K\rangle|n\rangle$, one finds that $\langle n|K\rangle$ is the wave function in the representation of the basis $|n\rangle$, according to the principle of quantum mechanics. An average of the quantity f on the Kth system is thus calculated as $f_K=\langle K|f|K\rangle$, and the ensemble expectation over f_K is

$$\boxed{\langle f\rangle=\frac{1}{N}\sum_{K=1}^{N}\langle K|f|K\rangle=\frac{1}{N}\sum_{K=1}^{N}\sum_{m,n}\langle K|m\rangle\langle m|f|n\rangle\langle n|K\rangle,} \tag{3.1}$$

where $\langle m|f|n\rangle$ is the matrix element of the operator f in the n-representation. Let's define the matrix element of the density matrix ρ as $\rho_{mn}=\sum_K\langle m|K\rangle\langle K|n\rangle/N$, and thus $\langle f\rangle=\sum_{m,n}f_{mn}\rho_{nm}=\mathrm{tr}(\rho f)$. In quantum statistical problems, the ensemble average of any quantity could be expressed as the trace of the product between the operator and the density matrix, and this is the quadratic average namely both quantum-mechanically and statistically. If one writes the density matrix in the form independent of the representation used, then $\rho=\sum_K|K\rangle\langle K|/N$. A few properties of the density matrix:

(a) The density matrix is Hermitian, i.e., $\rho_{mn}=\rho^*_{nm}$.

(b) The trace is 1, and the diagonal elements are non-negative, i.e., $\sum_n\rho_{nn}=1, 0\le\rho_{nn}\le 1$.

Selecting the representation in which the density matrix is diagonal, i.e., $\rho_{mn} = \rho_m \delta_{mn}$. Since,

$$\mathrm{tr}\left(\rho^2\right) = \sum_m \rho_m^2 \leq \left(\sum_m \rho_m\right)^2 = 1, \tag{3.2}$$

and the trace of a matrix is invariant under the unitary transform, thus the ρ in the non-diagonal representation,

$$\sum_{n,m} \rho_{mn}\rho_{nm} = \sum_{m,n} |\rho_{mn}|^2 \leq 1, \tag{3.3}$$

which puts constraints on each element of the density matrix. The diagonal element could be written explicitly as

$$\rho_{nn} = \frac{1}{N}\sum_K \langle n|K\rangle\langle K|n\rangle = \frac{1}{N}\sum_K |\langle n|K\rangle|^2. \tag{3.4}$$

According to quantum mechanics, $|\langle n|K\rangle|^2$ is the probability of the Kth system on the state $|n\rangle$, and averagely the probability of any system of the ensemble on the state $|n\rangle$ is ρ_{nn}. In this sense, the diagonal element of the density matrix characterizes the probability of the system of the ensemble staying on a certain state, and consequently it is very likely that the density matrix shares the similarity of the probability density in classical physics.

There are two ensembles namely the pure ensemble and the mixed ensemble in quantum statistics. If every system of the ensemble is staying at the same quantum state, we call the ensemble the pure ensemble. In this case, wave function is enough to describe the ensemble, otherwise the ensemble is mixed. Naturally for the pure ensemble, we have $\rho^2 = \rho$, i.e., only one of the diagonal elements of the density matrix is 1 and all the others are zero. In the non-diagonal representation, the pure density corresponds to

$$\rho_{mn} = \frac{1}{N}\sum_{K=1}^{N} \langle m|K\rangle\langle K|n\rangle \equiv \langle m|K\rangle\langle K|n\rangle, \tag{3.5}$$

$$\rho_{mn}^2 = \sum_l \rho_{ml}\rho_{ln} = \sum_l \langle m|K\rangle\langle K|l\rangle\langle l|K\rangle\langle K|n\rangle = \langle m|K\rangle\langle K|n\rangle = \rho_{mn}. \tag{3.6}$$

Let H be the Hamiltonian function of the system, then

$$i\hbar\frac{\partial}{\partial t}\rho = i\hbar\frac{\partial}{\partial t}\left(\frac{1}{N}\sum_K |K\rangle\langle K|\right) = \sum_K \frac{1}{N}H|K\rangle\langle K| - \sum_K \frac{1}{N}|K\rangle\langle K|H = [H,\rho], \tag{3.7}$$

which is called the quantum Liouville's equation. From the quantum Liouville's equation, one can immediately obtain the time evolution of the average of the physical quantity

$$i\hbar\frac{\mathrm{d}\langle f\rangle}{\mathrm{d}t} = \mathrm{tr}\left(i\hbar\frac{\partial\rho}{\partial t}f + i\hbar\rho\frac{\partial f}{\partial t}\right) = \mathrm{tr}\left([H,\rho]f + i\hbar\rho\frac{\partial f}{\partial t}\right) = \mathrm{tr}\left(\rho\left[i\hbar\frac{\partial f}{\partial t} + [f,H]\right]\right) = i\hbar\left\langle\frac{\partial f}{\partial t}\right\rangle + \langle[f,H]\rangle, \tag{3.8}$$

If one knows the density matrix, then all the properties of the physical quantities could be obtained. For a system in equilibrium, we have $\partial\rho/\partial t = 0$, i.e., $[\rho,H] = 0$, indicating that ρ is a function of H. In addition, if the Hamiltonian H is time-independent, one can choose the eigenstate of H., i.e., $|n\rangle$ to do the calculations, and in this case $\rho_{mn} = \rho_n\delta_{mn}$.

Two frequently-used ensembles are the micro-canonical and the canonical ensembles. In the micro-canonical ensemble, the energy E is fixed, thus $\rho_{mn} = \rho_n\delta_{mn}$, where $\rho_n = W^{-1}$ for $E \leq E_K \leq E + \delta$. All the thermodynamic properties of the system/ensemble could be determined by the entropy $S = k_\mathrm{B}\ln W$. For the pure ensemble, the number of microstates is 1, thus $S = 0$. In the canonical ensemble, the energy E is not fixed, but could change by exchanging with the external system. The density matrix is $\rho_{mn} = \rho_n\delta_{mn}$, where $\rho_n = Z^{-1}e^{-\beta E_n}$, here

$$\boxed{Z = \mathrm{tr}\left(e^{-\beta H}\right) = \sum_n e^{-\beta E_n},} \tag{3.9}$$

is the partition function. Moreover,

$$\rho = \frac{1}{N}\sum_K |K\rangle\langle K| = \frac{1}{N}\sum_{mn}\sum_K |E_m\rangle\langle E_m|K\rangle\langle K|E_n\rangle\langle E_n| = \sum_n \rho_n|E_n\rangle\langle E_n| = \frac{e^{-\beta H}}{Z}\sum_n |E_n\rangle\langle E_n| = \frac{e^{-\beta H}}{\mathrm{tr}(e^{-\beta H})}. \tag{3.10}$$

The average of the physical quantity f in the canonical ensemble is

$$\langle f\rangle = \mathrm{tr}\left(\rho f\right) = \frac{\mathrm{tr}(fe^{-\beta H})}{\mathrm{tr}(e^{-\beta H})} = \frac{\sum_n f_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}, \tag{3.11}$$

where f_n is the eigenvalue of the f corresponding to the eigenstate E_n. The density matrix in the coordinate representation could be calculated as:

$$\boxed{\rho\left(\mathbf{x}^N,\mathbf{x}^{N'}\right)=\langle\mathbf{x}^N|\rho|\mathbf{x}^{N'}\rangle=\sum_n e^{-\varphi-\beta E_n}\langle\mathbf{x}^N|E_n\rangle\langle E_n|\mathbf{x}^{N'}\rangle=\sum_n e^{-\varphi-\beta E_n}\phi_n(\mathbf{x}^N)\phi_n^*(\mathbf{x}^{N'}),} \tag{3.12}$$

here $\langle\mathbf{x}^N|E_n\rangle\equiv\phi_n(\mathbf{x}^N)$ is the expression for the energy eigenstate in the coordinate representation (with N particles).

Example – 1. We calculate the density matrix of the ensemble consisting of free particles. The eigen-function of the free particle with mass m placed in the cube with side length L is given by $\phi_E(\mathbf{x})=L^{-3/2}e^{i\mathbf{k}\cdot\mathbf{x}}$ under the periodic boundary condition, and the eigenvalue is $E=\hbar^2k^2/2m$. The density matrix of the canonical ensemble in the coordinate representation is

$$\langle\mathbf{x}|e^{-\beta H}|\mathbf{x}'\rangle=\sum_E\langle\mathbf{x}|E\rangle e^{-\beta E}\langle E|\mathbf{x}'\rangle=\sum_n e^{-\beta E}\phi_E(\mathbf{x})\phi_E^*(\mathbf{x}')=\frac{1}{L^3}\sum_{\mathbf{k}}\exp\left[-\frac{\beta\hbar^2k^2}{2m}+i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')\right]. \tag{3.13}$$

One can approximate the sum here by integration if the volume V is very large, using $\sum_{\mathbf{k}}\to L^3\int\mathrm{d}\mathbf{k}/(2\pi)^3$,

$$\langle\mathbf{x}|e^{-\beta H}|\mathbf{x}'\rangle=\frac{1}{(2\pi)^3}\int\exp\left[-\frac{\beta\hbar^2k^2}{2m}+i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')\right]\mathrm{d}\mathbf{k}=\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2}\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right], \tag{3.14}$$

therefore

$$\boxed{\mathrm{tr}\left(e^{-\beta H}\right)=\int\langle\mathbf{x}|e^{-\beta H}|\mathbf{x}\rangle\mathrm{d}\mathbf{x}=V\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2}.} \tag{3.15}$$

This is the partition function of the free particle, from which one can calculate the density matrix as

$$\boxed{\rho(\mathbf{x},\mathbf{x}')=\langle\mathbf{x}|\rho|\mathbf{x}'\rangle=\frac{\langle\mathbf{x}|e^{-\beta H}|\mathbf{x}'\rangle}{\mathrm{tr}(e^{-\beta H})}=\frac{1}{V}\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right].} \tag{3.16}$$

EXERCISE 13: Derive the partition function (3.15) using conventional method.

It could be found that the diagonal element of the density matrix is $\rho(\mathbf{x},\mathbf{x})=1/V$, which is independent of the position $\mathbf{x}$, indicating the probability the particle being at any position in the box is the same. Moreover, the off-diagonal element of the density matrix $\rho(\mathbf{x},\mathbf{x}')$ characterizes the spontaneous transition probability between position $\mathbf{x}$ and $\mathbf{x}'$, and this correlation effect is a pure quantum behavior. If the temperature T is high, the above expression approaches to a δ function, i.e., the system is classical. We can then calculate the average of the Hamiltonian as

$$\begin{aligned}\langle H\rangle=\mathrm{tr}(\rho H)&=\int\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}'\langle\mathbf{x}|\rho|\mathbf{x}'\rangle\langle\mathbf{x}'|H|\mathbf{x}\rangle\\&=-\frac{\hbar^2}{2mV}\int\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}'\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right]\nabla_{\mathbf{x}}^2\delta(\mathbf{x}-\mathbf{x}')\\&=-\frac{\hbar^2}{2mV}\int\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}'\delta(\mathbf{x}-\mathbf{x}')\nabla_{\mathbf{x}}^2\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right]\\&=-\frac{\hbar^2}{2mV}\int\mathrm{d}\mathbf{x}'\left[\nabla_{\mathbf{x}}^2\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right]\right]\Big|_{\mathbf{x}=\mathbf{x}'}=\frac{3}{2}k_{\mathrm{B}}T.\end{aligned} \tag{3.17}$$

Example – 2. We now calculate the density matrix of the harmonic oscillator. The density matrix takes the form of $\rho=e^{-\beta H}/\mathrm{tr}(e^{-\beta H})$, which could be re-expressed in the energy representation as $\rho_{nm}\sim\delta_{nm}e^{-\beta E_n}$. Taking the derivative with respective to β gives $-\partial\rho_{nm}/\partial\beta=\delta_{nm}E_ne^{-\beta E_n}=E_n\rho_{nm}$, which is the same as $-\partial\rho/\partial\beta=H\rho$. This is the Bloch's equation for ρ, with the initial condition $\rho(0)=1$. In the coordinate representation, we have

$$\boxed{-\frac{\partial\rho(q,q';\beta)}{\partial\beta}=H\rho(q,q';\beta),\quad\rho(q,q';0)=\delta(q-q').} \tag{3.18}$$

For the harmonic oscillator, the Bloch's equation reads

$$-\frac{\partial\rho}{\partial\beta}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}\rho+\frac{1}{2}m\omega^2q^2\rho. \tag{3.19}$$

The solution of it is given by,

$$\boxed{\rho(q,q';\beta)=\left(\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}\right)^{1/2}\times\exp\left[-\frac{m\omega}{2\hbar\sinh\beta\hbar\omega}\left[(q^2+q'^2)\cosh\beta\hbar\omega-2qq'\right]\right].} \tag{3.20}$$

EXERCISE 14: Solve Bloch's equation for the harmonic oscillator by transforming to $\xi=(m\omega/\hbar)^{1/2}q, f=\hbar\omega\beta/2$ and considering the appropriate limit of $f\to 0$.

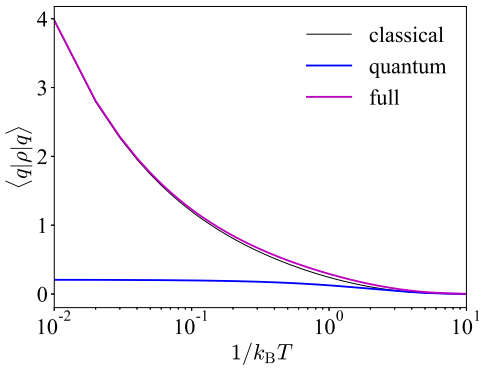

Fig. C: $\langle q|\rho|q\rangle$ as a function of $1/k_BT$.

If one takes $q=q'$ in the above expression, then

$$\rho(q,q;\beta)=\left(\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}\right)^{1/2}\times\exp\left(-\frac{m\omega q^2}{\hbar}\tanh\frac{\beta\hbar\omega}{2}\right), \tag{3.21}$$

thus

$$\mathrm{tr}\left(e^{-\beta H}\right)=\int\rho(q,q;\beta)\mathrm{d}q=\frac{1}{2\sinh(\beta\hbar\omega/2)}=\frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}, \tag{3.22}$$

which is the partition function for a single oscillator. In addition,

$$\langle q^2\rangle=\int q^2\rho(q,q;\beta)\mathrm{d}q\Big/\int\rho(q,q;\beta)\mathrm{d}q=\frac{\hbar}{2m\omega}\coth\frac{\beta\hbar\omega}{2}, \tag{3.23}$$

and consequently,

$$\langle U\rangle=\frac{1}{2}m\omega^2\langle q^2\rangle=\frac{\hbar\omega}{4}\coth\frac{\beta\hbar\omega}{2}, \tag{3.24}$$

$$\langle K\rangle=\left\langle-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}\right\rangle=\frac{\hbar\omega}{4}\coth\frac{\beta\hbar\omega}{2}. \tag{3.25}$$

The total energy is

$$\boxed{\langle E\rangle=\langle U\rangle+\langle K\rangle=\frac{\hbar\omega}{2}\coth\frac{\beta\hbar\omega}{2}.} \tag{3.26}$$

EXERCISE 15: Discuss the high- and low-temperature limits of the density matrix (3.21).
EXERCISE 16: The behavior of a system is either classical or quantum-mechanical is determined by the thermal wavelength,

$$\lambda_{\mathrm{th}}=\sqrt{\frac{h^2}{2\pi mk_BT}}. \tag{3.27}$$

Estimate at which temperature the de Broglie wavelength is comparable to the thermal wavelength.

D *Imaginary Time $\beta\hbar\leftrightarrow it$, Path Integral Simulations

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There exists close connection between the density matrix and the transition probability. For example, for the 1D free particle, the transition amplitude from q_{i} to q_{f} is given by

$$\langle q_{\mathrm{f}}|e^{-iHt/\hbar}|q_{\mathrm{i}}\rangle=\left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\exp\left[\frac{i}{\hbar}\frac{m(q_{\mathrm{f}}-q_{\mathrm{i}})^2}{2t}\right], \tag{4.1}$$

see Eq. (1.12). Similarly, the density matrix for the free particle $\langle q_{\mathrm{f}}|e^{-\beta H}|q_{\mathrm{i}}\rangle$ is

$$\langle q_{\mathrm{f}}|e^{-\beta H}|q_{\mathrm{i}}\rangle=\left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2}\exp\left[-\frac{m(q_{\mathrm{f}}-q_{\mathrm{i}})^2}{2\beta\hbar^2}\right], \tag{4.2}$$

see Eq. (3.16). We can easily find if one uses $\beta\hbar = it$ in Eq. (4.2), then Eq. (4.1) is naturally obtained. This means the density matrix in statistical mechanics can be obtained from the transition probability in quantum mechanics (and vice versa). We often call $\beta = 1/k_{\rm B}T$ the imaginary time, which fundamentally encapsulates the physics of temperature (therefore it describes equilibrium states.

EXERCISE 17: Establish this connection for the harmonic oscillator similarly.

Since the density matrix and the transition probability is strongly related via the imaginary time, one can also formulate the path integral for the density matrix. Since the structures of $\langle q_{\rm f}|e^{-\beta H}|q_{\rm i}\rangle$ and $\langle q_{\rm f}|e^{-iHt/\hbar}|q_{\rm i}|\rangle$ are very similar, we start from the following probability,

$$\langle q_{\rm f}|e^{-iH(t_{\rm f}-t_{\rm i})/\hbar}|q_{\rm i}\rangle = \int \mathcal{D}q \exp\left[\frac{i}{\hbar}\int_{t_{\rm i}}^{t_{\rm f}}\left[\frac{1}{2}m\dot{q}^2 - U(q)\right]\right], \tag{4.3}$$

here the factor appeared in the exponential is the action. Making $t = -i\tau$(which is also called the Wick's rotation, here we find $\beta\hbar \sim it \sim \tau$) gives

$$iS|_{t=-i\tau} = \int_{\tau_{\rm i}}^{\tau_{\rm f}} {\rm d}\tau \left[-\frac{m}{2}\left(\frac{{\rm d}q}{{\rm d}\tau}\right)^2 - U(q)\right] = -S_{\rm E}. \tag{4.4}$$

After introducing the Euclidean action $S_{\rm E}$, we transform the factor $e^{iS/\hbar}$ to $e^{-S_{\rm E}/\hbar}$(sometimes we also write it as $e^{S_{\rm E}/\hbar}$ which has a sign difference). The partition function is obtained as its path integral representation,

$$\boxed{Z(\beta) = {\rm tr}\left(e^{-\beta H}\right) = \int {\rm d}q\langle q|e^{-\beta H}|q\rangle = \int_{q(0)=q(\beta)} \mathcal{D}[q(\tau)] \exp\left[-\frac{1}{\hbar}\int_0^{\beta}{\rm d}\tau\left[\frac{1}{2}m\dot{q}(\tau) + U(q(\tau))\right]\right]}, \tag{4.5}$$

here the measure $\mathcal{D}[q(\tau)]$ contains the product of N terms and $\dot{q}$ represents the derivative with respect to τ. The trace operation sets the initial and final states equal and so the functional integral should be worked out over all paths with the periodic boundary condition $q(0) = q(\beta)$. Eq. (4.5) also tells that the Euclidean quantum field theory in $(d+1)$-dimensional space-time with $0 \le \tau \le \beta$ is equivalent to quantum statistical mechanics in d-dimensional space. In order to investigate a field theory at finite temperature all one needs to do is rotate it to Euclidean space and impose the corresponding periodic boundary condition.

The periodic boundary condition $q(0) = q(\beta)$ means only periodic orbits make contribution to the partition function. The path integral formulation of the partition function finds wide applications in field theory problems, like the decay of meta-stable states, the instanton statistical problem, etc. We can use the above idea to do Monte Carlo simulation and find certain properties of the system under consideration. Firstly, we denote iG by K and introduce $\epsilon = i\delta t$, then the propagator for the system under influence $U(q)$ could be written as

$$K(q,q_0;N,\epsilon) = \left(\frac{m}{2\pi\hbar\epsilon}\right)^{N/2}\int {\rm d}q_1\cdots{\rm d}q_{N-1} \times \exp\left[\frac{\epsilon}{\hbar}\sum_{j=1}^{N}\left[\frac{m}{2}\left(\frac{q_j - q_{j-1}}{\delta t}\right)^2 - U(q_j)\right]\right], \tag{4.6}$$

here $N\epsilon = \tau$ (imaginary time), this is a high-dimensional integration which could be evaluated by efficient Monte Carlo algorithm (e.g., the Metropolis). Next by introducing $\tau = it$ and $t_0 = 0$, we can write the propagator $K(q,\tau;q,0)$ as $K(q,\tau;q,0) = \sum_n \phi_n(q)\phi_0(q_0)e^{-\tau E_n/\hbar}$. If one now lets the imaginary time τ approach to infinity, then only the information on the ground state will be kept. More precisely, we have for the density

$$\phi_0^2(q) = \lim_{\tau\to\infty} e^{-\tau E_0/\hbar}K(q,\tau;q,0), \tag{4.7}$$

where $q_0 = q$ (the periodic boundary condition) is also used. Since the ground state wave function should be normalized, we obtain $\phi_0^2(q) = K(q,\tau;q,0)/\int_{-\infty}^{\infty}{\rm d}qK(q,\tau;q,0)$. It is very important to remember that in order to evaluate the wave function, the periodic condition and the imaginary-time scheme are adopted. In the followed steps, one can do the standard Monte Carlo simulation like the Metropolis to fulfill the above algorithm by treating the fact appeared in the exponential

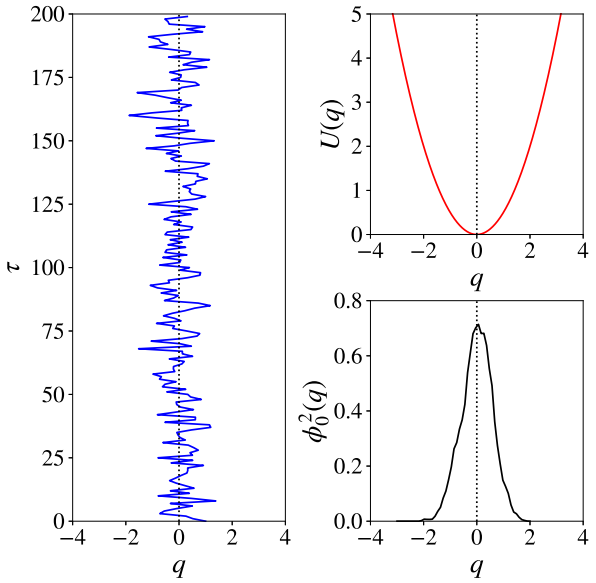


Fig. D: Monte Carlo simulation for path integral for harmonic oscillator (adopting Metropolis algorithm).

the effective energy. In Fig. D, we show the calculated results using the Metropolis algorithm for the harmonic oscillator with $U(q) = q^2/2$, here the left panel is the path in the imaginary time, and the right-lower panel shows the squared wave function $\phi_0^2(q)$. One can also study the ground state wave function of a double-well function, e.g., $U(q) = q^4 + \lambda q^2$ where $\lambda < 0$ is an control parameter. The non-trivial vacuum states of this function are given by $q = \pm(-\lambda/2)^{1/2}$. In Fig. E the paths in the imaginary-time domain with decreasing λ (from left to right) are shown. As one can see when the control parameter becomes more negative, the two equilibrium configurations $\sqrt{\lambda/2}$ and $-\sqrt{\lambda/2}$ become more separable. Fig. F shows the squared wave functions with three typical λ's, i.e., $\lambda = 0, -6$ and -12 (from left to right). The squared wave function in the left panel is very similar as the one obtained for the harmonic oscillator since the overall shape of q^4 is similar like that of q^2. However as a nonnegative λ emerges, the double-peak wave function also emerges naturally. The imaginary-time formalism is the foundation of many quantum Monte Carlo algorithms.

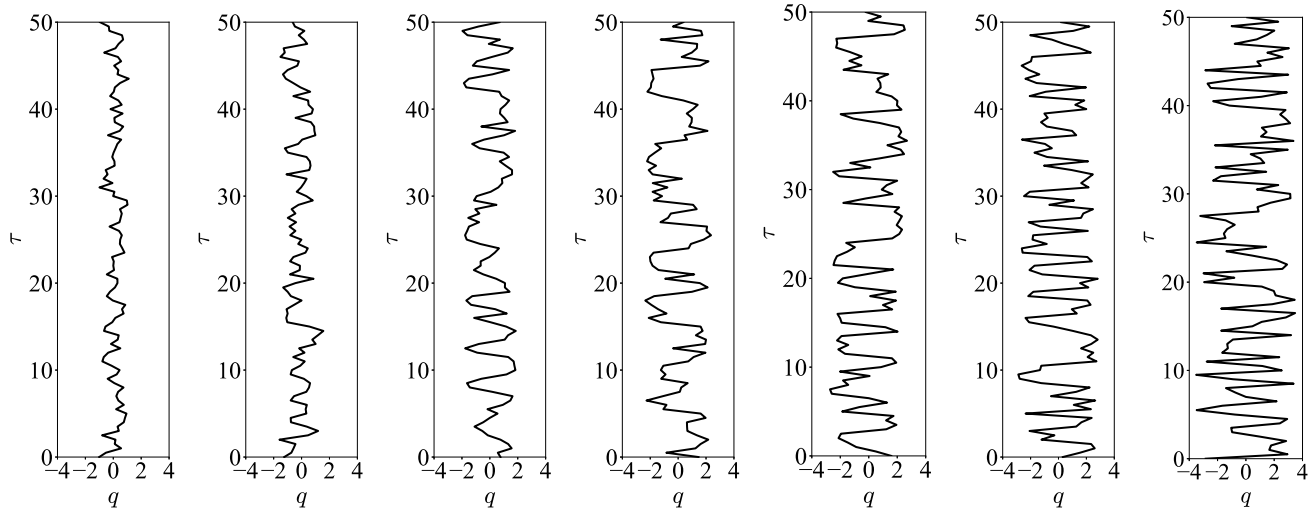


Fig. E: Paths in the imaginary-time domain with decreasing λ (from left to right) of the potential $U(q) = q^4 + \lambda q^2$ (with $\lambda < 0$).

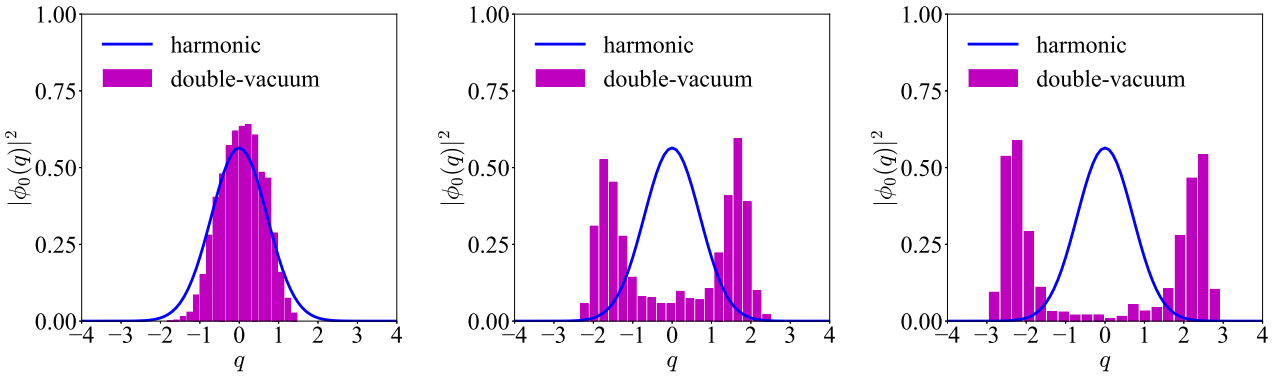


Fig. F: Squared wave functions with $\lambda = 0, -6$ and -12.

EXERCISE 18: How to obtain the ground state energy E_0 from evaluating the imaginary-time path integral?
EXERCISE 19: For the harmonic oscillator, the first-excited energy level could be obtained from,

$$E_1 - E_0 = \Delta E = -\frac{1}{\epsilon} \ln\left(\frac{\langle q(0)q(\tau+\epsilon)\rangle}{\langle q(0)q(\tau)\rangle}\right). \tag{4.8}$$

Explain this formula. Then evaluate the first-excited energy in the harmonic oscillator for $U(q) = q^2/2$.

E *Matsubara Frequency, Thermal Mass of a Scalar Field

RELEVANT REFERENCES:

- J. Kapusta, *Quantum Field Theory at Finite Temperature*, Cambridge University Press, 1989, Chapters 2 and 3.
- M. Laine and A. Vuorinen, *Basics of Thermal Field Theory: A Tutorial on Perturbative Computations*, Springer International Publishing, 2016, Chapters 2 and 3.

The imaginary-time formalism of the last section (e.g., Eq. (4.5)) could be generalized to the situation of a continuous field theory. For example, for a real scalar field with Lagrangian (we adopt $\hbar = c = 1$),

$$\mathcal{L}_0 = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 = \frac{1}{2}\left[(\partial_t\phi)^2 - (\nabla\phi)^2 - m^2\phi\right], \tag{5.1}$$

one can obtain the partition function,

$$\boxed{Z_0 = \mathrm{tr}\left[e^{-\beta(H_0-\mu N)}\right] = \int \mathrm{d}\phi\langle\phi|e^{-\beta(H_0-\mu N)}|\phi\rangle = \int \mathcal{D}\pi\int_{\phi(\mathbf{x},0)=\phi(\mathbf{x},\beta)}\mathcal{D}\phi\exp\left(-\int_0^\beta \mathrm{d}\tau\int \mathrm{d}\mathbf{x}(\mathcal{H}_0 - \mu\mathcal{N} - i\pi\partial_\tau\phi)\right),} \tag{5.2}$$

where $\tau = it$, $\pi = \partial_t\phi$ is the canonical momentum and $\mathcal{H}_0 = \pi\partial_t\phi - \mathcal{L}_0 = [\pi^2 + (\nabla\phi)^2 + m^2\phi^2]/2$. Notice the periodic boundary condition $\phi(\mathbf{x},0) = \phi(\mathbf{x},\beta)$. After integrating the momentum part, we shall obtain

$$\boxed{Z_0 = \overline{\mathcal{N}}\int\mathcal{D}\phi\exp\left(-\int_0^\beta \mathrm{d}\tau\int\mathrm{d}\mathbf{x}\mathcal{L}_0\right) = \overline{\mathcal{N}}\int\mathcal{D}\phi e^{-S_0} \sim \int\mathcal{D}\phi e^{-S_0},} \tag{5.3}$$

here $\overline{\mathcal{N}}$ is an integration constant (due to the momentum). The Lagrangian appearing in Eq. (5.3) is Euclidean, i.e.,

$$\mathcal{L}_{0,\mathrm{E}} = \frac{1}{2}\left[(\partial_\tau\phi)^2 + (\nabla\phi)^2 + m^2\phi^2\right]. \tag{5.4}$$

However, we will frequently omit the subscript "E".

We introduce $X \equiv (x^0,\mathbf{x}) = (t,\mathbf{x}) = (-i\tau,\mathbf{x})$ and $K \equiv (k^0,\mathbf{k}) = (-i\omega_n,\mathbf{k})$, here ω_n is called the Matsubara frequency. The Fourier transform of $\phi(X)$ is defined as

$$\phi(X) = \frac{1}{\sqrt{TV}}\sum_K e^{-iK\cdot X}\phi(K) = \frac{1}{\sqrt{TV}}\sum_{n,\mathbf{k}} e^{i(\omega_n\tau+\mathbf{k}\cdot\mathbf{x})}\phi(K), \tag{5.5}$$

where $K\cdot X = KX = k^0x^0 - \mathbf{k}\cdot\mathbf{x}$, we also have $\phi(-K) = \phi^*(K)$ since $\phi(X)$ is real. The boundary condition $\phi(0,\mathbf{x}) = \phi(\beta,\mathbf{x})$ gives $e^{i\omega_n\beta} = 1$, or

$$\boxed{\omega_n = 2\pi nT, \quad n\in\mathrm{Z}.} \tag{5.6}$$

Now, the action in momentum space becomes,

$$\boxed{S_0 = \int_X\mathcal{L}_0 = \frac{1}{2}\int_X\left[(\partial_\tau\phi)^2 + (\nabla\phi)^2 + m^2\phi^2\right] = \frac{1}{2}\sum_K\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K), \quad \int_X \equiv \int_0^\beta\mathrm{d}\tau\int\mathrm{d}\mathbf{x},} \tag{5.7}$$

where $D_0(K)$ is the free propagator in momentum space,

$$\boxed{D_0^{-1}(K) = \omega_n^2 + |\mathbf{k}|^2 + m^2,} \tag{5.8}$$

since

$$\begin{aligned}\int_X(\partial_\tau\phi)^2 &= \frac{1}{TV}\int_X\sum_{K,Q}\left[\partial_\tau e^{i(\omega_n\tau+\mathbf{k}\cdot\mathbf{x})}\phi(K)\right]\left[\partial_\tau e^{i(\omega_m\tau+\mathbf{q}\cdot\mathbf{x})}\phi(Q)\right]\\ &= -\frac{1}{TV}\int_X\sum_{K,Q}\omega_n\omega_m e^{-i(K+Q)X}\phi(K)\phi(Q) = \frac{1}{T^2}\sum_K\omega_n^2\phi(-K)\phi(K),\end{aligned} \tag{5.9}$$

$$\begin{aligned}\int_X(\nabla\phi)^2 &= \frac{1}{TV}\int_X\sum_{K,Q}\left[\nabla e^{i(\omega_n\tau+\mathbf{k}\cdot\mathbf{x})}\phi(K)\right]\left[\nabla e^{i(\omega_m\tau+\mathbf{q}\cdot\mathbf{x})}\phi(Q)\right]\\ &= -\frac{1}{TV}\int_X\sum_{K,Q}\mathbf{k}\cdot\mathbf{q}e^{-i(K+Q)X}\phi(K)\phi(Q) = \frac{1}{T^2}\sum_K|\mathbf{k}|^2\phi(-K)\phi(K),\end{aligned} \tag{5.10}$$

$$\begin{aligned}\int_X m^2\phi^2 &= \frac{m^2}{TV}\int_X\sum_{K,Q}\left[e^{i(\omega_n\tau+\mathbf{k}\cdot\mathbf{x})}\phi(K)\right]\left[e^{i(\omega_m\tau+\mathbf{q}\cdot\mathbf{x})}\phi(Q)\right]\\ &= -\frac{m^2}{TV}\int_X\sum_{K,Q}e^{-i(K+Q)X}\phi(K)\phi(Q) = \frac{m^2}{T^2}\sum_K\phi(-K)\phi(K).\end{aligned} \tag{5.11}$$

The partition function is given by

$$\boxed{Z_0 = \overline{\mathcal{N}} \int \mathcal{D}\phi(K) \exp\left[-\frac{1}{2}\sum_K \phi^*(K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right].} \tag{5.12}$$

Considering the multi-dimensional Gaussian integration $\int \mathrm{d}q_1 \cdots \mathrm{d}q_d e^{-qXq/2} = \sqrt{(2\pi)^d/\det X}$, we further write

$$\boxed{Z_0 = \left(\det \frac{D_0^{-1}(K)}{T^2}\right)^{-1/2},} \tag{5.13}$$

where another constant is omitted for simplicity. Consequently,

$$\boxed{\ln Z_0 = -\frac{1}{2}\ln\det\frac{D_0^{-1}(K)}{T^2} = -\frac{1}{2}\ln\prod_K \frac{D_0^{-1}(K)}{T^2} = -\frac{1}{2}\sum_K \ln\frac{D_0^{-1}(K)}{T^2}.} \tag{5.14}$$

By using the theorem of residue one can perform the sum over Matsubara frequency, then

$$\boxed{\ln Z_0 = -\frac{1}{2}\sum_{n,\mathbf{k}}\frac{\omega_n^2+\epsilon_k^2}{T^2} = -V\int\frac{\mathbf{dk}}{(2\pi)^3}\left[\frac{\epsilon_k}{2T} + \ln\left(1-e^{-\epsilon_k/T}\right)\right],\ \ \epsilon_k = \sqrt{k^2+m^2},} \tag{5.15}$$

the first term here is divergent (zero-point energy).

EXERCISE 20: Argue that $\phi(K)$ is dimensionless, and show that $\int_X e^{iKX} = (V/T)\delta_{K0}$.

EXERCISE 21: Finish the process leading to Eq. (5.15) using complex integration techniques.

EXERCISE 22: Thermodynamic quantities can be obtained via the partition function,

$$\Omega_0 = -T\ln Z_0 = TV\int\frac{\mathbf{dk}}{(2\pi)^3}\left[\frac{\epsilon_k}{2T} + \ln\left(1-e^{-\epsilon_k/T}\right)\right],\ \ P_0 = T\frac{\partial \ln Z_0}{\partial V} = -T\int\frac{\mathbf{dk}}{(2\pi)^3}\left[\frac{\epsilon_k}{2T} + \ln\left(1-e^{-\epsilon_k/T}\right)\right], \tag{5.16}$$

$$E_0 = -\frac{\partial \ln Z_0}{\partial\beta} = V\int\frac{\mathbf{dk}}{(2\pi)^3}\left[\frac{\epsilon_k}{2} + \frac{\epsilon_k}{1-e^{-\epsilon_k/T}}\right],\ \ C_V = \left(\frac{\partial E_0}{\partial T}\right)_V = V\int\frac{\mathbf{dk}}{(2\pi)^3}\frac{\epsilon_k^2 e^{-\epsilon_k/T}}{T^2(1-e^{-\epsilon_k/T})^2}. \tag{5.17}$$

Discuss their high- and low-temperature behaviors. Show that after omitting the vacuum part, the pressure at high temperature is

$$P_0 \approx \frac{\pi^2 T^4}{90} - \frac{m^2T^2}{24} + \frac{m^3T}{12\pi} + \frac{m^4}{2(4\pi)^2}\left(\ln\frac{me^\gamma}{4\pi T} - \frac{3}{4}\right) - \frac{m^6\zeta(3)}{3(4\pi)^4T^2} + \cdots, \tag{5.18}$$

here γ is the Euler constant. What is its low-temperature limit?

The propagator in coordinate space can be obtained as,

$$\begin{aligned} D_0(X) &= \langle\phi(X)\phi(0)\rangle_0 = \left\langle \frac{1}{TV}\sum_{K,Q} e^{-iKX}\phi(K)\phi(Q)\right\rangle_0 = \frac{T}{V}\frac{1}{T^2}\left\langle\sum_{K,Q} e^{-iKX}\phi(K)\phi(Q)\right\rangle_0 \\ &= \frac{T}{V}\sum_K e^{-iKX}\frac{1}{T^2}\sum_Q\langle\phi(K)\phi(Q)\rangle_0 = \frac{T}{V}\sum_K e^{-iKX}\frac{1}{T^2}\langle\phi(K)\phi(-K)\rangle_0, \end{aligned} \tag{5.19}$$

where in the last step one considers the fact that the ensemble average is nonzero only when $K+Q=0$:

$$\langle\phi(P)\phi(Q)\rangle_0 = \frac{\prod_K\int \mathrm{d}\phi(K)\exp\left[-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right]\phi(P)\phi(Q)}{\prod_K\int \mathrm{d}\phi(K)\exp\left[-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right]} = \delta_{P+Q,0}. \tag{5.20}$$

Since

$$D_0(Q) = \frac{1}{T^2}\frac{\prod_K\int \mathrm{d}\phi(K)\exp\left[-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right]\phi(Q)\phi(-Q)}{\prod_K\int \mathrm{d}\phi(K)\exp\left[-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right]} = \frac{1}{T^2}\langle\phi(Q)\phi(-Q)\rangle_0, \tag{5.21}$$

we have

$$D_0(X) = \frac{T}{V}\sum_K e^{-iKX} D_0(Q), \tag{5.22}$$

which could be further written as using Eq. (5.8),

$$\boxed{D_0(X) = T\sum_n \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \frac{e^{i\omega_n\tau + i\mathbf{k}\cdot\mathbf{x}}}{\omega_n^2 + \epsilon_k^2}, \quad \omega_n = 2\pi n T.} \tag{5.23}$$

EXERCISE 23: Prove that in d dimensions, $D_0(X)$ is given by

$$D_0(X) = \int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{2\epsilon_k} \frac{\cosh[(\beta/2 - |x^0|)\epsilon_k]}{\sinh(\beta\epsilon_k/2)}\bigg|_{\epsilon_k = \sqrt{|\mathbf{k}|^2 + m^2}}. \tag{5.24}$$

Discuss its short- and large-distance behaviors.

Interaction may introduce extra novel features to the problem. Here, we consider the ϕ^4 interaction in the form of $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\text{int}} = 2^{-1}\partial_\mu\phi\partial^\mu\phi - 2^{-1}m^2\phi^2 - \lambda\phi^4$. The partition function is similarly given as (the in-front constant is omitted),

$$Z = \int \mathcal{D}\phi e^{-S}, \quad S = S_0 + S_{\text{int}} = \int_X \mathcal{L}_0 + \int_X \mathcal{L}_{\text{int}}, \quad S_{\text{int}} = \lambda\int_X \phi^4. \tag{5.25}$$

Assuming λ is small, then

$$\boxed{\ln Z = \ln\int \mathcal{D}\phi e^{-S_0 - S_{\text{int}}} = \ln\left(\int \mathcal{D}\phi e^{-S_0}\sum_{n=0}^{\infty}\frac{(-S_{\text{int}})^n}{n!}\right),} \tag{5.26}$$

which becomes after subtracting and adding $\ln Z_0$,

$$\boxed{\ln Z = \ln Z_0 + \ln\left(\frac{\int \mathcal{D}\phi e^{-S_0}\sum_{n=0}^{\infty}\frac{(-S_{\text{int}})^n}{n!}}{\int \mathcal{D}\phi e^{-S_0}}\right) = \ln Z_0 + \ln Z_{\text{int}},} \tag{5.27}$$

where

$$\boxed{\ln Z_{\text{int}} \equiv \ln\left(1 + \sum_{n=1}^{\infty}\frac{1}{n!}\frac{\int \mathcal{D}\phi e^{-S_0}}{\int \mathcal{D}\phi e^{-S_0}(-S_{\text{int}})^n}\int \mathcal{D}\phi e^{-S_0}\right) = \ln\left(1 + \sum_{n=1}^{\infty}\frac{\langle(-S_{\text{int}})^n\rangle_0}{n!}\right).} \tag{5.28}$$

Here, $\langle\cdots\rangle_0$ implies that the ensemble average is taken in the free Lagrangian. For example, we have to order λ^3 that

$$\begin{aligned}\ln Z_{\text{int}} &\approx \ln\left(1 - \langle S_{\text{int}}\rangle_0 + \frac{\langle S_{\text{int}}^2\rangle_0}{2} - \frac{\langle S_{\text{int}}^3\rangle_0}{6}\right)\\ &\approx -\langle S_{\text{int}}\rangle_0 + \frac{1}{2}\left(\langle S_{\text{int}}^2\rangle_0 - \langle S_{\text{int}}\rangle_0^2\right) - \frac{1}{6}\left(\langle S_{\text{int}}^3\rangle_0 - 3\langle S_{\text{int}}\rangle_0\langle S_{\text{int}}^2\rangle_0 + 2\langle S_{\text{int}}\rangle_0^3\right).\end{aligned} \tag{5.29}$$

Let's discuss in more details the perturbation at linear order of λ. Since,

$$\langle S_{\text{int}}\rangle_0 = \lambda\frac{\int \mathcal{D}\phi e^{-S_0}\int_X \phi^4(X)}{\int \mathcal{D}\phi e^{-S_0}}, \tag{5.30}$$

where

$$e^{-S_0} = \exp\left(-\frac{1}{2}\sum_K \phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right) = \prod_K \exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right), \tag{5.31}$$

$$\int_X \phi^4(X) = \frac{1}{T^2V^2}\sum_{K_1,\cdots,K_4}\int_X e^{i(K_1+\cdots+K_4)X}\phi(K_1)\cdots\phi(K_4) = \frac{1}{T^3V}\sum_{K_1,\cdots,K_4}\delta(K_1+\cdots+K_4)\phi(K_1)\cdots\phi(K_4), \tag{5.32}$$

we have

$$\langle S_{\rm int}\rangle_0 = \frac{\lambda}{T^3V}\frac{\sum\limits_{K_1,\cdots,K_4}\delta(K_1+\cdots+K_4)\prod\limits_K\int \mathrm{d}\phi(K)\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right)\phi(K_1)\cdots\phi(K_4)}{\prod\limits_K\int \mathrm{d}\phi(K)\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right)}. \tag{5.33}$$

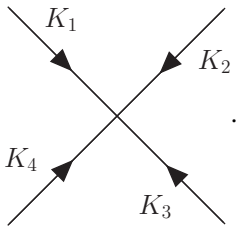
In order to simplify this expression, we notice the integration is nonzero only when K_1, K_2, K_3 and K_4 cancel each other. There are three choices on contracting two momenta (lines) from four, therefore

$$\begin{aligned}\langle S_{\rm int}\rangle_0 =& \frac{3\lambda}{T^3V}\sum_{Q,P}\frac{\prod\limits_K\int \mathrm{d}\phi(K)\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right)\phi(-Q)\phi(Q)\phi(-P)\phi(P)}{\prod\limits_K\int \mathrm{d}\phi(K)\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right)}\\ =& \frac{3\lambda}{T^3V}\left[\sum_Q\frac{\prod\limits_Q\int \mathrm{d}\phi(Q)\exp\left(-\frac{1}{2}\phi(-Q)\frac{D_0^{-1}(Q)}{T^2}\phi(Q)\right)\phi(Q)\phi(-Q)}{\prod\limits_Q\int \mathrm{d}\phi(Q)\exp\left(-\frac{1}{2}\phi(-Q)\frac{D_0^{-1}(Q)}{T^2}\phi(Q)\right)}\right]^2.\end{aligned} \tag{5.34}$$

Using the expression for $D_0(Q)$ leads us to

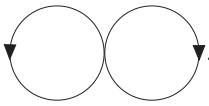
$$\ln Z_{\rm int}^{(1)} = -\langle S_{\rm int}\rangle_0 = -3\lambda\frac{T}{V}\left[\sum_Q D_0(Q)\right]^2. \tag{5.35}$$

Graphically, we use the following diagram to represent the interaction $\lambda\phi^4$ (vertex),



. (5.36)

Contracting the four external lines then gives the corresponding contribution,

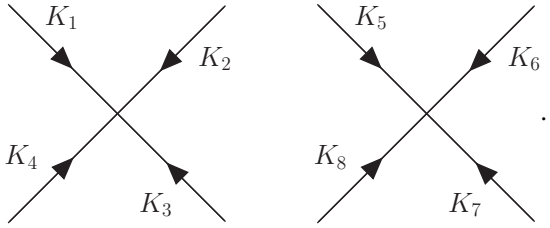
$$-\langle S_{\rm int}\rangle_0 = -3\lambda\frac{T}{V}\left[\sum_Q D_0(Q)\right]^2 = 3$$  . (5.37)

Here, each vertex induces the coupling constant $-\lambda$ one time and each closed loop corresponds to $T/V\sum_Q D_0(Q)$. Moreover, momentum conservation gives the factor $V/T\delta(K_{\rm in}-K_{\rm out})$, and "3" is the combinatorial factor.

There is only one linked diagram in the first-order approximation. The un-linked diagrams in $\ln Z$ would be canceled with each other, e.g., in the second-order approximation, we have

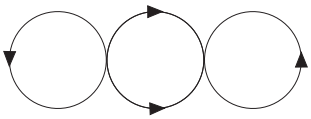
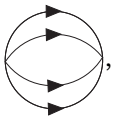
$$\ln Z_{\rm int}^{(2)} = \frac{1}{2}\left(\langle S_{\rm int}^2\rangle_0 - \langle S_{\rm int}\rangle_0^2\right). \tag{5.38}$$

Here the diagram corresponding to $\langle S_{\rm int}^2\rangle_0$ should be constructed from $(-\lambda\phi)^2$, namely from the following diagrams,

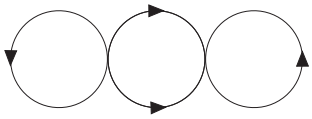


. (5.39)

One possibility is contracting the left and diagram separably and obtaining two bubble diagrams, which cancel the contribution from the term $\langle S_{\rm int}\rangle_0^2$, and the remaining contribution is given by

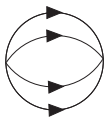
$$\ln Z_{\rm int}^{(2)} = 36$$  $$+ 12$$  , (5.40)

here "36" and "12" are other related combinatorial factors. In particular, we have the following "translations",



$$= (-\lambda)^2 \left(\frac{T}{V}\right)^4 \left(\frac{V}{T}\right)^2 \sum_{K_1,\cdots,K_4} \delta(K_2+K_3) D_0(K_1)\cdots D_0(K_4)$$

$$= \lambda^2 \frac{T^2}{V^2} \left[\sum_K D_0(K)\right]^2 \sum_{K_2,K_3} \delta(K_2+K_3) D_0(K_2) D_0(K_3), \tag{5.41}$$

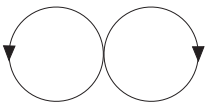
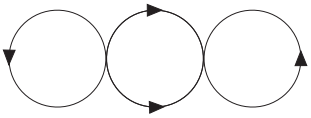
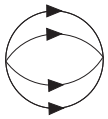


$$= (-\lambda)^2 \left(\frac{T}{V}\right)^4 \left(\frac{V}{T}\right)^2 \sum_{K_1,\cdots,K_4} \delta(K_1+\cdots+K_4) D_0(K_1)\cdots D_0(K_4). \tag{5.42}$$

One can prove mathematically that

$$\boxed{\ln Z_{\rm int} = \sum_{n=1}^{\infty} \frac{(-)^n \langle S_{\rm int}^n\rangle_{0,\text{connected}}}{n!},} \tag{5.43}$$

which is called the linked-cluster theorem. Consequently, we have to order λ^2 that,

$$\ln Z_{\rm int} \approx 3$$  $$+ 36$$  $$+ 12$$  $$+ \mathcal{O}(\lambda^3).$$ (5.44)

We will see in the following that these diagrams are not complete, and there would be terms proportional to $\lambda^{3/2}$.

The full propagator could be decomposed into the free part and the interaction part (i.e., self-energy),

$$\boxed{D^{-1}(K) = D_0^{-1}(K) + \Pi(K).} \tag{5.45}$$

The connection between Π and $\ln Z_{\rm int}$ could be established as follows. Since $\ln Z = \ln \int \mathcal{D}\phi e^{-S_0 - S_{\rm int}}$, we have

$$\begin{aligned}
\frac{\delta \ln Z}{\delta D_0^{-1}(Q)} &= \frac{1}{\int \mathcal{D}\phi e^{-S_0-S_{\rm int}}} \frac{\delta}{\delta D_0^{-1}(Q)} \int \mathcal{D}\phi e^{-S_0} e^{-S_{\rm int}} \\
&= \frac{1}{\int \mathcal{D}\phi e^{-S_0-S_{\rm int}}} \frac{\delta}{\delta D_0^{-1}(Q)} \prod_K \int \mathrm{d}\phi(K) \exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right) e^{-S_{\rm int}} \\
&= -\frac{1}{2T^2} \frac{\int \mathcal{D}\phi e^{-S_0-S_{\rm int}} \phi(-Q)\phi(Q)}{\int \mathcal{D}\phi e^{-S_0-S_{\rm int}}} = -\frac{1}{2} D(Q),
\end{aligned} \tag{5.46}$$

therefore

$$\boxed{D(Q) = -2\frac{\delta \ln Z}{\delta D_0^{-1}} = 2D_0^2 \frac{\delta \ln Z}{\delta D_0}.} \tag{5.47}$$

According to the definition of (5.45), we obtain $D = [D_0^{-1} + \Pi]^{-1} = D_0[1 + D_0\Pi]^{-1}$. From the relation (5.47) we then have

$$\boxed{\frac{1}{1+\Pi D_0} = 2D_0 \frac{\delta \ln Z}{\delta D_0}.} \tag{5.48}$$

By expanding both sides of Eq. (5.48) over λ and writing the self-energy in the series of $\Pi = \sum_{n=1}^{\infty} \Pi_n$, one can find that Π_n is proportional to λ^n. For instance, we have at order λ^2 that,

$$\frac{1}{1+\Pi D_0} = 1 - D_0\Pi_1 - D_0\Pi_2 + D_0\Pi_1 D_0\Pi_1 + \mathcal{O}(\lambda^3). \tag{5.49}$$

Eq. (5.14) gives $\delta \ln Z_0/\delta D_0 = 2^{-1} D_0^{-1}$, and therefore

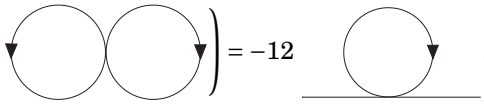
$$2D_0 \frac{\delta \ln Z}{\delta D_0} = 2D_0 \left(\frac{\delta \ln Z_0}{\delta D_0} + \frac{\delta \ln Z_{\rm int}}{\delta D_0} \right) = 1 + 2D_0 \frac{\delta \ln Z_{\rm int}}{\delta D_0} \approx 1 + 2D_0 \left[-\frac{\delta \langle S_{\rm int}\rangle_0}{\delta D_0} + \frac{1}{2} \frac{\delta(\langle S_{\rm int}^2\rangle_0 - \langle S_{\rm int}\rangle_0^2)}{\delta D_0} \right]. \tag{5.50}$$

We consequently obtain,

$$\boxed{\Pi_1 + \Pi_2 - \Pi_1 D_0 \Pi_1 + \cdots = -2 \frac{\delta \ln Z_{\rm int}}{\delta D_0}, \ \text{with} \ \ \Pi_1 = 2 \frac{\delta \langle S_{\rm int}\rangle_0}{\delta D_0}, \ \ \Pi_2 - \Pi_1 D_0 \Pi_1 = -\frac{\delta(\langle S_{\rm int}^2\rangle_0 - \langle S_{\rm int}\rangle_0^2)}{\delta D_0}.} \tag{5.51}$$

One can express the self-energy Π_1 graphically as

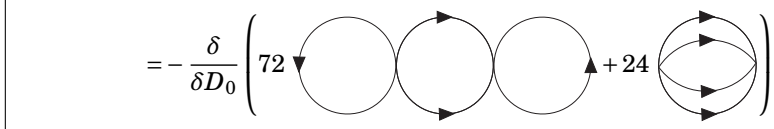
$$\boxed{\Pi_1 = 6\lambda \frac{T}{V} \frac{\delta}{\delta D_0} \left[\sum_K D_0(K) \right]^2 = 12\lambda \frac{T}{V} \sum_K D_0(K) = -2 \frac{\delta}{\delta D_0} \left(3 \right) = -12} \ \ .$$



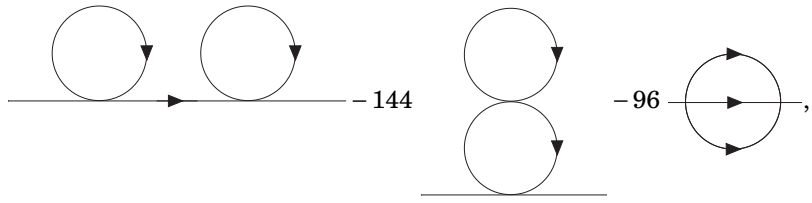
We find calculating the functional derivative with respect to the propagator is equivalent to cutting a line. Similarly,

$$\Pi_2 - \Pi_1 D_0 \Pi_1 = -\frac{\delta(\langle S_{\rm int}^2\rangle_0 - \langle S_{\rm int}\rangle_0^2)}{\delta D_0} \tag{5.53}$$

$$= -\frac{\delta}{\delta D_0} \left(72 \ + 24 \right) \tag{5.54}$$

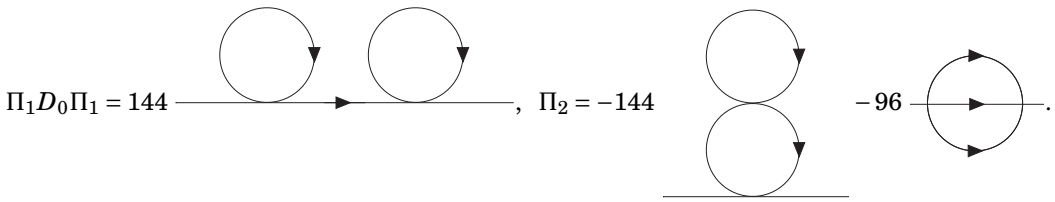


$$= -144 \ - 144 \ - 96 \ , \tag{5.55}$$



therefore

$$\Pi_1 D_0 \Pi_1 = 144 \ , \quad \Pi_2 = -144 \ - 96 \ . \tag{5.56}$$



The self-energy is in fact constructed from the one–particle–irreducible (1PI), i.e.,

$$\boxed{\Pi = -2 \left(\frac{\delta \ln Z_{\rm int}}{\delta D_0} \right)_{\rm 1PI}.} \tag{5.57}$$

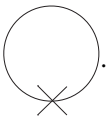
Check Π_1 and Π_2 for this relation.

We calculate the contribution from Π_1 to the pressure. In order to do that, we first write out the expression for Π_1,

$$\Pi_1 = 12\lambda \frac{T}{V} \sum_K \frac{1}{\omega_n^2 + \epsilon_k^2} = \Pi_1^{\rm vac} + \Pi_1^T = 6\lambda \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\epsilon_k} + 12\lambda \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{f(\epsilon_k)}{\epsilon_k}, \ \ f(\epsilon_k) = \frac{1}{e^{\epsilon_k/T} - 1}. \tag{5.58}$$

The temperature-dependent part is convergent while the vacuum contribution diverges. We can remove the divergent

vacuum contribution by using the renormalized self-energy, $\Pi_1^{\rm ren} = \Pi_1 - \Pi_1^{\rm vac}$. Then the modified propagator is given by $D^{-1}(K) = \omega_n^2 + k^2 + m^2 + \Pi_1$. We see that the self-energy plays a similar role as the mass squared term in the Lagrangian, and we can account for this effect by adding the a contribution in the original Lagrangian as $\mathcal{L} \to \mathcal{L} - 2^{-1}\delta m^2 \phi^2$. This added new term could be treated as another interaction and δm^2 has the same order as λ. Its graph is represented as

$\delta m^2 \langle \phi^2 \rangle_0 =$  . (5.59)

The cutting rule then gives the corresponding contribution to the self-energy as

$\delta m^2 =$  . (5.60)

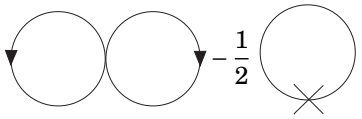
In this sense, we can obtain finite result by selecting the renormalized scheme $\delta m^2 = -\Pi_1^{\rm vac}$.

For massless Boson ($m = 0$), which is equivalent to high temperature $T \gg m$, we have

$$\boxed{\Pi_1^{\rm ren} = 12\lambda \int \frac{{\rm d}\mathbf{k}}{(2\pi)^3} \frac{f(\epsilon_k)}{\epsilon_k} \approx \lambda T^2,} \tag{5.61}$$

where the relation $\int_0^\infty x{\rm d}x/(e^x - 1) = \pi^2/6$ is used. We see that the massless Boson acquires a thermal mass λT^2 at high temperatures. The $\ln Z_{\rm int}$ at order λ is given by including the mass-correction term as,

$$\ln Z_{\rm int}^{(1)} = 3 \quad - \frac{1}{2} \quad = -3\lambda \frac{V}{T} \left[\frac{T}{V} \sum_Q D_0(Q) \right]^2 - \frac{1}{2} \delta m^2 \sum_Q D_0(Q)$$



$$= -\frac{V}{T} \frac{1}{48\lambda} \left(\Pi_1^{\rm vac} + \Pi_1^T \right)^2 + \frac{V}{T} \frac{1}{24\lambda} \Pi_1^{\rm vac} \left(\Pi_1^{\rm vac} + \Pi_1^T \right) = \frac{V}{T} \frac{1}{48\lambda} \left(\Pi_1^{{\rm vac},2} - \Pi_1^{T,2} \right), \tag{5.62}$$

therefore we obtain (after removing the vacuum part),

$$\boxed{\frac{T}{V} \ln Z_{\rm int}^{(1)} = -3\lambda \left[\int \frac{{\rm d}\mathbf{k}}{(2\pi)^3} \frac{f(\epsilon_k)}{\epsilon_k} \right]^2 \approx -\frac{\lambda T^4}{48}.} \tag{5.63}$$

The corresponding expression for the pressure is then,

$$\boxed{P = \frac{\pi^2 T^4}{90} \left(1 - \frac{15}{8} \frac{\lambda}{\pi^2} + \cdots \right).} \tag{5.64}$$

We have already seen that the first-order perturbation adds a thermal mass λT^2 to the massless particle. At low momentum/energy (near the thermal mass scale), i.e., $\omega_n^2, |\mathbf{k}|^2 \sim \lambda T^2$, the free propagator $D_0^{-1} = \omega_n^2 + k^2$ itself is on the order of λT^2. However, the contribution from the self-energy is also on such order, implying the above perturbative calculation is unreasonable. Actually, we need to consider an infinite series of graphs to remove the infrared divergence, a technique sometimes called resummation. The full propagator should be used instead of the free one, i.e.,

$$\Pi = 12\lambda \frac{T}{V} \sum_K D(K) = 12\lambda \frac{T}{V} \sum_K \frac{1}{D_0^{-1}(K) + \Pi}, \tag{5.65}$$

this is a self-consistent equation for Π. We expand the term above to obtain,

$$\frac{1}{D_0^{-1}(K) + \Pi} = D_0 \sum_{n=0}^\infty (-\Pi D_0)^n, \quad \Pi = 12\lambda \frac{T D_0}{V} \sum_K \sum_{n=0}^\infty (-\Pi D_0)^n. \tag{5.66}$$

If one uses Π_1 to approximate Π in (5.65) then there would be a large loop on which n small loops are attached. Such diagram is often called a daisy diagram. Iterating the process further, one should obtain the so-called super-daisy diagram. We would like to point out that although there are many many loops in the diagram the overall structure of the self-energy is still one-loop. We now write Eq. (5.65) in the following more apparent form,

$$\Pi = 12\lambda \int \frac{{\rm d}\mathbf{k}}{(2\pi)^3} T \sum_n \frac{1}{\omega_n^2 + k^2 + \Pi} = 12\lambda \int \frac{{\rm d}\mathbf{k}}{(2\pi)^3} \frac{f\left(\sqrt{k^2 + \Pi}\right)}{\sqrt{k^2 + \Pi}}, \tag{5.67}$$

where the sum over Matsubara is used and the zero-temperature is removed. By introducing a new integration variable $x = \sqrt{k^2/\Pi + 1}$ we can obtain the equation $1 = (6\lambda/\pi^2)\int_1^\infty \mathrm{d}x\,\sqrt{x^2-1} f(\sqrt{\Pi}x)$. According to the formula,

$$\int_1^\infty \mathrm{d}x\,\sqrt{x^2-1} f(ux) = \frac{2\pi^2 T^2}{u^2}\left[\frac{1}{12} - \frac{u}{4\pi T} + \mathcal{O}\left(\frac{u^2}{T^2}\ln\frac{u}{T}\right)\right], \tag{5.68}$$

we obtain

$$\boxed{\Pi = \lambda T^2 - \frac{3T^2\lambda^{3/2}}{\pi} + \cdots.} \tag{5.69}$$

We find that the next-order contribution is proportional to $\lambda^{3/2}$ instead of λ^2.

EXERCISE 24: Plot $\Pi^{1/2}/T$ as a function of λ using the exact solution, the solutions at orders λ and $\lambda^{3/2}$.

The partition function including interaction could similarly be obtained,

$$\boxed{\ln Z_{\rm int} = -\langle S_{\rm int}\rangle_0 + \sum_{N=2}^\infty \frac{(-1)^N \langle S_{\rm int}^N\rangle_{0,\rm c}}{N!},} \tag{5.70}$$

here "c" abbreviates for "connected", and

$$\begin{aligned}
\sum_{N=2}^\infty \frac{(-1)^N\langle S_{\rm int}^N\rangle_{0,\rm c}}{N!} &= \sum_{N=2}^\infty \frac{(-)^N}{N!} 6^N 2^{N-1}(N-1)! \quad \text{(}N\text{ loops)} \\
&= \sum_{N=2}^\infty \frac{1}{N!} 6^N 2^{N-1}(N-1)! V \sum_n \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \frac{(-\Pi_1)^N}{12^N} D_0^N(K) = \frac{V}{2}\sum_n \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \sum_{N=2}^\infty \frac{1}{N}[-\Pi_1 D_0(K)]^N \\
&= -\frac{V}{2}\sum_n \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\{\ln[1+\Pi_1 D_0(K)] - \Pi_1 D_0(K)\} = -\frac{V}{2}\sum_n \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\left[\ln\left(1+\frac{\lambda T^2}{\omega_n^2+k^2}\right) - \frac{\lambda T^2}{\omega_n^2+k^2}\right].
\end{aligned} \tag{5.71}$$

The pressure is given by combining the zero-temperature contribution and the mode of $n = 0$ above, i.e.,

$$\boxed{P \approx \frac{\pi^2 T^4}{90} - \frac{\lambda T^4}{48} - \frac{T}{2}\int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\left[\ln\left(1+\frac{\lambda T^2}{k^2}\right) - \frac{\lambda T^2}{k^2}\right] \approx \frac{\pi^2 T^4}{90}\left[1 - \frac{15}{8}\frac{\lambda}{\pi^2} + \frac{15}{2}\left(\frac{\lambda}{\pi^2}\right)^{3/2} + \cdots\right].} \tag{5.72}$$

We see again that the next-order contribution to the pressure is $\lambda^{3/2}$.

EXERCISE 25: Prove the relation:

$$\int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\left[\ln\left(1+\frac{\lambda T^2}{k^2}\right) - \frac{\lambda T^2}{k^2}\right] = -\frac{\lambda^{3/2}T^3}{6\pi}. \tag{5.73}$$

Discuss how the potential divergence maybe removed.

Perturbatively determining/analyzing different types of correction to a given quantity is a central theme in physical calculations. Finally, we give a few examples and point out certain important ingredients when necessary.

Example – 1. The main feature of the estimation on the order of magnitude and approximated perturbative calculations could be clearly demonstrated in some very elementary mathematical problems. For instance, it could be shown when trying to solve the following simple algebraic equation,

$$x^n(t) = \Omega + t x(t)/\Lambda, \quad x(t) \in \mathrm{R}^+, \quad n \in \mathrm{N}^+, \quad n \geq 5, \quad t \geq 0, \tag{5.74}$$

where t and Λ are two parameters (e.g., t is the time) with Λ a positive constant. As we all know there is no closed formula for the simple algebraic equation if the order of the equation is larger than or equal to five. In this sense we need use either numerical algorithms or approximated methods to investigate the root of the equation like (5.74). If the "time" t is small near zero, the second term on the left hand side of Eq. (5.74) could be treated as a perturbation and in this case we could assume $x(t) \approx x_0[1+\delta(t)] = \Omega^{1/n}[1+\delta(t)]$ with $\delta(t)$ a small correction to the leading order solution "1". Expanding both sides of Eq. (5.74) to order $\delta(t)$, one obtains $\delta(t) = t\Omega^{1/n-1}/n\Lambda$ and then,

$$x(t) \approx \Omega^{1/n}\left(1 + \frac{1}{n\Lambda}\Omega^{1/n-1}t\right). \tag{5.75}$$

The above (approximated) theory will be broken if $t \lesssim n\Lambda\Omega^{1-1/n}$. The approximated theory here is often called the linear perturbation and the basic requirement is that the t should not be larger than $n\Lambda\Omega^{1-1/n}$, e.g., $t \lesssim t_{\max} \approx sn\Lambda\Omega^{1-1/n}, s \ll 1$. Moreover, if one considers the next contribution to the solution, i.e., $x(t) = \Omega^{1/n}(1+\alpha t+\beta t^{\sigma})$, where $\alpha = \Omega^{1/n-1}/n\Lambda$, then after some straightforward calculations, one obtains that $\sigma = 2$ and consequently,

$$x(t) \approx \Omega^{1/n}\left(1+\frac{1}{n\Lambda}\Omega^{1/n-1}t-\frac{n-3}{2n^2\Lambda^2}\Omega^{2/n-2}t^2\right). \tag{5.76}$$

One has that $t \ll n\Lambda\Omega^{1-1/n}$ from the first-order theory. If higher order corrections are taken into consideration, e.g., the second-order contribution appeared in (5.76), the condition for the perturbation theory is obtained as $|(n-3)\delta^2(t)/2| \ll |\delta(t)|$, or equivalently $|(n-3)\delta(t)/2| \ll 1$, or $t \ll 2n\Lambda\Omega^{1-1/n}/(n-3)$. It becomes $t \ll 2\Lambda\Omega^{1-1/n} \sim 2\Lambda\Omega$ if n is large, which is weaker than the criterion $t \ll n\Lambda\Omega^{1-1/n}$, indicating the effective perturbative region shrinks as the order of the expansion increases. The perturbation element (or the small quantity in general) of the Eq. (5.74) is $\delta(t) = \alpha t = \Omega^{1/n-1}t/n\Lambda$, and consequently $x(t) \approx \Omega^{1/n}[1+\delta(t)-(n-3)\delta^2(t)/2]$. It is obvious that it could not be treated as small when the t is large, indicating that either the linear theory or the theory with higher order terms breaks down at large t. However, on the other hand, in the limit that the t approaches to infinity, another perturbative scheme for Eq. (5.74) emerges. In that situation, the term Ω on the right hand side of the equation (5.74) could be safely neglected, leading to $x_\infty(t) = (t/\Lambda)^{1/(n-1)}$, and it is called the asymptotic solution (large-t) of Eq. (5.74). Assuming that $x(t) \approx x_\infty(t)[1+\phi(t)]$ based on the asymptotic solution and the factor $|\phi(t)| \ll 1$, one could obtain,

$$x(t) \approx \left(\frac{t}{\Lambda}\right)^{\frac{1}{n-1}}\left[1+\frac{\Omega}{n-1}\left(\frac{\Lambda}{t}\right)^{\frac{n}{n-1}}\right], \quad \phi(t) = \frac{\Omega}{n-1}\left(\frac{\Lambda}{t}\right)^{\frac{n}{n-1}}, \tag{5.77}$$

with the condition that

$$t \gg t_{\rm asp} \equiv \Lambda\exp\left(-\frac{n-1}{n}\ln\left(\frac{n-1}{\Omega}\right)\right). \tag{5.78}$$

Moreover, considering that $x(t) \approx x_\infty(t)[1+\phi(t)+\mu(t)]$ to even higher order with $\mu(t)$ the contribution smaller than $\phi(t)$, we have

$$x(t) \approx \left(\frac{t}{\Lambda}\right)^{\frac{1}{n-1}}\left[1+\frac{\Omega}{n-1}\left(\frac{\Lambda}{t}\right)^{\frac{n}{n-1}}-\frac{n\Omega^2}{2(n-1)^2}\left(\frac{\Lambda}{t}\right)^{\frac{2n}{n-1}}\right], \tag{5.79}$$

and thus $x(t) \approx x_\infty(t)[1+\phi(t)-n\phi^2(t)/2]$, i.e., $\mu(t) = -n\phi^2(t)/2$. The exact solution of the algebraic equation (5.74) could be numerically constructed (e.g., iterative scheme or the Newton's algorithm).

Example – 2: an effective Hooke's "constant". Consider the particle moves under a potential having a minimum x_0. For motion around x_0, the potential acting on the particle could be approximated by expanding the potential $U(x)$ as,

$$U(x) \approx U(x_0)+\dot{U}|_{x=x_0}\delta x+2^{-1}\ddot{U}|_{x=x_0}\delta x^2, \tag{5.80}$$

where $\delta x^n = (x-x_0)^n$, $\dot{U} = {\rm d}U/{\rm d}x$, and $\ddot{U} = {\rm d}^2U/{\rm d}x^2$, and since the first-order derivative of the potential at the equilibrium x_0 is zero, one obtains

$$\boxed{U_{\rm harm}(\delta x) = 2^{-1}k^2\delta x^2+{\rm const.}, \quad k = [U''(x_0)]^{1/2},} \tag{5.81}$$

where the constant is the zero point of the potential (which actually has no fundamental effects on the dynamics processes). The above one is called the harmonic potential, and the solution of which could be obtained exactly. Now, if one tries to study the behavior of the particle far from the equilibrium position x_0, the natural treatment is investigating the effects from the high order terms (e.g., the term δx^3) perturbatively based on the harmonic solution. This is the frequently-used method in physical problems: Firstly obtaining the solution via the simple approximation (here it is given by $U_{\rm harm}(\delta x)$, the terms like this are often called the non-interacting terms), and then perturbatively computing the high order effects based on the simple solution. The oscillation around the meta-stable states if they exist is also important and the transition from the meta-stable states to the global ground state is an exciting issue in modern field calculations.[1] Consider the extra force $f^\delta(x)$ based on Hooke's force in the harmonic system, $\delta x \to x$. In this situation the energy conservation equation becomes $2^{-1}m\dot{x}^2+2^{-1}kx^2+U^\delta(x) = 2^{-1}kd_{\max}^2+U^\delta(d_{\max})$, where $d_{\max}$ the maximum distance the oscillator could reach, and $U^\delta(x)$ is the potential due to the extra force. If the extra potential is homogeneous with order α, i.e., $U^\delta(\lambda x) = \lambda^\alpha U^\delta(x)$, the period of the system could be given generally by

$$\boxed{T = 4\sqrt{\frac{m}{k}}\int_0^{\pi/2}{\rm d}\eta\left[1+\frac{2U^\delta(d_{\max})[1-\sin^\alpha\eta]}{kd_{\max}^2\cos^2\eta}\right]^{-1/2}.} \tag{5.82}$$

[1] The tunneling between the true and false vacuum states was investigated in S. Coleman, *Fate of the False Vacuum: Semiclassical Theory*, Phys. Rev. D **15**, 2929 (1977); C. Callan and S. Coleman, *Fate of the False Vacuum. II: First Quantum Corrections*, Phys. Rev. D **16**, 1762 (1977).

In certain situations one can do perturbative calculations based on $\xi = 2U^\delta(d_{\max})[1-\sin^\alpha\eta]/kd_{\max}^2\cos^2\eta$. By taking the extra force as $f^\delta(x) = -ax^3 (a>0)$, $\xi = (ad_{\max}^2/2k)(1+\sin^2\eta)$, the effective potential is then given by $U_{\rm eff}(x) = U_{\rm tot}(x) = 2^{-1}kx^2 + 4^{-1}ax^4$, characterizing the cubic response to the perturbation. However, such effective potential has actually little use since the high order term here still contains the dynamical variable "x". One could obtain to order a^2 that,

$$T \approx 2\pi\sqrt{\frac{m}{k}} \times \left(1 - \frac{3ad_{\max}^2}{8k} + \frac{57a^2d_{\max}^4}{256k^2}\right), \tag{5.83}$$

and the perturbative condition is $\sigma = ad_{\max}^2/k \ll 1$, or equivalently $U^\delta(d_{\max}) \ll U(d_{\max})/2$. In this formula, if the replacements, $m/k \leftrightarrow \ell/g$, $d_{\max} = \chi_{\max}\ell$ and $a = -mg/6\ell^3$ are made, one immediately obtains the first-order correction coefficient 1/16 in the period of the simple pendulum, namely

$$\boxed{T \approx 2\pi\sqrt{\frac{\ell}{g}} \times \left(1 + \frac{1}{16}\chi_{\max}^2 + \frac{11}{3072}\chi_{\max}^4 + \cdots\right),} \tag{5.84}$$

where $\chi_{\max}$ is the maximum angle of the simple pendulum. However the even higher order corrections could not be obtained simply through (5.83), since the period of the simple pendulum contains higher order corrections from $\sin\chi$. The correction directly from the term ax^3 corresponds to the conventional perturbation theories, and the one characterized by the factor $1 + 16^{-1}\chi_{\max}^2 + (11/3072)\chi_{\max}^4 + \cdots$ corresponds to the improved perturbations. The fourth-order correction $(11/3072)\chi_{\max}^4$ in the period of the simple pendulum could be decomposed into two terms: the $\chi_{\max}^2$ term and the $\chi_{\max}^4$ term from the interacting energy $E(\chi_{\max}) = -mg\ell\cos\chi_{\max} \approx -mg\ell(1 - 2^{-1}\chi_{\max}^2 + 24^{-1}\chi_{\max}^4 + \cdots)$, or equivalently the terms proportional to χ and to χ^3 in the force $F(\chi) = -mg\sin\chi \approx -mg(\chi - 6^{-1}\chi^3)$. One could obtain the corresponding nonlinear effects simply by considering the χ^3 term based on the harmonic approximation, but the coefficient is 19/3072 (via the formula (5.83)) instead of 11/3072. Improved perturbation indicates that besides the "direct" term — χ^3, the higher order term originated from χ (e.g., the first term in $\sin\chi \approx \chi - \chi^3/6$) also contributes to the coefficient 11/3072. This latter one is denoted as the "indirect" contribution; in other words, there exists the mode-coupling between the low modes (here characterized by χ) and the high modes (characterized by χ^3), in the sense $\chi^3 \leftarrow (\chi^3)^1$ (direct term) + $(\chi^1)^3$ (indirect high order terms). As the index "n" appearing in χ^n becomes large, the mode-coupling pattern will also become more fruitful. We introduce the very basic concept of effective theories. In the case of the force ax^3, one could derive an effective Hooke's constant through the period of the system. In particular, according to the general period formula, one has $T = 2\pi(m/k_{\rm eff})^{1/2} = 2\pi m^{1/2}k_{\rm eff}^{-1/2}$ where the effective spring constant is $k_{\rm eff} \approx k(1 + s_1\sigma + s_2\sigma^2) + \mathcal{O}(\sigma^3)$ with $\sigma = ad_{\max}^2/k \ll 1$. In order to reproduce the first two terms as shown in the formula (5.83), i.e., $-3\sigma/8$ and $57\sigma^2/256$, one obtains the two coefficients $s_1 = 3/4$ and $s_2 = -3/128$. The effective Hooke's constant is thus[2]

$$\boxed{k_{\rm eff} \approx k \times \left(1 + \frac{3}{4}\frac{ad_{\max}^2}{k} - \frac{3}{128}\frac{a^2d_{\max}^4}{k^2}\right),} \tag{5.85}$$

and in other applications one could use the effective potential $U_{\rm eff}(x) = 2^{-1}k_{\rm eff}x^2$. Here the high order effects characterized by the coefficient a appears in the low-order coefficient and the "dynamical" variable "x" disappears at the fourth order. However, there exist other approaches to construct the effective parameters, e.g., the Hooke's constant in the presence of the nonlinear force could also be obtained as $\bar{k}_{\rm eff} = k + ad_{\max}^2/2$ by considering the maximum distance, indicating other mechanisms need to be taken into account in the construction of an effective theory. We have no attempt to introduce/discuss these advanced issues in the present lecture. The effective theories with the high order degrees of freedom integrated out are often called the "low-energy effective theories".

Example – 3: equation of state of a unitary Fermi gas. The unitary limit refers to $ak_{\rm F} \to \infty$ where a is the scattering length and $k_{\rm F} = p_{\rm F}$ is the Fermi momentum of the system under consideration. Obviously, the conventional perturbative schemes based on the small quantity $ak_{\rm F}$ does not apply for the unitary Fermi gas. Conventionally, the equation of state (defined as the energy per particle) for small $ak_{\rm F}$ is given by

$$\boxed{\text{EOS} \approx \frac{k_{\rm F}^2}{2m}\left(\frac{3}{5} + \frac{2}{3\pi}k_{\rm F}a + \frac{4}{35\pi^2}(11 - 2\ln 2)(k_{\rm F}a)^2 + 0.23(k_{\rm F}a)^3 + \cdots\right),} \tag{5.86}$$

here $k_{\rm F} = (3\pi^2\rho)^{1/3}$ with ρ being the density. The first term here, namely $3k_{\rm F}^2/10m$ is the free-gas result and $E_{\rm F} \equiv k_{\rm F}^2/2m$ is the Fermi energy. We want to analyze $\xi \equiv \mu/E_{\rm F}$, the Bertsch parameter. Theoretical analysis tells us that besides the limit $ak_{\rm F} \to 0$, the 4D system is also free. The wave function of a pair of Fermions with opposite spins in dimensions d is $R(r) \sim r^{2-d}$, here d is the distance between the Fermions. When calculating relevant quantities, one needs $\int d\mathbf{x}|R(r)|^2 \sim$

[2] See, B.J. Cai and B.A. Li, *Auxiliary Function Approach for Determining Symmetry Energy at Suprasaturation Densities*, Phys. Rev. C **103**, 054611 (2021), Section III.

$\int \mathrm{d}r r^{d-1} r^{4-2d} \sim \int \mathrm{d}r r^{3-d}$, implying the probability of emergence of such pair near $r=0$ for $d \geq 4$ is large (singularity). In this sense, we say that the system in 4D is the non-interacting, $\xi = 0$, and one can develop effective theories in 4D and extrapolate the corresponding equation of state to 3D; the idea of Nishida–Son effective theory.[3] The Lagrangian is

$$\boxed{\mathcal{L} = \sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^\dagger \left(i\partial_t + \frac{\nabla^2}{2m} + \mu_\sigma \right) \psi_\sigma + c_0 \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow = \Psi^\dagger \left(i\partial_t + \frac{\sigma_3 \nabla^2}{2m} + \mu\sigma_3 + \delta\mu \right) \Psi - \frac{1}{c_0} \phi^\dagger \phi + \Psi^\dagger \sigma_+ \Psi \phi + \Psi^\dagger \sigma_- \Psi \phi^\dagger,} \tag{5.87}$$

where $\Psi = (\psi_\uparrow, \psi_\downarrow^\dagger)^{\mathrm{T}}$ are the two-component Nabmu–Gorkov field, σ_i with $i = 1 \sim 3$ are the three Pauli matrices, $\sigma_\pm = (\sigma_1 \pm \sigma_2)/2$, $\mu = (\mu_\uparrow + \mu_\downarrow)/2$, $\delta\mu = (\mu_\uparrow - \mu_\downarrow)/2$, and c_0 is the interaction strength between two Fermions. By introducing $\phi = \phi_0 + g\varphi$ where $g = [(8\pi^2\epsilon)^{1/2}/m](m\phi_0/2\pi)^{\epsilon/4}$, $\epsilon = 4-d$ and φ being the fluctuating field and ϕ_0 the ground state (condensate), one can expand the Lagrangian as $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1 + \mathcal{L}_2$:

$$\mathcal{L}_0 = \Psi^\dagger \left(i\partial_t + \frac{\sigma_3 \nabla^2}{2m} + \sigma_+ \phi_0 + \sigma_- \phi_0 \right) \Psi + \varphi^\dagger \left(i\partial_t + \frac{\nabla^2}{4m} \right) \varphi, \tag{5.88}$$

$$\mathcal{L}_1 = g\Psi^\dagger \sigma_+ \Psi \varphi + g\Psi^\dagger \sigma_- \Psi \varphi^\dagger + \mu \Psi^\dagger \sigma_3 \Psi + 2\mu\varphi^\dagger \varphi, \quad \mathcal{L}_2 = -\varphi^\dagger \left(i\partial_t + \frac{\nabla^2}{4m} \right) \varphi - 2\mu\varphi^\dagger\varphi. \tag{5.89}$$

Here, $\mathcal{L}_0$ is the free part and the mass of a Fermion pair is $2m$, $\mathcal{L}_1$ and $\mathcal{L}_2$ define the vertices. The Fermion and the Boson propagators are given by,

$$G(p_0, \mathbf{p}) = \frac{1}{p_0^2 - \varepsilon^2(\mathbf{p}) + i0^+} \begin{pmatrix} p_0 + E(\mathbf{p}) & -\phi_0 \\ -\phi_0 & p_0 - E(\mathbf{p}) \end{pmatrix}; \; D(p_0, \mathbf{p}) = \left(p_0 - \frac{E(\mathbf{p})}{2} + i0^+ \right)^{-1}, \tag{5.90}$$

where $E(\mathbf{p}) = \mathbf{p}^2/2m$ is the single-particle energy, $\varepsilon(\mathbf{p}) = [E^2(\mathbf{p}) + \phi_0^2]^{1/2}$ is the dispersion relation. Based on this effective theory, one can show that the 1-loop and 2-loop potentials are,

$$U_{\mathrm{eff}}^{(1)}(\phi_0) = \frac{\phi_0}{3} \left[1 + \frac{7 - 3(\gamma + \ln 2)}{6} \epsilon \right] \left(\frac{m\phi_0}{2\pi} \right)^{d/2} - \frac{\mu}{\epsilon} \left[1 + \frac{1 - 2(\gamma - \ln 2)}{4} \epsilon \right] \left(\frac{m\phi_0}{2\pi} \right)^{d/2}; \; U_{\mathrm{eff}}^{(2)}(\phi_0) = -C\epsilon\phi_0 \left(\frac{m\phi_0}{2\pi} \right)^{d/2}, \tag{5.91}$$

where $C \approx 0.14424$ is a constant. The total effective potential to this order is then $U_{\mathrm{eff}}(\phi_0) = U_{\mathrm{eff}}^{(1)}(\phi_0) + U_{\mathrm{eff}}^{(2)}(\phi_0)$, the minimum of which gives the condensate field ϕ_0 as $\phi_0 = (2\mu/\epsilon)[1 + (3C - 1 + \ln 2)\epsilon]$. One sees μ is really on the order of ϵ. After obtaining the effective potential, one can evaluate the pressure $P = -U_{\mathrm{eff}}(\phi_0)$ and then $\rho = \partial P/\partial\mu$, therefore

$$\boxed{\xi \equiv \frac{\mu}{E_{\mathrm{F}}} = \frac{1}{2} \epsilon^{3/2} \exp\left(\frac{\epsilon \ln \epsilon}{8 - 2\epsilon} \right) \left[1 - \left(3C - \frac{5}{4}(1 - \ln 2)\epsilon \right) \right] \approx 2^{-1}\epsilon^{3/2} + 16^{-1}\epsilon^{5/2} \ln\epsilon - 0.0246\epsilon^{5/2}.} \tag{5.92}$$

Taking $\epsilon = 1$ gives $\xi \approx 0.475$, which is close to the experimental result ≈ 0.376.[4] The Nishida–Son theory was later expanded by including higher-order terms in ϵ and the prediction is even closer to the experimental result.

Example – 4: corrections to gravitational potential. The gravitational potential between two masses m_1 and m_2 with distance r given by $U_{\mathrm{G}}(r) = -Gm_1m_2/r$ should be modified to be when considering the relevant corrections:[5]

$$\boxed{U_{\mathrm{G}}^{\mathrm{eff}}(r) \approx -\frac{Gm_1m_2}{r} \left[1 - \frac{G(m_1 + m_2)}{rc^2} - \frac{127}{30\pi^2} \frac{G\hbar}{r^2c^3} \right],} \tag{5.93}$$

here the second (third) term is the special-relativity correction characterized by c (quantum correction by $\hbar$).

EXERCISE 26: Derive the analytic expressions for the $x(t)$ of Eq. (5.74) to order $\delta^3(t)$ and $\phi^3(t)$. Discuss their applicable conditions; consider the equation by generalizing Eq. (5.74) to be $x^n(t) = \Omega + tx^m(t)/\Lambda$ with $m < n$, develop its approximated solutions.

EXERCISE 27: Assume the effective spring constant is $k_{\mathrm{eff}} \approx k(1 + s_1\sigma + s_2\sigma^2 + s_3\sigma^3 + s_4\sigma^4)$, work out the values of s_3 and s_4.

EXERCISE 28: The Coleman–Weinberg potential[6] is the effective potential when including radiative corrections. For a scalar field, the Coleman–Weinberg potential is given by,

$$\boxed{U_{\mathrm{eff}}(\phi_{\mathrm{cl}}) = U(\phi_{\mathrm{cl}}) - \frac{i\hbar}{2} \int \frac{\mathrm{d}^4k}{(2\pi)^4} \ln\left[1 - \frac{U''(\phi_{\mathrm{cl}})}{k^2} \right] \to U_{\mathrm{eff}}(\phi_{\mathrm{cl}}) = U(\phi_{\mathrm{cl}}) + \frac{\hbar}{2} \int \frac{\mathrm{d}^4k_{\mathrm{E}}}{(2\pi)^4} \ln\left[1 + \frac{U''(\phi_{\mathrm{cl}})}{k_{\mathrm{E}}^2} \right],} \tag{5.94}$$

[3] Y. Nishida and D.T. Son, *ϵ Expansions for a Fermi Gas at Infinite Scattering Length*, Phys. Rev. Lett. **97**, 050403 (2006).

[4] M. Ku et al., *Revealing the Superfluid Lambda Transition in the Universal Thermodynamics of a Unitary Fermi Gas*, Science **335**, 563 (2012).

[5] J. Donoghue, *Leading Quantum Correction to the Newtonian Potential*, Phys. Rev. Lett. **72**, 2996 (1994).

[6] S. Coleman and E. Weinberg, *Radiative Corrections as the Origin of Spontaneous Symmetry Breaking*, Phys. Rev. D **7**, 1888 (1973); S. Coleman, *Aspects of Symmetry*, Cambridge University Press, 1985, Chapter 5; for a recent relevant discussion, see, e.g., A. Andreassen, W. Frost, and M. Schwartz, *Consistent Use of Effective Potentials*, Phys. Rev. D **91**, 016009 (2015).

where the second expression follows from using $k^0 = ik_0^{\rm E}$ and $\mathbf{k} = \mathbf{k}_{\rm E}$, and therefore $d^4k = id^4k_{\rm E}$ as well as $k^2 = -k_{\rm E}^2$. Obviously, (5.94) is a semi-classical expansion based on $\hbar$. Adopting $U(\phi) = 2^{-1}\mu^2\phi^2 + \lambda\phi^4/4!$, considering the counter-terms $B\phi_{\rm cl}^2 + C\phi_{\rm cl}^4$ in the effective potential and the renormalization conditions $d^2U_{\rm eff}(\phi_{\rm cl})/d\phi_{\rm cl}^2|_{\phi_{\rm cl}=0} = 0$ together with $d^4U_{\rm eff}(\phi_{\rm cl})/d\phi_{\rm cl}^4|_{\phi_{\rm cl}=M} = \lambda(M)$ to show

$$U_{\rm eff}(\phi_{\rm cl}) = \frac{1}{24}\lambda(M)\phi_{\rm cl}^4 + \frac{\lambda^2(M)\phi_{\rm cl}^4}{256\pi^2}\left[\ln\left(\frac{\phi_{\rm cl}^2}{M^2}\right) - \frac{25}{6}\right] + \mathcal{O}[\lambda^2(M)]. \tag{5.95}$$

For the (0+1)-dimensional problem, show that $U_{\rm eff}(\phi_{\rm cl}) = U(\phi_{\rm cl}) + 2^{-1}\hbar\mu[1 + \lambda\phi_{\rm cl}^2/2\mu^2]^{1/2}$. Obviously, $U_{\rm eff}(0)$ is the zero-point energy.

F Linear Perturbations, Retarded Response and Correlation Functions

Relevant Reference:

- D. Forster, *Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions*, CRC Press, 1975.
- P. Chaikin and T. Lubensky, *Principles of Condensed Matter Physics*, Cambridge University Press, 1995, Chapter 7.
- X.G. Wen, *Quantum Field Theory of Many-body Systems*, Oxford University Press, 2004, Chapter 2.
- J. Negele and H. Orland, *Quantum Many-particle Systems*, Westview Press, 1988, Chapter 5.
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- R. Kubo, *The Fluctuation-dissipation Theorem*, Rep. Prog. Phys. **29**, 255 (1966).
- L. Kadanoff and P. Martin, *Hydrodynamic Equations and Correlation Functions*, Ann. Phys. **24**, 419 (1963).

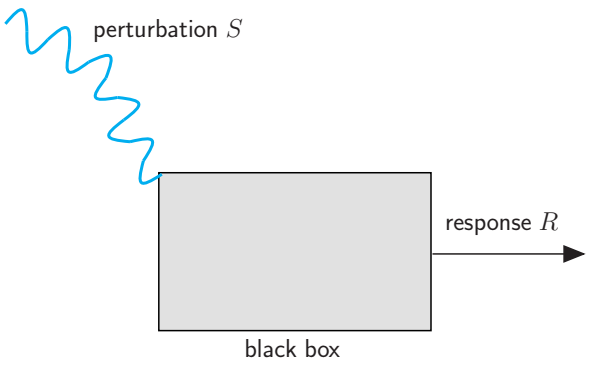

Fig. G: The black box executes a response R when a perturbation S is applied on it.

When we perturb a system (nuclear matter, solid, etc.), generally treated as a black box, the system would response correspondingly. Let us execute a perturbation S on the black box, then the latter generally responses characterized by R. If the perturbation is not quite strong (weak), the response R is expected to be proportional to S, i.e.,

$$R = \beta S, \tag{6.1}$$

where β is the corresponding proportionality coefficient. An elementary example is the Hooke's force applied on a spring with coefficient k, i.e., $F = -kx$ where x is the distance from the equilibrium position. By measuring the linear response F with a distance x, one can straightforwardly determine Hooke's constant k, therefore linear responses could be measured. To develop a theory for a given system, it is therefore extremely important to calculate various linear responses from the theory, because these results are usually the easiest to check by experiment. Consider a 1D harmonic oscillator with Hamiltonian $H_0 = p^2/2m + 2^{-1}mW^2x^2$ and a dipole interaction $\delta H = -e{\rm E}x$, here E is the electric field. The induced dipole momentum is given by $d = \langle\overline{n}|ex|\overline{n}\rangle$, here $|\overline{n}\rangle$ is the ground state of $H_0 + \delta H$. To the first order of perturbation theory, $|\overline{n}\rangle$ is given by

$$|\overline{n}\rangle = |0\rangle + \sum_{n=1,2,\cdots} |n\rangle\frac{\langle n|\delta H|0\rangle}{E_0 - E_n}, \tag{6.2}$$

here $|n\rangle$ is the ground state of H_0. The dipole momentum is then obtained as (χ is the susceptibility)

$$d = -2{\rm E}\sum_{n=1,2,\cdots}\frac{\langle 0|ex|n\rangle\langle n|ex|0\rangle}{E_0 - E_n} = \frac{2e^2}{W}\langle 0|x^2|0\rangle{\rm E} \equiv \chi{\rm E}. \tag{6.3}$$

The above result can be expressed in terms of correlation functions. To understand the general relationship between linear response and correlation functions, we consider a general quantum system described by H_0. We then turn the perturbation on and off slowly and calculate the linear response using standard time-dependent perturbation theory. After including a time-dependent perturbation $f(t)\mathcal{O}_1$, the total Hamiltonian is given as

$$H(t) = H_0 + f(t)\mathcal{O}_1, \tag{6.4}$$

Here, $f(t) = 0$ for t less than a starting time. To obtain the response of an H_0 eigenstate $|\psi_n\rangle$ under the perturbation $f(t)\mathcal{O}_1$, we start with $|\psi_n\rangle$ at $t_{-\infty} = -\infty$. Then, at a finite time t,

$$\boxed{|\psi_n(t)\rangle = {\rm T}\exp\left(-i\int_{-\infty}^{t} dt' H(t')\right)|\psi_n\rangle,} \tag{6.5}$$

where T is the time-ordering operator which puts the latest operator on the leftest side. We can expand $|\psi_n(t)\rangle$ to first order in $\mathcal{O}_1$ as,

$$|\psi_n(t)\rangle = \exp\left(-i\int_{-\infty}^{t} \mathrm{d}t' H_0\right)|\psi_n\rangle + \delta|\psi_n(t)\rangle, \tag{6.6}$$

where

$$\delta|\psi_n(t)\rangle = -i\int_{-\infty}^{t} \mathrm{d}t' f(t') e^{-iH_0(t-t')}\mathcal{O}_1 e^{-iH_0(t'-t_{-\infty})}|\psi_n\rangle = -i\int_{-\infty}^{t} \mathrm{d}t' f(t') e^{-iH_0(t-t_{-\infty})} \underbrace{e^{iH_0(t'-t_{-\infty})}\mathcal{O}_1 e^{-iH_0(t'-t_{-\infty})}}_{\mathcal{O}_1(t')}|\psi_n\rangle \tag{6.7}$$

To obtain the change of the physical quantity $\mathcal{O}_2$ in the response to the perturbation $f(t)\mathcal{O}_1$, we calculate

$$\begin{aligned}\boxed{\begin{aligned}\delta\langle\psi_n(t)|\mathcal{O}_2|\psi_n(t)\rangle &\equiv \langle\psi_n(t)|\mathcal{O}_2|\psi_n(t)\rangle - \langle\psi_n|e^{iH_0(t-t_{-\infty})}\mathcal{O}_2 e^{-iH_0(t-t_{-\infty}}|\psi_n\rangle \\ &\approx -i\int_{-\infty}^{t} \mathrm{d}t' f(t')\langle\psi_n|[\mathcal{O}_2(t),\mathcal{O}_1(t')]|\psi_n\rangle + \cdots \\ &= \int_{-\infty}^{\infty} \mathrm{d}t' D(t,t') f(t'),\end{aligned}}\end{aligned} \tag{6.8}$$

where $D(t,t')$ is the response function defined by

$$\boxed{iD(t,t') = \Theta(t-t')\langle\psi_n|[\mathcal{O}_2(t),\mathcal{O}_1(t')]|\psi_n\rangle.} \tag{6.9}$$

At zero temperature, one can take $|\psi_n\rangle$ to be the ground state $|\psi_0\rangle$. If H_0 is time independent, then $D(t,t')$ would be a function of $t-t'$ only, which could be written as $D(t-t')$. The response $\delta\langle\mathcal{O}_2\rangle$ for the ground state is given by

$$\boxed{\delta\langle\mathcal{O}_2\rangle = \int_{-\infty}^{\infty} \mathrm{d}t' D(t-t') f(t').} \tag{6.10}$$

The factor $\Theta(t-t')$ in $D(t-t')$ tells only when $t > t'$ it is nonzero, implying the retarded nature.

We now use the formula (6.10) to deal with the dipole momentum of the above harmonic oscillator. In this case, $-e\mathrm{E}$ plays the role of $f(t)$ and $\mathcal{O}_2 = \mathcal{O}_1 = ex$, so the response function is

$$D(t-t') = -i\Theta(t-t')\langle 0|[x(t),x(t')]|0\rangle = -2\langle 0|x^2|0\rangle\Theta(t-t')\sin W(t-t'). \tag{6.11}$$

Moreover, we should turn on the electric field slowly in the sense that $\mathrm{E}(t) = \mathrm{E}e^{-\epsilon|t|}$, therefore

$$d = \int_{-\infty}^{\infty} \mathrm{d}t' e^2 D(t-t') e^{\epsilon t'}(-\mathrm{E}) = -e^2\int \mathrm{d}t D(t)\mathrm{E} = \frac{2e^2}{W}\langle 0|x^2|0\rangle\mathrm{E}. \tag{6.12}$$

If we introduce the Fourier transform of $D(t)$ as

$$\boxed{D(\omega) = \int \mathrm{d}t D(t) e^{i\omega t},} \tag{6.13}$$

then $d = -e^2 D(\omega = 0)\mathrm{E}$. We see that the linear response of an electric dipole to an electric field is related to the correlation of the dipole operator ex. In fact, all of the other linear responses have a similar structure, namely the coefficients of the linear responses can be calculated from the correlation functions of appropriate operators, e.g., the conductivity can be calculated from the correlation function of the current operators. A few examples:

(a) Density: the corresponding operator is $\psi^\dagger\psi$ and the response function is charge susceptibility.

(b) Spin density, then the operator and response function are $\psi_a^\dagger\vec{\sigma}_{ab}\psi_b$ and spin susceptibility, respectively.

(c) For current density, we have $(e/m)\psi^\dagger(-i\nabla - e\mathbf{A})\psi$ for the operator and the response function is conductivity.

The retarded response function (6.9) could be generalized to finite temperature,

$$\boxed{iD_{\mathrm{R}}(t-t') = \sum_n \Theta(t-t')\langle\psi_n|[\mathcal{O}(t),\mathcal{O}(t')]|\psi_n\rangle\frac{e^{-\beta E_n}}{Z} \equiv \Theta(t-t')\langle[\mathcal{O}(t),\mathcal{O}(t')]\rangle,} \tag{6.14}$$

where Z is the partition function and subscript "R" is added, (6.14) is often called the Kubo Formula. In the remaining of this section we take $\mathcal{O}_2 = \mathcal{O}_1 = \mathcal{O}$, and $\langle\cdots\rangle$ indicates the ensemble average. Then a similar formula as (6.10) could be

written out,

$$\boxed{\langle \mathcal{O}(t)\rangle = \langle \mathcal{O}\rangle + \int \mathrm{d}t D(t-t')f(t').} \tag{6.15}$$

We define the correlation $C(t-t')$ as

$$\boxed{C(t-t') = \langle \mathcal{O}(t)\mathcal{O}(t')\rangle = \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega(t-t')} C(\omega).} \tag{6.16}$$

Therefore $C(t) = \langle \mathcal{O}(t)\mathcal{O}(0)\rangle$ represents the fluctuation of the operator $\mathcal{O}$ after time t.

Inserting a complete set of energy eigenstates $|n\rangle$ of H with energy E_n and considering gives

$$\langle n|\mathcal{O}(t)|m\rangle = \langle n|e^{iHt}\mathcal{O}e^{-iHt}|m\rangle = e^{-it(E_m-E_n)}\langle n|\mathcal{O}|m\rangle, \tag{6.17}$$

we can write the correlation function as

$$C(t-t') = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} \langle n|\mathcal{O}(t)|m\rangle\langle m|\mathcal{O}(t')|n\rangle = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} |\langle n|\mathcal{O}|m\rangle|^2 e^{-i(E_m-E_n)(t-t')}. \tag{6.18}$$

The frequency-dependent correlation function can be written

$$\boxed{C(\omega) = \int \mathrm{d}t e^{i\omega t} C(t) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} |\langle n|\mathcal{O}|m\rangle|^2 2\pi\delta(E_m - E_n - \omega).} \tag{6.19}$$

Using the similar technique, we can write out the spectral decomposition of the retarded response function,

$$iD_{\mathrm{R}}(t-t') = \Theta(t-t') \sum_{n,m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z} |\langle n|\mathcal{O}|m\rangle|^2 e^{-i(E_m-E_n)(t-t')}, \tag{6.20}$$

equivalently, we have

$$\boxed{D_{\mathrm{R}}(t) = -i\Theta(t) \sum_{n,m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z} |\langle n|\mathcal{O}|m\rangle|^2 e^{-it(E_m-E_n)}.} \tag{6.21}$$

By introducing the spectral function (the meaning of $\overline{D}$ will become clear later)

$$\overline{D}(\omega) = -\pi\left(1 - e^{-\beta\omega}\right) \sum_{n,m} \frac{e^{-\beta E_n}}{Z} |\langle n|\mathcal{O}|m\rangle|^2 \delta(\omega - (E_m - E_n)), \tag{6.22}$$

the retarded response function becomes,

$$D_{\mathrm{R}}(t) = i \int \frac{\mathrm{d}\omega}{\pi} e^{-i\omega t} \Theta(t) \overline{D}(\omega). \tag{6.23}$$

Fourier transforming this result, one could read off,

$$D_{\mathrm{R}}(\omega) = \int \frac{\mathrm{d}\omega'}{\pi} \frac{\overline{D}(\omega')}{\omega' - \omega - i\epsilon}. \tag{6.24}$$

This is know as a Kramers–Kronig relation, which could be used to extend the response function into the complex plane by writing

$$\boxed{D(z) = \int \frac{\mathrm{d}\omega'}{\pi} \frac{\overline{D}(\omega')}{\omega' - z}.} \tag{6.25}$$

We call this the dynamical susceptibility. If one can do an experiment to determine how much the system absorbs at all frequencies, then from this information one can determine the response of the system at zero frequency, which is known as the thermodynamic sum rule. When we evaluate $D(z)$ just above the real axis, we get the retarded response function $D_{\mathrm{R}} = D(\omega + i\epsilon)$. The upper half-plans is therefore the analytic extension of $D_{\mathrm{R}}(\omega)$. When considering about the lower half-plane, the concept of advanced response function emerges such that $D_{\mathrm{A}}(\omega) = D(\omega - i\epsilon)$. From the definition of $D(z)$, we could find that its poles are located exclusively along the real axis at $z = \omega'$, so that $D(z)$ is analytic everywhere except the real axis. Substituting the basic relation

$$\frac{1}{\omega - \omega' \pm i\epsilon} = \mathcal{P}\left(\frac{1}{\omega - \omega'}\right) \mp \pi i \delta(\omega - \omega'), \tag{6.26}$$

where $\mathcal{P}$ denotes the principal part, we can obtain

$$D(\omega \pm i\epsilon) = \int \frac{d\omega'}{\pi} \mathcal{P}\left(\frac{1}{\omega' - \omega}\right) \overline{D}(\omega') \pm i\overline{D}(\omega). \tag{6.27}$$

So that the real part of $D(z)$ is continuous across the real axis, but the dissipative imaginary part has a discontinuity:

$$\overline{D}(\omega) \equiv \mathrm{Im} D(\omega + i\epsilon) = \frac{1}{2i}[D(\omega + i\epsilon) - D(\omega - i\epsilon)] = \frac{i}{2}[D(\omega - i\epsilon) - D(\omega + i\epsilon)] \tag{6.28}$$

We often introduce the notations $D(\omega) = \mathrm{Re} D(\omega) + i\mathrm{Im} D(\omega) \equiv D'(\omega) + iD''(\omega)$. The imaginary part $D''(\omega)$ is called the dissipative or absorptive part of the response function. It is also known as the spectral function, which will become apparent after we discuss Green's function theories in the next section.

EXERCISE 29: Show the real (imaginary) part of the response function is even (odd), and argue the imaginary part is dissipative.
EXERCISE 30: Show that the Kramers–Kronig relation could also be written in the following form,

$$\boxed{\mathrm{Re} D(\omega) = \mathcal{P}\int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\mathrm{Im} D(\omega')}{\omega - \omega}, \quad \mathrm{Im} D(\omega) = -\mathcal{P}\int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\mathrm{Re} D(\omega')}{\omega - \omega},} \tag{6.29}$$

implying the two parts are not independent.

Combining (6.19) and (6.21) leads to

$$\boxed{C(\omega) = -2[1 + n_{\mathrm{B}}(\omega)]\mathrm{Im} D(\omega), \quad n_{\mathrm{B}} = \frac{1}{e^{\beta\omega} - 1}.} \tag{6.30}$$

This is the famous fluctuation–dissipation theorem, n_{B} is the Bose distribution. We see explicitly two terms contribute to the fluctuations, namely the $n_{\mathrm{B}}(\omega)$ factor is due to thermal effects while the "1" can be thought of as due to inherently quantum fluctuations. As usual, the classical limit occurs for high temperatures with $\beta\omega \ll 1$ where $n_{\mathrm{B}} \approx k_{\mathrm{B}}T/\omega$. In this regime, the fluctuation–dissipation theorem reduces to its classical counterpart $C(\omega) = -2k_{\mathrm{B}}T\mathrm{Im} D(\omega)/\omega$.

The fluctuation–dissipation theorem could be established in a classical harmonic oscillator. Suppose that thermal fluctuations give rise to a random force, acting on the oscillator according to the equation of motion,

$$\boxed{m\ddot{x} + mW^2 x + \gamma\dot{x} = F(t),} \tag{6.31}$$

here $\gamma > 0$ is the damping coefficient. Fourier transforming both sides and considering $\int x^{(n)} e^{i\omega t} dt = (-i\omega)^n x(\omega)$, we may obtain the equation of motion in ω space,

$$x(\omega) = \chi(\omega)F(\omega), \quad \chi(\omega) = \frac{1}{m(W^2 - \omega^2) - i\omega\gamma}. \tag{6.32}$$

Here $\chi(\omega)$ is the response function or susceptibility to the external force. The imaginary part of the susceptibility is,

$$\boxed{\chi''(\omega) = \frac{\omega\gamma}{m^2(W^2 - \omega^2)^2 + \omega^2\gamma^2} = |\chi(\omega)|^2 \omega\gamma,} \tag{6.33}$$

which governs the dissipation (since it is proportional to γ). Over long time periods, one expects that the two-point correlation function to be purely a function of the time difference, namely $S(t,t') = \langle x(t)x(t)'\rangle = \langle x(t-t')x(0)\rangle$. The power spectrum of fluctuations $\langle |x(\omega)|^2\rangle$ is defined as the Fourier transform of $\langle x(t)x(0)\rangle$, therefore its inverse transform gives

$$\boxed{\langle x(t)x(t')\rangle = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \langle |x(\omega)|^2\rangle.} \tag{6.34}$$

Under thermal equilibrium, the equipartition equilibrium theorem tells us that $2^{-1}mW^2\langle x^2\rangle = k_{\mathrm{B}}T/2$, or equivalently

$$\langle x^2\rangle = \int \frac{d\omega}{2\pi} \langle |x(\omega)|^2\rangle = \int \frac{d\omega}{2\pi} |\chi(\omega)|^2 \langle |F(\omega)|^2\rangle = \frac{k_{\mathrm{B}}T}{mW^2}. \tag{6.35}$$

Since the integration over ω is very sharply peaked around $|\omega| = W$, one can replace $\langle |F(\omega)|^2\rangle \to \langle |F(W)|^2\rangle$ when doing the relevant calculations. Replacing $|\chi(\omega)|^2$ with $\chi''(\omega)/\omega\gamma$, we then have

$$\frac{k_{\mathrm{B}}T}{mW^2} = \frac{\langle |F(W)|^2\rangle}{2\gamma} \int \frac{d\omega}{\pi} \frac{\chi''(\omega)}{\omega} = \frac{\langle |F(W)|^2\rangle}{2\gamma mW^2}. \tag{6.36}$$

So the spectrum of the fluctuations is determined by the damping force (viscosity γ) as,

$$\boxed{\langle |F(W)|^2 \rangle = 2\gamma k_{\rm B} T.} \tag{6.37}$$

If we assume that the noise spectrum depends only on the properties of the damping medium in which the oscillator is embedded, and not fundamentally on the properties of the oscillator itself, (6.37) is expected to hold for any frequency W. In this sense, we conclude that the power spectrum of the force is a flat function of frequency. This consequently implies that in thermal equilibrium the force coupling the system to the environment is a source of white noise of an amplitude which depends on the viscosity of the medium,

$$\boxed{\langle F(t)F(t')\rangle = \int \frac{{\rm d}\omega}{2\pi} e^{-i\omega(t-t')} \langle |F(\omega)|^2 \rangle = 2\gamma k_{\rm B} T \delta(t-t').} \tag{6.38}$$

The noise spectrum of fluctuations is given by

$$\boxed{S(\omega) \equiv \langle |x(\omega)|^2 \rangle = |\chi(\omega)|^2 \langle |F(\omega)|^2 \rangle = \langle |F(\omega)|^2 \rangle \frac{\chi''(\omega)}{\omega\gamma} = \frac{2k_{\rm B}T}{\omega} \chi''(\omega),} \tag{6.39}$$

or inversely

$$\boxed{\overbrace{S(t) = \langle x(t)x(0)\rangle}^{\text{fluctuations}} = 2k_{\rm B}T \int \frac{{\rm d}\omega}{2\pi} e^{-i\omega t} \underbrace{\frac{\chi''(\omega)}{\omega}}_{\text{dissipation}},} \tag{6.40}$$

which says that fluctuations in a classical harmonic oscillator are directly related to the dissipative response function via the fluctuation–dissipation theorem. This form of fluctuation–dissipation theorem is consistent with (6.30) at high temperatures (using $S \leftrightarrow -C$ for the notation consistency).

EXERCISE 31: Solve the damped harmonic oscillator (with $F(t) = 0$) under appropriate initial conditions; use the imaginary part $\chi''(\omega)$ to obtain the real part $\chi'(\omega)$ via the Kramers–Kronig relation; define $\tan\Phi(\omega) = \chi''(\omega)/\chi'(\omega)$, what's the meaning of Φ?

EXERCISE 32: Show that in hydrodynamic problems, the response function takes the form of

$$D_{\rm sound}(\omega) \sim \frac{1}{\omega^2 - v_{\rm s}^2 k^2}, \tag{6.41}$$

where $v_{\rm s}$ is the speed of sound. Argue how the viscosity could be obtained from the response function.

EXERCISE 33: Define the advanced response function, $iD_{\rm A}(t-t') = \Theta(t'-t)\langle [\mathcal{O}(t), \mathcal{O}(t')]\rangle$, show that

$$D_{\rm A}(\omega) = \int \frac{{\rm d}\omega'}{\pi} \frac{{\rm Im} D(\omega')}{\omega' - \omega + i\epsilon}. \tag{6.42}$$

What's the physical meaning of this response function?

Finally, we derive the imaginary-time response function. The partition function in the presence of a perturbation of the form $f(\tau)\mathcal{O}$ is evaluated as,

$$Z = Z_0 \left\langle {\rm T} \exp\left(-\int_0^\beta {\rm d}\tau f(\tau)\mathcal{O}(\tau)\right)\right\rangle. \tag{6.43}$$

The expectation value of $\mathcal{O}(\tau)$ is then given by to linear order,

$$\langle \mathcal{O}(\tau)\rangle = \frac{\delta \ln Z}{\delta f(\tau)} = \frac{\left\langle {\rm T}\mathcal{O}(\tau)\exp\left(-\int_0^\beta {\rm d}\tau' f(\tau')\mathcal{O}(\tau')\right)\right\rangle}{\left\langle {\rm T}\exp\left(-\int_0^\beta {\rm d}\tau' f(\tau')\mathcal{O}(\tau')\right)\right\rangle} \approx \langle \mathcal{O}\rangle - \int_0^\beta {\rm d}\tau' \left[\langle {\rm T}\mathcal{O}(\tau)\mathcal{O}(\tau')\rangle - \langle\mathcal{O}\rangle^2\right] f(\tau'). \tag{6.44}$$

Therefore,

$$\boxed{\langle \mathcal{O}(\tau)\rangle = \langle\mathcal{O}\rangle - \int_0^\beta {\rm d}\tau' D^{\rm (im)}(\tau-\tau') f(\tau'),\ \ D^{\rm (im)}(\tau-\tau') = \langle {\rm T}\mathcal{O}(\tau)\mathcal{O}(\tau')\rangle - \langle\mathcal{O}\rangle^2.} \tag{6.45}$$

Using the similar technique as in the real-time situation, one can show

$$\boxed{D^{\rm (im)}(i\omega_n) = \int \frac{{\rm d}\omega}{\pi} \frac{1}{\omega - i\omega_n} {\rm Im} D^{\rm (im)}(\omega),} \tag{6.46}$$

where ω_n is the Matsubara frequency. Compared with (6.25), we find that (6.46) is nothing more than the dynamical susceptibility $D(z)$, evaluated at $z = i\omega_n$. In other words, $D^{(\mathrm{im})}(i\omega_n)$ is the unique analytic extension of $D(\omega)$ into the complex plane. It therefore provides a procedure to calculate response functions, namely writing $D^{\mathrm{im}}(i\omega_n)$ in the form (6.46), and using this to read off $D''(\omega)$ which in turn reconstructs the dynamical response function via (6.25).

G General Theories on Propagators and Spectral Functions

RELEVANT REFERENCE:

- L. Kadanoff and G. Baym, *Quantum Statistical Mechanics*, Westview Press, 1962, Chapters 1-6.
- A. Fetter and J. Walecka, *Quantum Theory Many-particle Systems*, Dover Press, 2003, Chapters 3 and 4.
- J. Negele and H. Orland, *Quantum Many-particle Systems*, Westview Press, 1988, Chapter 5.

Since the fundamental definition of the Green's functions (e.g., see Section A and the amplitude $\langle q_f|e^{-iHt}|q_i\rangle$) describes the propagation of the system, this is expected to have strong relations with the transport aspects of the system under consideration. In this section, we plan to introduce this aspect of Green's function in some more details. The properties of a quantum mechanical system composed of many identical particles are most conveniently described in terms of the second-quantized, Heisenberg representation, particle-creation, and annihilation operators. The creation operator $\psi^\dagger(\mathbf{x},t)$, when acting to the right on a state of the system, adds a particle to the state at the space-time point $\mathbf{x},t$; the annihilation operator $\psi(\mathbf{x},t)$, the adjoint of the creation operator, acting to the right, removes a particle from the state at the point $\mathbf{x},t$. The macroscopic operators of direct physical interest can all be expressed in terms of products of a few ψ's and $\psi^\dagger$'s. For example, the density of particles at the point $\mathbf{x};t$ is $n(\mathbf{x},t) = \psi^\dagger(\mathbf{x},t)\psi(\mathbf{x},t)$. Since the act of removing and then immediately replacing a particle at $\mathbf{x},t$ measures the density of particles at that point, the operator for the total number of particles is given by

$$N(t) = \int d\mathbf{x}\psi^\dagger(\mathbf{x},t)\psi(\mathbf{x},t). \tag{7.1}$$

Similarly, the total energy of a system of particles of mass m interacting through a two-body potential $v(\mathbf{x})$ is

$$H(t) = \int d\mathbf{x}\frac{\nabla\psi^\dagger(\mathbf{x},t)\cdot\nabla\psi(\mathbf{x},t)}{2m} + \frac{1}{2}\int d\mathbf{x}d\mathbf{x}'\psi^\dagger(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t)v(|\mathbf{x}-\mathbf{x}'|)\psi(\mathbf{x}',t)\psi(\mathbf{x},t), \quad \hbar = 1. \tag{7.2}$$

The equation of any operator $X(t)$ in the Heisenberg representation is

$$\frac{\partial X(t)}{\partial t} = \frac{1}{i}[X(t),H(t)]. \tag{7.3}$$

Since $[H(t),H(t)] = 0$, we see that the Hamiltonian is independent of time. Also the Hamiltonian does not change the number of particles, $[H,N(t)] = 0$, and therefore $N(t)$ is also independent of time. Because of the time independence of H, (7.3) may be integrated in the form

$$X(t) = e^{iHt}X(0)e^{-iHt}. \tag{7.4}$$

Particles may be classified into one of two types: Fermi–Dirac particles, also called Fermions, which obey the exclusion principle, and Bose–Einstein particles, or Bosons, which do not. The wave function of any state of a collection of Bosons must be a symmetric function of the coordinates of the particles, whereas, for Fermions, the wave function must be antisymmetric. One of the main advantages of the second-quantization formalism is that these symmetry requirements are very simply represented in the equal-time commutation relations of the creation and annihilation operators. These commutation relations are

$$\psi(\mathbf{x},t)\psi(\mathbf{x}',t) \mp \psi(\mathbf{x}',t)\psi(\mathbf{x},t) = [\psi(\mathbf{x},t),\psi(\mathbf{x}',t)]_\mp = 0, \tag{7.5}$$

$$\psi^\dagger(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t) \mp \psi^\dagger(\mathbf{x}',t)\psi^\dagger(\mathbf{x},t) = [\psi^\dagger(\mathbf{x},t),\psi^\dagger(\mathbf{x}',t)]_\mp = 0, \tag{7.6}$$

$$\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t) \mp \psi^\dagger(\mathbf{x}',t)\psi(\mathbf{x},t) = [\psi(\mathbf{x},t),\psi^\dagger(\mathbf{x}',t)]_\mp = \delta(\mathbf{x}-\mathbf{x}'), \tag{7.7}$$

where the upper sign ("–") refers to Bose-Einstein particles and the lower sign ("+") refers to Fermi-Dirac particles. We see, for Fermions, that $\psi^2(\mathbf{x},t) = 0$. This is an expression of the exclusion principle in space: It is impossible to find two identical Fermions at the same point in space and time.

We shall be interested in describing the behavior of many-particle systems at finite temperature. For a system in thermodynamic equilibrium the expectation value of any operator X may be computed by using the grand-canonical ensemble of statistical mechanics. Thus

$$\langle X\rangle = \frac{\mathrm{tr}\left[e^{-\beta(H-\mu N)}X\right]}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]} = \frac{\sum_i\langle i|X|i\rangle e^{-\beta(E_i-\mu N_i)}}{\sum_i e^{-\beta(E_i-\mu N_i)}}, \tag{7.8}$$

here $|i\rangle$ represents a state of the system, normalized to unity, with energy E_i and number of particles N_i. The sum runs over all states of the system with all possible numbers of particles. The thermodynamic state of the system is now defined by the parameters μ, the chemical potential, and β^{-1}, the inverse temperature measured in energy units, i.e., $\beta = 1/k_{\rm B}T$, where $k_{\rm B}$ is Boltzmann's constant. Zero temperature, or $\beta \to \infty$, describes the ground state of the system.

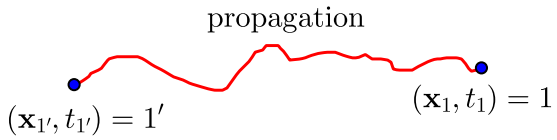

Fig. H: Single Green's function describes the propagation of a particle in spacetime.

The Green's functions, which shall form the base of our discussion of many-particle systems, are thermodynamic averages of products of the operators $\psi(1)$ and $\psi(1')$. We use the abbreviated notation 1 to mean $\mathbf{x}_1, t_1$ and $1'$ to mean $\mathbf{x}_{1'}, t_{1'}$, etc. The one-particle Green's function is defined by

$$\boxed{G(1,1') = \frac{1}{i}\langle \mathrm{T}(\psi(1)\psi^\dagger(1'))\rangle,} \tag{7.9}$$

while the two-particle Green's function is defined by

$$\boxed{G(12,1'2') = \frac{1}{i^2}\langle \mathrm{T}(\psi(1)\psi(2)\psi^\dagger(2')\psi^\dagger(1'))\rangle.} \tag{7.10}$$

In these Green's functions, T represents the Wick time-ordering operation. When applied to a product of operators it arranges them in chronological order with the earliest time appearing on the right and the latest on the left. For Bosons, this is the full effect of T. For Fermions, however, it is convenient to define T to include an extra factor, ± 1, depending on whether the resulting time-ordered product is an even or odd permutation of the original order. In addition to the one-particle Green's function we define the correlation functions

$$\boxed{G^>(1,1') = \frac{1}{i}\langle \psi(1)\psi^\dagger(1')\rangle, \quad G^<(1,1') = \pm\frac{1}{i}\langle \psi^\dagger(1')\psi(1)\rangle,} \tag{7.11}$$

The notation ">" and "<" is intended as a reminder that for $t_1 > t_{1'}$, $G = G^>$, while for $t_1 < t_{1'}$, $G = G^<$.

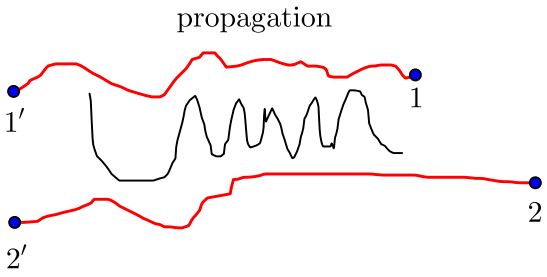

Fig. I: Physical meaning of the two-particle Green's function: propagation of two particles.

The one-particle Green's function $G(1,1')$ has a direct physical interpretation. It describes the propagation of disturbances in which a single particle is either added to or removed from the many-particle equilibrium system, see Fig. H. For example, when $t_1 > t_{1'}$ the creation operator acts first, producing a disturbance by adding a particle at the space-time point $\mathbf{x}_1, t_1$. This disturbance then propagates to the later time $t_{1'}$, when a particle is removed at $\mathbf{x}_{1'}$, ending the disturbance and returning the system to its equilibrium state. For $t_1 < t_{1'}, \psi$ acts first. The disturbance, which is now produced by the removal of a particle at $\mathbf{x}_1, t_1$, propagates to time $t_{1'}$, when it is terminated by the addition of a particle at the point $\mathbf{x}_{1'}$. Similarly, the two-particle Green's function describes, for the various time orders, disturbances produced by the removal or addition of two particles. For example, when t_1 and t_2 are both later than $t_{1'}$ and $t_{2'}$, $G_2(12,1'2')$ describes the addition of two particles and the subsequent removal of two particles. Yet when t_1 and $t_{1'}$ are later than t_2 and $t_{2'}$, the two-particle Green's function describes the disturbance produced by the addition of one particle and the removal of one particle, and the subsequent return to equilibrium by the removal of a particle and the addition of a particle, see Fig. I, where the black line represents the fluctuations caused by the medium. We shall make extensive use of this physical interpretation of the Green's functions.

The function $G^>$, which we may write as

$$G^>(1,1') = \frac{1}{i}\frac{\mathrm{tr}\left[e^{-\beta(H-\mu N)}e^{it_1 H}\psi(\mathbf{x}_1,0)e^{-i(t_1-t_{1'})H}\psi^\dagger(\mathbf{x}_{1'},0)e^{-it_{1'}H}\right]}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]}, \tag{7.12}$$

is an analytic function for complex values of the time arguments in the region $0 > \mathrm{Im}(t_1 - t_{1'}) > -\beta$. This analyticity follows directly from the assumption that the $e^{-\beta(H-\mu N)}$ factor is sufficient to guarantee the absolute convergence of the trace for real time, i.e.,

$$-\beta(H-\mu N) < (\mathrm{Im}\, t_1 - \mathrm{Im}\, t_{1'})\underbrace{(H-\mu N)}_{K} < 0, \quad e^{-\beta(H-\mu N)} \to 0. \tag{7.13}$$

Similarly $G^<(1,1')$ is an analytic function in the region $0 < \mathrm{Im}(t_1 - t_{1'}) < \beta$.

To derive the relation between $G^>$ and $G^<$ we notice that the expression

$$G^<(1,1')\big|_{t_1=0} = \pm\frac{1}{i}\frac{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\psi^\dagger(\mathbf{x}_{1'},t_{1'})\psi(\mathbf{x}_1,0)\right]}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]} \tag{7.14}$$

may be rearranged, using the cyclic invariance of the trace ($\mathrm{tr}(AB)=\mathrm{tr}(BA)$), to become

$$\begin{aligned} G^<(1,1')\big|_{t_1=0} &= \pm\frac{1}{i}\frac{\mathrm{tr}\left[\psi(\mathbf{x}_1,0)e^{-\beta(H-\mu N)}\psi^\dagger(\mathbf{x}_{1'},t_{1'})\right]}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]} \\ &= \pm\frac{1}{i}\frac{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\left[e^{\beta(H-\mu N)}\psi(\mathbf{x}_1,0)e^{-\beta(H-\mu N)}\psi^\dagger(\mathbf{x}_{1'},t_{1'})\right]\right]}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]} \\ &= \pm\frac{1}{i}\left\langle e^{\beta(H-\mu N)}\psi(\mathbf{x}_1,0)e^{-\beta(H-\mu N)}\psi^\dagger(\mathbf{x}_{1'},t_{1'})\right\rangle. \end{aligned} \tag{7.15}$$

Because $\psi(\mathbf{x}_1,0)$ removes a particle, we have $\psi(\mathbf{x}_1,0)f(N)=f(N+1)\psi(\mathbf{x}_1,0)$, where $f(N)$ is any function of the number operator N. In particular, $\psi(\mathbf{x}_1,0)e^{\beta\mu N}=e^{\beta\mu(N+1)}\psi(\mathbf{x}_1,0)$, i.e., $e^{-\beta\mu N}\psi(\mathbf{x}_1,0)e^{\beta\mu N}=e^{\beta\mu}\psi(\mathbf{x}_1,0)$. From the time evolution of X, it follows that $e^{\beta H}\psi(\mathbf{x}_1,0)e^{-\beta H}=\psi(\mathbf{x}_1,-i\beta)$, thus

$$\boxed{G^<(1,1')\big|_{t_1=0} = \pm\frac{1}{i}\langle\psi(\mathbf{x}_1,-i\beta)\psi^\dagger(1')\rangle e^{\beta\mu} = \pm e^{\beta\mu}\,G^>(1,1')\big|_{t_1=-i\beta}.} \tag{7.16}$$

This relationship is crucial to all our Green's function analysis.

Notice that (7.16) follows directly from the cyclic invariance of the trace and the structure of the time dependence of $\psi(1)$. Since G_2 is also defined as a trace, we can go through an entirely similar analysis for it, splitting it into several non-time-ordered expectation values of ψ's and $\psi^\dagger$'s and proving a set of relations similar to (7.16). However, this analysis is much too complicated because G_2 is composed of too many different analytic pieces, corresponding to all the different possible time orderings of its four time variables. We employ the following simple device to exhibit a relation like (7.16) for G_2. We consider the time variable to be restricted to the interval $0\le it\le\beta$. To complete the definition of the Green's functions in this time domain, we extend the definition of the time-ordering symbol T to mean "$i\times t$" ordering when the times are imaginary. The further down the imaginary axis a time is, the "later" it is, see Fig. J. Then the Green's functions are well defined in the interval $0\le it\le\beta$, e.g., the one-particle Green's function is

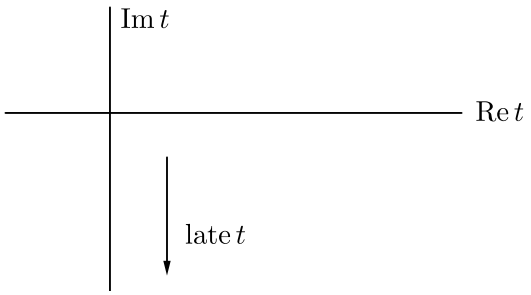

Fig. J: Time-ordering on the imaginary axis.

$$G(1,1') = \begin{cases} G^>(1,1'), & it_1 > it_{1'}, \\ G^<(1,1'), & it_1 < it_{1'}. \end{cases} \tag{7.17}$$

For $0<it_{1'}<\beta$, we have the relation $G(1,1')\big|_{t_1=0}=G^<(1,1')\big|_{t_1=0}$ since $0=it_1<it_{1'}$ for all $t_{1'}$. Similarly, we have $G(1,1')\big|_{t_1=-i\beta}=G^>(1,1')\big|_{t_1=-i\beta}$ since $\beta=it_1>it_{1'}$. Therefore (7.16) can be restated as,

$$\boxed{G(1,1')\big|_{t_1=0} = \pm e^{\beta\mu}\,G(1,1')\big|_{t_1=-i\beta}.} \tag{7.18}$$

Moreover, we can see immediately that G_2 on the imaginary-time axis obeys exactly this same boundary condition,

$$G_2(12,1'2')\big|_{t_1=0} = \pm e^{\beta\mu}\,G_2(12,1'2')\big|_{t_1=-i\beta},\quad G_2(12,1'2')\big|_{t_{1'}=0} = \pm e^{-\beta\mu}\,G_2(12,1'2')\big|_{t_{1'}=-i\beta}. \tag{7.19}$$

These boundary conditions on G and G_2 will be used over and over again in the subsequent analysis. It is only at a later stage that we shall need the imaginary-time Green's functions. Now we shall restrict our attention to the one-particle function, for which (7.16) is a suitable representation of the boundary condition. Because of the translational and rotational invariance of the Hamiltonian (7.2) in space and its translational invariance in time, $G^>$ and $G^<$ depend only on $|\mathbf{x}_1-\mathbf{x}_{1'}|$ and $|t_1-t_{1'}|$. When we want to emphasize that these functions depend only on the difference variables, we shall write them as $G^{>,<}(1-1')$ or as $G^{>,<}(|\mathbf{x}_1-\mathbf{x}_{1'}|,|t_1-t_{1'}|)$. In terms of the difference variables, (7.16) is

$$\boxed{G^<(\mathbf{x},t) = \pm e^{\beta\mu}G^>(\mathbf{x},t-i\beta).} \tag{7.20}$$

We now introduce the Fourier transforms of $G^>$ and $G^<$, defined by

$$G^>(\mathbf{p},\omega) = i\int \mathrm{d}\mathbf{x}\int_{-\infty}^{+\infty} \mathrm{d}t e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}G^>(\mathbf{x},t),\quad G^<(\mathbf{p},\omega) = \pm i\int \mathrm{d}\mathbf{x}\int_{-\infty}^{+\infty} \mathrm{d}t e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}G^<(\mathbf{x},t). \tag{7.21}$$

Note the explicit factors of "i" and "$\pm i$" that we have included here to make $G^>(\mathbf{p},\omega)$ and $G^<(\mathbf{p},\omega)$ real nonnegative quantities. Equation (7.16) then becomes the simple relationship

$$\boxed{G^<(\mathbf{p},\omega) = e^{-\beta(\omega-\mu)}G^>(\mathbf{p},\omega).} \tag{7.22}$$

It is useful to introduce the spectral function $A(\mathbf{p},\omega)$ defined by

$$\boxed{A(\mathbf{p},\omega) = G^>(\mathbf{p},\omega) \mp G^<(\mathbf{p},\omega),} \tag{7.23}$$

and the boundary condition on G can then be represented by writing

$$G^>(\mathbf{p},\omega) = [1\pm f(\omega)]A(\mathbf{p},\omega),\quad G^<(\mathbf{p},\omega) = f(\omega)A(\mathbf{p},\omega),\quad f(\omega) = \frac{1}{e^{\beta(\omega-\mu)}\mp 1}. \tag{7.24}$$

The function f can be recognized as the average occupation number in the grand-canonical ensemble of a mode with energy ω: When the Hamiltonian can be diagonalized to the form $\sum_\lambda \epsilon_\lambda \psi_\lambda^\dagger \psi_\lambda$, then $\psi_\lambda^\dagger$ is a creation operator for a mode of the system with energy ϵ_λ. The average occupation number of the mode λ is $\langle \psi_\lambda^\dagger \psi_\lambda\rangle = f(\epsilon_\lambda)$.

From the definitions of $G^>$ and $G^<$ it follows that

$$\boxed{A(\mathbf{p},\omega) = \int \mathrm{d}\mathbf{x}\int_{-\infty}^{+\infty} \mathrm{d}t e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}\left\langle [\psi(\mathbf{x},t)\psi^\dagger(\mathbf{0},0) \mp \psi^\dagger(\mathbf{0},0)\psi(\mathbf{x},t)]\right\rangle.} \tag{7.25}$$

Thus, as a consequence of the equal-time commutation relation, A satisfies the sum rule

$$\boxed{\int \frac{\mathrm{d}\omega}{2\pi}A(\mathbf{p},\omega) = \int \mathrm{d}\mathbf{x}e^{-i\mathbf{p}\cdot\mathbf{x}}\left\langle [\psi(\mathbf{x},0)\psi^\dagger(\mathbf{0},0) \mp \psi^\dagger(\mathbf{0},0)\psi(\mathbf{x},0)]\right\rangle = \int \mathrm{d}\mathbf{x}\delta(\mathbf{x}) = 1.} \tag{7.26}$$

Example – free particles. We can use the relations that we have just derived to find G for the trivial case of free particles, for which the Hamiltonian is

$$H_0 = \int \mathrm{d}\mathbf{x}\frac{\nabla\psi^\dagger(\mathbf{x},t)\cdot\nabla\psi(\mathbf{x},t)}{2m}. \tag{7.27}$$

We notice that,

$$G^<(\mathbf{p},\omega) = \int \mathrm{d}\mathbf{x}\mathrm{d}t e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}[\pm iG^<(\mathbf{x},t)] = \int \mathrm{d}\mathbf{x}\mathrm{d}t e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}\langle\psi^\dagger(\mathbf{0},0)\psi(\mathbf{x},t)\rangle = \int \frac{e^{i\omega t}\mathrm{d}t}{\Omega}\langle\psi^\dagger(\mathbf{p},0)\psi(\mathbf{p},t)\rangle, \tag{7.28}$$

where Ω is the volume of the system and $\psi(\mathbf{p},t)$ is the spatial Fourier transform of $\psi(\mathbf{x},t)$, i.e., $\psi(\mathbf{p},t) = \int \mathrm{d}\mathbf{x}e^{-i\mathbf{p}\cdot\mathbf{x}}\psi(\mathbf{x},t)$. Since $\psi(\mathbf{p},0)$ removes a free particle with momentum $\mathbf{p}$, it must remove energy $\mathbf{p}^2/2m$ from the system. Thus,

$$\psi(\mathbf{p},t) = e^{iHt}\psi(\mathbf{p},0)e^{-iHt} = \exp\left(-i\frac{\mathbf{p}^2}{2m}t\right)\psi(\mathbf{p},0),\quad \text{since } \psi(\mathbf{p},0)e^{-iHt} = e^{-iHt-itE_{\text{single}}} = \exp\left(-iHt - i\frac{\mathbf{p}^2}{2m}t\right)\psi(\mathbf{p},0). \tag{7.29}$$

Consequently,

$$G^<(\mathbf{p},\omega) = \frac{2\pi}{\Omega}\delta\left(\omega - \frac{\mathbf{p}^2}{2m}\right)\langle\psi^\dagger(\mathbf{p},0)\psi(\mathbf{p},0)\rangle. \tag{7.30}$$

Hence $A(\mathbf{p},\omega)$ is proportional to $\delta(\omega-\mathbf{p}^2/2m)$, and the constant of proportionality is determined from the sum rule (7.26) to be 2π. Thus, for free particles, $A(\mathbf{p},\omega) = A_0(\mathbf{p},\omega) = 2\pi\delta(\omega-\mathbf{p}^2/2m)$, and

$$\begin{aligned} G_0^>(\mathbf{x},t) &= \int \frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{d}\mathbf{p}}{(2\pi)^3}\frac{G^>(\mathbf{p},\omega)}{i}e^{i\mathbf{p}\cdot\mathbf{x}-i\omega t} = \int \frac{\mathrm{d}\omega}{2\pi i}\frac{\mathrm{d}\mathbf{p}}{(2\pi)^3}e^{i\mathbf{p}\cdot\mathbf{x}-i\omega t}[1\pm f(\omega)]A_0(\mathbf{p},\omega) \\ &= \frac{1}{i}\int \frac{\mathrm{d}\omega\mathrm{d}\mathbf{p}}{(2\pi)^3}e^{i\mathbf{p}\cdot\mathbf{x}-i\omega t}[1\pm f(\omega)]\delta\left(\omega-\frac{\mathbf{p}^2}{2m}\right) = -i\int \frac{\mathrm{d}\mathbf{p}}{(2\pi)^3}\exp\left(i\mathbf{p}\cdot\mathbf{x} - i\frac{\mathbf{p}^2}{2m}t\right)\left[1\pm f\left(\frac{\mathbf{p}^2}{2m}\right)\right], \end{aligned} \tag{7.31}$$

$$G_0^<(\mathbf{x},t) = \pm i\int \frac{\mathrm{d}\mathbf{p}}{(2\pi)^3}f\left(\frac{\mathbf{p}^2}{2m}\right)\exp\left(i\mathbf{p}\cdot\mathbf{x} - i\frac{\mathbf{p}^2}{2m}t\right). \tag{7.32}$$

Since $\psi^\dagger(\mathbf{p},0)\psi(\mathbf{p},0)$ is the operator representing the density of particles with momentum $\mathbf{p}$, it follows that for free particles the average number of particles with momentum $\mathbf{p}$ is

$$\langle n(\mathbf{p})\rangle = \frac{\langle\psi^\dagger(\mathbf{p},0)\psi(\mathbf{p},0)\rangle}{\Omega} = f\left(\frac{\mathbf{p}^2}{2m}\right) = \left[\exp\left(\frac{\beta\mathbf{p}^2}{2m} - \beta\mu\right) \mp 1\right]^{-1}. \tag{7.33}$$

This is a result familiar from elementary statistical mechanics.

The Fourier transform of the field operator $\psi(\mathbf{x},t)$, given by $\psi(\mathbf{p},\omega) = \int d\mathbf{x}\int dt e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}\psi(\mathbf{x},t)$, is an operator which annihilates a particle with momentum $\mathbf{p}$ and energy ω. Thus $G^<(\mathbf{p},\omega)$ can be identified as the average density of particles in the system with momentum $\mathbf{p}$ and energy ω, i.e.,

$$G^<(\mathbf{p},\omega) = \langle n(\mathbf{p},\omega)\rangle = A(\mathbf{p},\omega)f(\omega). \tag{7.34}$$

The interpretation of this result is evident: $f(\omega)$ is the average occupation number of a mode with energy ω; the spectral function $A(\mathbf{p},\omega)$ is a weighting function with total weight unity, which whenever it is nonzero defines the spectrum of possible energies ω, for a particle with momentum $\mathbf{p}$ in the medium. To check this result, we note the density of particles,

$$\boxed{\langle n(\mathbf{x},t)\rangle = \langle\psi^\dagger(\mathbf{x},t)\psi(\mathbf{x},t)\rangle = \pm iG^<(\mathbf{x}t,\mathbf{x}t) = \int\frac{d\omega}{2\pi}\frac{d\mathbf{p}}{(2\pi)^3}G^<(\mathbf{p},\omega).} \tag{7.35}$$

This says that the total density of particles is equal to the integral over all $\mathbf{p}$ and ω of the density of particles with momentum $\mathbf{p}$ and energy ω. Since $\langle n(\mathbf{x},t)\rangle$ is independent of $\mathbf{x}$ and t, we shall represent it simply as n.

EXERCISE 34: Consider the degenerate Fermi system at zero temperature, work out the expression for $G(\mathbf{p},\omega)$:

$$G(\mathbf{p},\omega) = \frac{\Theta(p-p_\mathrm{F})}{\omega-\epsilon_\mathbf{p}+i0^+} + \frac{\Theta(p_\mathrm{F}-p)}{\omega-\epsilon_\mathbf{p}-i0^+} = \frac{1}{\omega-\epsilon_\mathbf{p}+i0^+\mathrm{sgn}(p-p_\mathrm{F})},\quad \epsilon_\mathbf{p} = \mathbf{p}^2/2m-\mu, \tag{7.36}$$

here $i0^+$ could be traced physically (mathematically) back to the principle of causality (Fourier transform of $\Theta(t)$). Therefore $G(\mathbf{p},\omega)$ has only a single pole, slightly below the real axis at $\omega = p^2/2m-\mu$ if $p > p_\mathrm{F}$ and above the real axis at the same value of ω if $p < p_\mathrm{F}$.

When there is an interaction between the particles, $A(\mathbf{p},\omega)$ will not be a single delta function. To see the detailed structure of A, let us compute $G^>(\mathbf{p},\omega)$ by explicitly introducing sums over states. Then $G^>(\mathbf{p},\omega)$ is

$$\begin{aligned}
G^>(\mathbf{p},\omega) &= A(\mathbf{p},\omega)[1\pm f(\omega)] = i\int d\mathbf{x}dte^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}G^>(\mathbf{x},t) = \int d\mathbf{x}dte^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}\langle\psi(\mathbf{x},t)\psi^\dagger(\mathbf{0},0)\rangle\\
&= \int\frac{d\mathbf{x}'}{\Omega}d\mathbf{x}dte^{-i\mathbf{p}\cdot\mathbf{x}+i\mathbf{p}\cdot\mathbf{x}'+i\omega t}\langle\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',0)\rangle = \int\frac{d\mathbf{x}'}{\Omega}d\mathbf{x}dte^{-i\mathbf{p}\cdot\mathbf{x}+i\mathbf{p}\cdot\mathbf{x}'+i\omega t}\frac{\mathrm{tr}\left[e^{-\beta(H-\mu N)}e^{iHt}\psi(\mathbf{x},0)e^{-iHt}\psi^\dagger(\mathbf{x}',0)\right]}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]}\\
&= \int dt\frac{e^{i\omega t}}{\Omega}\sum_i e^{-\beta(E_i-\mu N_i)}\frac{\langle i|e^{iHt}\psi(\mathbf{p})e^{-iHt}\psi^\dagger(\mathbf{p})|i\rangle}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]} = \int dt\frac{e^{i\omega t}}{\Omega}\sum_{i,j}e^{-\beta(E_i-\mu N_i)}\frac{\langle i|e^{iHt}\psi(\mathbf{p})e^{-iHt}|j\rangle\langle j|\psi^\dagger(\mathbf{p})|i\rangle}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]}\\
&= \sum_{i,j}\int\frac{dt}{\Omega}e^{it(\omega+E_i-E_j)}e^{-\beta(E_i-\mu N_i)}\frac{\langle i|\psi(\mathbf{p})|j\rangle\langle j|\psi^\dagger(\mathbf{p})|i\rangle}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]} = \frac{1}{\Omega}\sum_{i,j}e^{-\beta(E_i-\mu N_i)}\left|\langle j|\psi^\dagger(\mathbf{p})|i\rangle\right|^2\times\frac{2\pi\delta(\omega+E_i-E_j)}{\mathrm{tr}\left[e^{-\beta(H-\mu N)}\right]},
\end{aligned} \tag{7.37}$$

here $\left|\langle j|\psi^\dagger(\mathbf{p})|i\rangle\right|^2$ is the average transition probability among levels, the relations $H|i\rangle = E_i|i\rangle, \sum_j|j\rangle\langle j| = \mathbf{1}$ are used.

It is clear then that the values of ω for which $A(\mathbf{p},\omega)$ is nonvanishing are just the possible energy differences which result from adding a single particle of momentum $\mathbf{p}$ to the system. Almost always the energy spectrum of the system is sufficiently complex so that $A(\mathbf{p},\omega)$ finally appears to have no delta functions in it but is instead a continuous function of ω. However, there are often sharp peaks in A, see Fig. K. These sharp peaks represent coherent and long-lived excitations which behave in many ways like free or weakly interacting particles. These excitations are usually called quasi-particles. We can notice from (7.37) that $G^>(\mathbf{p},\omega)$ is proportional to the averaged transition probability for processes in which an extra particle with momentum $\mathbf{p}$, when added to the system, increases the energy of the system by ω. This transition probability measures the density of states available for an added particle. Therefore, $G^>(\mathbf{p},\omega)$ is the density of states available for the addition of an extra particle with momentum $\mathbf{p}$ and energy ω. Similarly $G^<(\mathbf{p},\omega)$ is proportional to the averaged transition probability for processes involving the removal of a particle with momentum $\mathbf{p}$, and leading to a decrease of the energy of the system by ω. Since the transition probability for

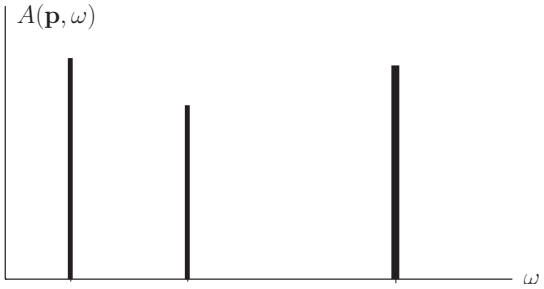

Fig. K: The structure of the spectral function for the system with interactions.

the removal of a particle is just a measure of the density of particles, we again see that $G^<(\mathbf{p},\omega)$ is the density of particles with momentum $\mathbf{p}$ and energy ω. The interpretation of $G^>$ as a density of states and $G^<$ as a density of particles will be used many times in our further work. In terms of these two transition probabilities, the boundary condition (7.22) is

$$\boxed{[A(1\pm f(\omega))]/Af(\omega) = e^{\beta(\omega-\mu)},} \tag{7.38}$$

This "detailed balancing condition", is a direct consequence of the use of an equilibrium ensemble.

In addition to the detailed dynamical information, G contains all possible information about the statistical mechanics of the system. We have already seen how we can write the expectation value of the density of particles in terms of $G^<$. Similarly we can express the total energy, i.e., the expectation value of the Hamiltonian (7.2), in terms of $G^<$. To do this we must make use of the equations of motion for ψ and $\psi^\dagger$. Using the equation of motion and the commutation relations, we shall obtain

$$\boxed{\left(i\frac{\partial}{\partial t}+\frac{\nabla^2}{2m}\right)\psi(\mathbf{x},t) = \int d\bar{\mathbf{x}} v(\mathbf{x}-\bar{\mathbf{x}})\psi^\dagger(\bar{\mathbf{x}},t)\psi(\bar{\mathbf{x}},t)\psi(\mathbf{x},t),} \tag{7.39}$$

$$\boxed{\left(-i\frac{\partial}{\partial t'}+\frac{\nabla'^2}{2m}\right)\psi^\dagger(\mathbf{x}',t') = \psi^\dagger(\mathbf{x}',t')\int d\bar{\mathbf{x}}' v(\mathbf{x}'-\bar{\mathbf{x}}')\psi^\dagger(\bar{\mathbf{x}}',t')\psi(\bar{\mathbf{x}}',t'),} \tag{7.40}$$

thus

$$\begin{aligned}\Phi &\equiv \frac{1}{4}\int d\mathbf{x}\left[\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}\right)\psi^\dagger(\mathbf{x},t')\psi(\mathbf{x},t)\right]_{t'=t}\\ &= \frac{1}{4}\int d\mathbf{x}\left[\left(-\frac{\nabla^2}{2m}-\frac{\nabla'^2}{2m}\right)\psi^\dagger(\mathbf{x}',t)\psi(\mathbf{x},t)\right]_{\mathbf{x}'=\mathbf{x}} + \frac{1}{2}\int d\mathbf{x}d\bar{\mathbf{x}}\psi^\dagger(\mathbf{x},t)\psi^\dagger(\bar{\mathbf{x}},t)v(\mathbf{x}-\bar{\mathbf{x}})\psi(\bar{\mathbf{x}},t)\psi(\mathbf{x},t).\end{aligned} \tag{7.41}$$

The right side of (7.41) is half the kinetic energy plus all the potential energy. When we add the other half of the kinetic energy we find that,

$$\boxed{\begin{aligned}\langle H\rangle &= \frac{1}{4}\int d\mathbf{x}\left[\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}+\frac{\nabla\cdot\nabla'}{m}\right)\psi^\dagger(\mathbf{x}',t')\psi(\mathbf{x},t)\right]_{\mathbf{x}'=\mathbf{x},t'=t}\\ &= \pm\frac{i}{4}\int d\mathbf{x}\left[\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}+\frac{\nabla\cdot\nabla'}{m}\right)G^<(\mathbf{x}t,\mathbf{x}'t')\right]_{\mathbf{x}'=\mathbf{x},t'=t}\\ &= \frac{1}{4}\int d\mathbf{x}\left[\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}+\frac{\nabla\cdot\nabla'}{m}\right)\times\int\frac{d\omega}{2\pi}\frac{d\mathbf{p}}{(2\pi)^3}e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')-i\omega(t-t')}G^<(\mathbf{p},\omega)\right]_{\mathbf{x}'=\mathbf{x},t'=t}\\ &= \frac{1}{4}\int d\mathbf{x}\left[i(-i\omega)-i(i\omega)+\frac{(i\mathbf{p})\cdot(-i\mathbf{p})}{m}\right]\times\left[\int\frac{d\omega}{2\pi}\frac{d\mathbf{p}}{(2\pi)^3}e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')-i\omega(t-t')}G^<(\mathbf{p},\omega)\right]_{\mathbf{x}'=\mathbf{x},t'=t}\\ &= \Omega\int\frac{d\omega}{2\pi}\frac{d\mathbf{p}}{(2\pi)^3}\frac{1}{2}\left(\omega+\frac{\mathbf{p}^2}{2m}\right)f(\omega)A(\mathbf{p},\omega),\end{aligned}} \tag{7.42}$$

where Ω is the volume of the system. Equation (7.42) is very useful for evaluating ground-state energies, etc.

EXERCISE 35: The pressure of a system could be obtained by $P(\beta,\mu) = \int_{-\infty}^{\mu} d\mu' n(\beta,\mu')$. Derive it for the free gas.

We have seen that the one-particle Green's function contains very useful dynamic and thermodynamic information. However, to extract this information we must first develop techniques for determining G. Our methods will be based on the equation of motion satisfied by the one-particle Green's function. We start from

$$\frac{1}{i}\left\langle \mathrm{T}\left[\left(i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}\right)\psi(1)\psi^\dagger(1')\right]\right\rangle = \pm\frac{1}{i}\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)\langle \mathrm{T}(\psi(1)\psi(2)\psi^\dagger(2^+)\psi^\dagger(1'))\rangle|_{t_2=t_1}, \tag{7.43}$$

here, the notation 2^+ is intended to serve as a reminder that the time argument of $\psi^\dagger(2)$ must be chosen to be infinitesimally larger than the time arguments of the ψ's in order that the time ordering in G_2 reproduce the order of factors that appears in (7.39). Since $\psi^\dagger$'s commute (or anticommute) at equal times, we do not have to worry about the time ordering of $\psi(1)$ and $\psi(2)$. In this way we find that (7.43) becomes an equation of motion for G:

$$\boxed{\left(i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}\right)G(1,1') = \delta(1-1')\pm i\int d\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)G_2(12,1'2^+)|_{t_2=t_1}.} \tag{7.44}$$

To convert (7.43) into an equation for G we must take the time derivatives outside the T-ordering symbol. The spatial derivatives commute with the time-ordering operation, but the time derivative does not. Since T changes the

time ordering when $t_1 = t_{1'}$, the difference

$$\frac{\partial}{\partial t_1}\langle \mathrm{T}(\psi(1)\psi^\dagger(1'))\rangle - \left\langle \mathrm{T}\left(\frac{\partial}{\partial t_1}\psi(1)\psi^\dagger(1')\right)\right\rangle \tag{7.45}$$

must be proportional to a delta function of $t_1 - t_{1'}$. The constant of proportionality is the discontinuity of $\langle T(\psi(1)\psi^\dagger(1'))\rangle$ as t_1 passes through $t_{1'}$, i.e.,

$$\underbrace{\langle \psi(1)\psi^\dagger(1')}_{\text{to } t_{1'}<t_1} \mp \underbrace{\psi^\dagger(1')\psi(1)\rangle}_{\text{to } t_{1'}>t_1}. \tag{7.46}$$

Thus,

$$\frac{\partial}{\partial t_1}\langle \mathrm{T}(\psi(1)\psi^\dagger(1'))\rangle - \left\langle \mathrm{T}\left(\frac{\partial}{\partial t_1}\psi(1)\psi^\dagger(1')\right)\right\rangle = \delta(t_1 - t_{1'})\underbrace{\langle \psi(1)\psi^\dagger(1') \mp \psi^\dagger(1')\psi(1)\rangle}_{\text{equal time}} = \delta(t_1 - t_{1'})\delta(\mathbf{x}_1 - \mathbf{x}_{1'}) = \delta(1-1'). \tag{7.47}$$

In a similar fashion we can also write an equation of motion for G_2 involving G_3, one for G_3 involving G_4, and so on. As we shall have no need for these equations we shall not write them down.

Starting from the equation of motion of $\psi^\dagger(1')$, we also derive the adjoint equation of motion,

$$\boxed{\left(-i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m}\right)G(1,1') = \delta(1-1') \mp i\int \mathrm{d}\mathbf{x}_2 G_2(12^-,1'2)v(\mathbf{x}_2 - \mathbf{x}_{1'}).} \tag{7.48}$$

Equations (7.44) and (7.48) are equally valid for the real-time and the imaginary-time Green's functions. The only difference between the two cases is that for imaginary times one has to interpret the delta function in time as being defined with respect to integrations along the imaginary-time axis. Equations (7.44) and (7.48) each determine G in terms of G_2. It is in general impossible to know G_2 exactly. We shall find G by making approximations for G_2 in the equations of motion (7.44) and (7.48), famous examples include Hartree and Hartree–Fock approximations. However, even if G_2 were precisely known, (7.44) and (7.48) would not be sufficient to determine G unambiguously. These equations are first-order differential equations in time, and thus a single supplementary boundary condition is required to fix their solution precisely. The necessary boundary condition is, of course, condition (7.18).

A very natural representation of G which automatically takes the quasi-periodic boundary condition into account is to express G as a Fourier series, which we write in momentum space as,

$$G(\mathbf{p}, t-t') = \frac{1}{-i\beta}\sum_\nu e^{-iz_\nu(t-t')}G(\mathbf{p}, z_\nu), \quad 0 \le it, it' \le \beta, \tag{7.49}$$

where $-i\beta$ is the imaginary period, $z_\nu = \pi\nu/(-i\beta) + \mu$ (Matsubara frequency, see (5.6) and **EXERCISE 37**). The sum is taken to run over all even integers for Bose statistics and over all odd integers for Fermi statistics in order to reproduce correctly the "±" in the boundary conditions. The equation of motion directly determines the Fourier coefficient $G(\mathbf{p}, \pi\nu/(-i\beta) + \mu)$. However we want to know the spectral weight function A. To relate G to A we invert the Fourier series (7.49):

$$G(\mathbf{p}, z_\nu) = \int_0^{-i\beta} \mathrm{d}t \exp\left[i\left(\frac{\pi\nu}{-i\beta} + \mu\right)\cdot(t-t')\right]G(\mathbf{p}, t-t'), \tag{7.50}$$

this integral must be independent of t' and is most simply evaluated by taking $t' = 0$. Then

$$G(\mathbf{p},t) = G^>(\mathbf{p},t) = \int \frac{\mathrm{d}\omega}{2\pi i}e^{-i\omega t}\underbrace{\frac{A(\mathbf{p},\omega)}{1 \mp e^{-\beta(\omega-\mu)}}}_{G^>(\mathbf{p},\omega)}, \quad G(\mathbf{p}, z_\nu) = \int \frac{\mathrm{d}\omega}{2\pi}\frac{A(\mathbf{p},\omega)}{z_\nu - \omega}, \tag{7.51}$$

i.e., the Fourier coefficient is the analytic function

$$G(\mathbf{p}, z) = \int \frac{\mathrm{d}\omega}{2\pi}\frac{A(\mathbf{p},\omega)}{z-\omega} \tag{7.52}$$

evaluated at $z = z_\nu = \pi\nu/(-i\beta) + \mu$. The procedure for finding A from the Fourier coefficients is then very simple: One merely continues the Fourier coefficients—a function defined on the points $z = \pi\nu/(-i\beta) + \mu$—to an analytic function for all (nonreal) z. The unique continuation which has no essential singularity at $z = \infty$ is the function (7.52). Then, $A(\mathbf{p},\omega)$ is given by the discontinuity of $G(\mathbf{p}, z)$ across the real axis, i.e.,

$$\boxed{A(\mathbf{p},\omega) = i\left[G(\mathbf{p},\omega + i\epsilon) - G(\mathbf{p},\omega - i\epsilon)\right],} \tag{7.53}$$

using the basic relation (6.27). Compare (7.53) with (6.28). Three concepts—equations of motion, boundary conditions, and analytic continuations—form the mathematical basis of all our techniques for determining Green's functions.

EXERCISE 36: Show that for free particles, the function $G(\mathbf{p},z)$ is given by $[z-\mathbf{p}^2/2m]^{-1}$, and then calculate $A_0(\mathbf{p},\omega)$.

EXERCISE 37: For even $\nu = 2n$, the factor z_ν is given by $z_\nu = i\pi\nu/\beta = i2\pi n/\beta = i\omega_n$ where $\omega_n = 2\pi n/\beta = 2\pi nT$ is the Matsubara frequency for Bosons, see (5.6). Show that this could produce the correct boundary condition for the Green's functions.

A typical form of the spectral function has the form (e.g., in the Hartree–Fock approximation),

$$A(\mathbf{p},\omega) = 2\pi\delta(\omega - E(\mathbf{p})), \tag{7.54}$$

i.e., there is just a single possible energy for each momentum. However, this result is physically quite unreasonable. The interaction between the particles should result in the existence of a spread in these possible energies. Perhaps the best way of seeing the necessity of this spread is to consider

$$\frac{1}{\Omega^2}\left|\langle\psi(\mathbf{p},t)\psi^\dagger(\mathbf{p},t')\right|^2 = \left|G^>(\mathbf{p},t-t')\right|^2 = \left|\int\frac{\mathrm{d}\omega}{2\pi}A(\mathbf{p},\omega)[1\pm f(\omega)]e^{-i\omega(t-t')}\right|^2. \tag{7.55}$$

If the expectation value in (7.55) involved only a single state, (7.55) would be the probability that one could add a particle with momentum $\mathbf{p}$ to this state at the time t', remove a particle at the time t, and then come back to the very same state as in the beginning. Clearly, as the addition and removal processes become very separated in time, i.e., $|t-t'|\to\infty$, this probability should decrease. The expectation value in (7.55) actually contains a sum over many different states. This sum should lead to a result decreasing even more strongly in time.

However, the right-hand side of (7.55) is independent of time, since

$$\left|\left[1\pm f\left(\frac{\mathbf{p}^2}{2m}+nv\right)\right]\cdot\exp\left[-i(t-t')\cdot\left(\frac{\mathbf{p}^2}{2m}+nv\right)\right]\right|^2 = \left|\left[1\pm f\left(\frac{\mathbf{p}^2}{2m}+nv\right)\right]\right|^2. \tag{7.56}$$

Therefore, this approximation predicts an infinite lifetime for any state produced by adding a single particle to the system. Thus, we must look for better approximations if we are to have an understanding of the lifetimes of single-particle excited states. It is possible to estimate this lifetime for a classical gas without doing any calculation. If we first add a particle and then remove a particle with the same momentum, we should come back to the same state only if, in the intervening time, the added particle has not collided with any of the other particles in the gas. Therefore, we should expect that the probability (7.55) should decay as $e^{-\Gamma(\mathbf{p})|t-t'|}$, where $\Gamma(\mathbf{p})$ is the collision rate for the added particle. This collision rate can be estimated as

$$\Gamma(\mathbf{p}) \sim \langle n\rangle\sigma(\overline{\mathbf{p}}/m) \sim \langle n\rangle\sigma\overline{\mathbf{v}},\quad \overline{\mathbf{v}} = \overline{\mathbf{p}}/m, \tag{7.57}$$

where σ is an average collision cross section, and $\overline{\mathbf{p}}/m$ is an average relative velocity of the added particle with respect to the other particles in the medium. This decay of single-particle excited states is an exceedingly important feature of many-particle systems. It is responsible for the return of the system to thermodynamic equilibrium after a disturbance. It is very easy to find a form for A that will lead to a proper decay of the probability (7.55). No A which is a sum of a finite number of delta functions will lead to exponential decay in (7.55). But any continuously varying A will lead to rapid decay. Consider, for example, the Lorentzian line shape,

$$A(\mathbf{p},\omega) = \frac{\Gamma(\mathbf{p})}{\left[\omega - E(\mathbf{p})\right]^2 + \left[\Gamma(\mathbf{p})/2\right]^2}. \tag{7.58}$$

When the dispersion in energy $\Gamma(\mathbf{p})$ is much less than β, we can perform (7.55) by replacing $f(\omega)$ by $f(E(\mathbf{p}))$:

$$\int\frac{\mathrm{d}\omega}{2\pi}\frac{\Gamma(\mathbf{p})}{[\omega-E(\mathbf{p})]^2+\Gamma^2(\mathbf{p})/4}[1\pm f(E(\mathbf{p}))]e^{-i\omega(t-t')} \sim \int\frac{e^{-i\omega(t-t')}\mathrm{d}\omega}{(\omega-\alpha)^2+\beta} \sim e^{-\sqrt{\beta}|t-t'|} \sim e^{-\Gamma(\mathbf{p})|t-t'|}. \tag{7.59}$$

Thus $\Gamma(\mathbf{p})$ represents both the energy dispersion and decay rate of the single-particle excited state with momentum $\mathbf{p}$.

The time-ordered Green's function (correlation function) can also defined for general operators besides $\psi(\mathbf{x},t)$,

$$iG(t_\mathrm{f},t_\mathrm{i}) = \langle 0|\mathrm{T}[\mathcal{O}_2(t_\mathrm{f})\mathcal{O}_1(t_\mathrm{i})]|0\rangle. \tag{7.60}$$

Importantly, we can use path integral formulation to re-express it as,

$$\boxed{iG(t_\mathrm{f},t_\mathrm{i}) = \int\mathcal{D}x\mathcal{O}_2(t_\mathrm{f})\mathcal{O}_1(t_\mathrm{i})\exp\left(i\int\mathrm{d}tL\right)\Big/\int\mathcal{D}x\exp\left(i\int\mathrm{d}tL\right) = \langle\mathcal{O}_2(t_\mathrm{f})\mathcal{O}(t_\mathrm{i})\rangle,} \tag{7.61}$$

here the time t contains a small imaginary part, namely $t\to te^{-i\epsilon}$. The coefficient in the path integral representation of

the propagator cancels out when we calculate the correlation function, which greatly simplifies the path integral calculations. We calculate the time-ordered correlation function for the harmonic oscillator. After including the small imaginary time, i.e., $t \to te^{-i\epsilon}$ with $\epsilon = 0^+$, the action becomes (W plays the role of fundamental frequency of the oscillator),

$$S = \int \mathrm{d}t \frac{e^{-i\epsilon}}{2} x \left[-me^{2i\epsilon} \left(\frac{\mathrm{d}}{\mathrm{d}t} \right)^2 - mW^2 \right] x, \tag{7.62}$$

and then

$$iG(t_\mathrm{f}, t_\mathrm{i}) = \frac{\int \mathcal{D}x x(t_\mathrm{f}) x(t_\mathrm{i}) \exp\left[i \int \mathrm{d}t \frac{e^{-i\epsilon}}{2} x \left(-me^{2i\epsilon} \left(\frac{\mathrm{d}}{\mathrm{d}t} \right)^2 - mW^2 \right) x \right]}{\int \mathcal{D}x \exp\left[i \int \mathrm{d}t \frac{e^{-i\epsilon}}{2} x \left(-me^{2i\epsilon} \left(\frac{\mathrm{d}}{\mathrm{d}t} \right)^2 - mW^2 \right) x \right]}. \tag{7.63}$$

Using Wick's theorem (see **EXERCISE 39** for a prototype example), one can find that

$$e^{-i\epsilon} \left(-me^{2i\epsilon} \left(\frac{\mathrm{d}}{\mathrm{d}t} \right)^2 - mW^2 \right) G(t - t') = \delta(t - t'). \tag{7.64}$$

Since $\epsilon = 0^+$, we have the solution

$$G(t - t') = -\frac{i}{2mW} \exp\left(-ie^{-i\epsilon} |t - t'| W \right) \to -\frac{i}{2mW} \exp\left[-i|t|W\left(1 - i0^+\right) \right]. \tag{7.65}$$

which is finite as $t - t' \to \pm\infty$, the second relation holds for $\epsilon \to 0^+$ while the first one for general $0 < \epsilon \leq \pi/2$. The ω-space correlation function is then

$$G(\omega) = \int \mathrm{d}t G(t, 0) e^{i\omega t} = \frac{m^{-1}}{\omega^2 - W^2 + i0^+}. \tag{7.66}$$

To summarize, $G(\omega)$ is the inverse of $-m\mathrm{d}^2/\mathrm{d}t^2 - mW^2$ appearing in the action $S = \int \mathrm{d}t 2^{-1} x(t)[-m\mathrm{d}^2/\mathrm{d}t^2 - mW^2]x(t)$.

Based on the definitions for the response function D and the time-ordered correlation function iG, one finds

$$D(t) = 2\Theta(t)\mathrm{Re}G(t), \tag{7.67}$$

if $\mathcal{O}_1$ and $\mathcal{O}_2$ are both Hermitian. Furthermore, if $\mathcal{O}_1 = \mathcal{O}_2 = \mathcal{O}_1^\dagger$, we have $G(t) = G(-t)$ and consequently,

$$\boxed{\mathrm{Re}D(\omega) = \mathrm{Re}G(\omega), \quad \mathrm{Im}D(\omega) = \mathrm{sgn}(\omega)\mathrm{Im}G(\omega).} \tag{7.68}$$

There exist standard methods for calculating G (path-integral and Feynman diagrams) since it is time-ordered and therefore Wick's theorem applies: $\mathrm{Im}G(\omega) \to \mathrm{Im}D(\omega) \to D(\omega)$ (see (6.25)), in this sense (7.68) are extremely important.

EXERCISE 38: Start from the standard definition for time-order correlation function, argue why there should be a small imaginary time in the calculation, i.e., $t \to te^{-i\epsilon}$ with $\epsilon = 0^+$. Prove the relations (7.67) and (7.68).

EXERCISE 39: Show that

$$\langle q_i q_j \cdots q_k q_l \rangle \equiv \int_{-\infty}^{+\infty} \mathrm{d}^n q q_i q_j \cdots q_k q_l e^{-qKq/2} \Big/ \int_{-\infty}^{+\infty} \mathrm{d}^n q e^{-qKq/2} = \sum_{\mathrm{Wick}} K^{-1}_{mn} \cdots K^{-1}_{st}. \tag{7.69}$$

For example, $\langle q_i q_j q_k q_l \rangle = K^{-1}_{ij} K^{-1}_{kl} + K^{-1}_{ik} K^{-1}_{jl} + K^{-1}_{il} K^{-1}_{kj}$.

As a short summary,

Linear responses can be calculated from the response functions of corresponding operators

Response functions can be expressed in terms of time-ordered correlation functions

Time-ordered correlation functions can be calculated through the path integral

Comments – details of using $i0^+$. We use the path integral formula to calculate the correlation function of the harmonic oscillator. Let $|n\rangle$ be the eigenstate of the energy operator H with eigenvalue E_n. We assume that the ground state energy E_0 is zero, then the evolution for the general state $|q'\rangle$ is

$$\boxed{|q', t'\rangle = e^{iHt'}|q'\rangle = \sum_{n=0}^{\infty} e^{iHt'}|n\rangle\langle n|q'\rangle = \sum_{n=0}^{\infty} \psi_n^*(q') e^{iE_n t'}|n\rangle,} \tag{7.70}$$

where $\psi_n(q) = \langle q|n\rangle$. Using $H(1 - i0^+)$ to replace H, then only the zeroth order term will be kept in the limit $t' \to -\infty$,

namely $\psi_0^*(q')|0\rangle$. Multiplying this result by an arbitrary function $\chi(q')$ and integrating over q' where $\langle 0|\chi\rangle \neq 0$, we obtain "const. $\times$ $|0\rangle$", here the constant could be absorbed into the definition of the path integral. In this sense, we have produced an in-state. Similarly, replacing H with $H(1-i0^+)$ and taking the limit $t''\to\infty$ could find the out-state from $\langle q'',t''| = \langle q''|e^{-iHt''}$. The scattering amplitude between the in-state and the out-state is thus expressed as $\langle 0|0\rangle$. In order to calculate this quantity, namely $\langle 0|0\rangle$, the theoretical term of 0^+ is very important and necessary. More generally,

$$\langle 0|0\rangle_{F,J} = \int \mathcal{D}p\mathcal{D}q \exp\left(i\int_{-\infty}^{+\infty} \mathrm{d}t \left(p\dot{q} - \left(1-i0^+\right)H(p,q) + Fq + Jp\right)\right), \tag{7.71}$$

where F, J are the external fields coupling to the coordinates and momenta, respectively.

For the case of harmonic oscillator, the scattering amplitude between the in-state and the out-state is given by after integrating out the momentum,

$$\boxed{\langle 0|0\rangle_F = \int \mathcal{D}q \exp\left(i\int_{-\infty}^{+\infty} \mathrm{d}t \left(\frac{1}{2}\left(1+i0^+\right)m\dot{q}^2 - \frac{1}{2}\left(1-i0^+\right)mW^2q^2\right)\right).} \tag{7.72}$$

The effect of replacing H by $H(1-i0^+)$ is equivalent to use$(1-i0^+)/m$ to replace $1/m$, or use $(1+i0^+)m$ to replace m, and in the following calculation we take $m=1$. Introducing $x(\omega) = q(\omega) + F(\omega)/[\omega^2 - W^2 + i0^+]$, we obtain,

$$S = \frac{1}{2}\int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{2\pi}\left[x(\omega)\left(\omega^2 - W^2 + i0^+\right)x(-\omega) - \frac{F(\omega)F(-\omega)}{\omega^2 - W^2 + i0^+}\right], \tag{7.73}$$

$$\langle 0|0\rangle_F = \exp\left[\frac{i}{2}\int \frac{\mathrm{d}\omega}{2\pi}\frac{F(\omega)F(-\omega)}{-\omega^2+W^2-i0^+}\right]\int \mathcal{D}x \exp\left(\frac{i}{2}\int \frac{\mathrm{d}\omega}{2\pi}\left(x(\omega)\left(\omega^2 - W^2 + i0^+\right)x(-\omega)\right)\right), \tag{7.74}$$

the second term is the value of $\langle 0|0\rangle$ in the absence of the external fields, which is 1, thus

$$\boxed{\langle 0|0\rangle_F = \exp\left[\frac{i}{2}\int \frac{\mathrm{d}\omega}{2\pi}\frac{F(\omega)F(-\omega)}{-\omega^2+W^2-i0^+}\right].} \tag{7.75}$$

Simultaneously by introducing

$$\langle 0|0\rangle_F = \exp\left[\frac{i}{2}\int \mathrm{d}t\mathrm{d}t' F(t)G(t-t')F(t')\right], \quad G(t-t') = -\int \frac{\mathrm{d}\omega}{2\pi}\frac{e^{-i\omega(t-t')}}{-\omega^2+W^2-i0^+}, \tag{7.76}$$

one can obtain by straightforward calculations that $G(t-t') = -ie^{-iW|t-t'|}/2W$, and $G(t-t')$ is the solution of the differential equation $\left(\partial^2/\partial t^2 + W^2\right)G(t-t') = -\delta(t-t')$. The result obtained here is the same as (7.65).

H Spectroscopy, Nucleon Momentum Distribution

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In this section, we discuss the spectral function in some more details which is closely related to certain experiments. We use the nucleon as an example and since nucleon is a Fermion, we may first rewrite the expressions developed in the last two sections. The relation (7.53) tells that,

$$\boxed{A(\mathbf{p},\omega)=2\mathrm{Im}G(\mathbf{p},\omega-i\epsilon),\quad \epsilon=0^{+}.} \tag{8.1}$$

There exists a Fermi energy (momentum) due to the Pauli principle for a Fermi system, in the following we will calculate the energy by subtracting the Fermi energy denoted by μ. Then the relations in (7.24) could be rewritten as,

$$G^{>}(\mathbf{p},\omega)=[1-f(\omega)]A(\mathbf{p},\omega),\quad G^{<}(\mathbf{p},\omega)=f(\omega)A(\mathbf{p},\omega),\quad f(\omega)=\frac{1}{e^{\beta\omega}+1}, \tag{8.2}$$

one shall notice that here ω is understood as $\omega-\mu$. Combining (8.1) and (8.2) gives us

$$\boxed{G^{<}(\mathbf{p},\omega)=\left(\frac{2}{e^{\beta\omega}+1}\right)\mathrm{Im}G(\mathbf{p},\omega-i\epsilon),\quad G^{>}(\mathbf{p},\omega)=\left(\frac{e^{\beta\omega}}{e^{\beta\omega}+1}\right)\mathrm{Im}G(\mathbf{p},\omega-i\epsilon).} \tag{8.3}$$

Notice that $G^{<}(\mathbf{p},\omega)$ or $G^{>}(\mathbf{p},\omega)$ is the Fourier transform of the correlation functions defined in (7.11), while $G(\mathbf{p},\omega)$ is the Fourier transform of the time-ordered correlation function. Comparing (8.3) with the fluctuation–dissipation theorem in Section F, in the following form,

$$\boxed{\begin{aligned} C(t-t')&=\langle\mathcal{O}(t)\mathcal{O}(t')\rangle\leftrightarrow G^{<}(1,1')=\pm\frac{1}{i}\langle\psi^{\dagger}(1')\psi(1)\rangle, &(8.4)\\ iD_{\mathrm{R}}(t-t')&=\Theta(t-t')\langle[\mathcal{O}(t),\mathcal{O}(t')]\rangle\leftrightarrow G(1,1')=\frac{1}{i}\langle\mathrm{T}(\psi(1)\psi^{\dagger}(1'))\rangle, &(8.5)\\ C(\omega)&=-2[1+n_{\mathrm{B}}(\omega)]\mathrm{Im}D(\omega+i\epsilon)\leftrightarrow G^{<}(\mathbf{p},\omega)=\left(\frac{2}{e^{\beta\omega}+1}\right)\mathrm{Im}G(\mathbf{p},\omega-i\epsilon), &(8.6)\end{aligned}}$$

see (6.14), (6.16), (6.30), (7.11) and notice that $\mathrm{Im}D(\omega)=\mathrm{sgn}(\omega)\mathrm{Im}G(\omega)$ of (7.68). In this sense, relations in (8.3) provide the Fermionic fluctuation–dissipation theorem, and $\mathrm{Im}D(\omega)$ is also called the spectral function. For high-temperature limit, we have $G^{<}(\mathbf{p},\omega)\approx A(\mathbf{p},\omega)=2\mathrm{Im}G(\mathbf{p},\omega-i\epsilon)$.

The spectral function provides a link to experimental data. For example, the reaction (e,e′p) could be used to study the hole spectral function for typical finite nuclei. Since the electron interacts weakly with the nucleons inside, it is an ideal probe to study nuclei. The dominant operators that excite the nucleus in electron scattering have a one-body character. When the incident electron has enough energy, the removed proton can be sufficiently energetic so that the impulse approximation may apply. If the electron transfers a substantial amount of energy the resulting excited state is expected to be dominated by a simple particle-hole state. It corresponds to the outgoing particle suitably influenced by the surrounding medium and the valence hole that is selected by the kinematics of the reaction. Moreover, additional interactions between this particle and the hole state play no role. In the impulse approximation, the energy ω and momentum $\mathbf{q}$ lost by the electron are transferred to a proton with binding (missing) energy E_{m} and (missing) momentum $-\mathbf{p}_{\mathrm{m}}$, which then leaves the nucleus with momentum $\mathbf{p}'=\mathbf{q}-\mathbf{p}_{\mathrm{m}}$ and kinetic energy $T_{\mathbf{p}'}$. The proton knockout cross section is proportional to the spectral function,

$$\mathrm{d}\sigma\sim A(\mathbf{p}_{\mathrm{m}},E_{\mathrm{m}}), \tag{8.7}$$

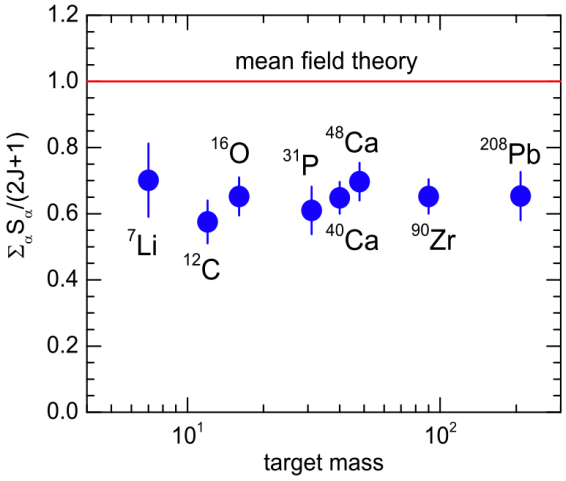

Fig. L: The spectroscopic factors from the (e,e′p) reaction as a function of target mass. The dotted line with a value of 1 is the mean-field model prediction.

here $A(\mathbf{p}_{\mathrm{m}},E_{\mathrm{m}})$ is the (hole) spectral function, i.e., the probability to find in the parent nucleus a proton with binding energy E_{m} and momentum $\mathbf{p}_{\mathrm{m}}$. The spectroscopic factor of the last valence orbit for different nuclei is shown in Fig. L, the results indicate that there is an essentially global reduction of the single-particle strength of about 30% for these valence holes in most nuclei. Such a substantial deviation from the predicted of mean-field models, then requires a detailed explanation on the basis of the correlations in nuclei. In quantum field theory, the cross section could be similarly calculated from the time-ordered correlation functions (S matrix), under certain conditions.

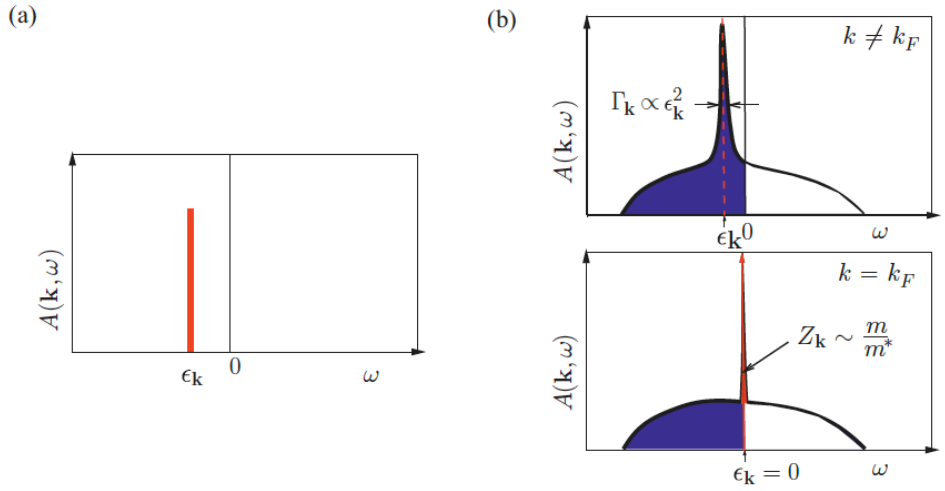

Fig. M: Sketch of the spectral function with interactions. Taken from Coleman (2016).

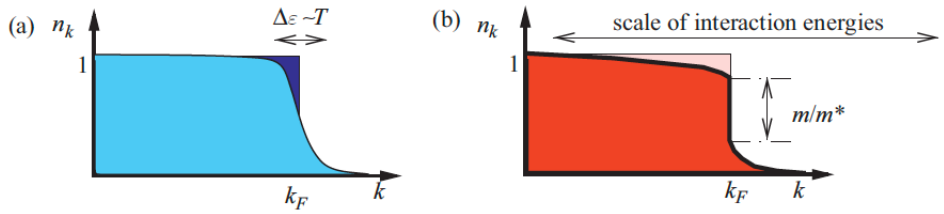

Fig. N: Nucleon momentum distribution function in a free Fermi gas model (left panel) and the one including interactions (right panel). Taken from Coleman (2016).

The nucleon (or other Fermions like electron) momentum distribution could be obtained from the Green's function or the spectral function as[7]

$$\boxed{n_\mathbf{k} = \int_{-\infty}^{0} \frac{\mathrm{d}\omega}{2\pi} A(\mathbf{k},\omega),} \tag{8.8}$$

here ω is counted below the Fermi surface. For a free Fermi gas, then the momentum distribution function takes the step-function form of $\Theta(\mu - E_\mathbf{k})$. With interactions included, a sharp quasi-particle in the spectral function may emerge,

$$\boxed{A(\mathbf{k},\omega)/2\pi = \frac{1}{\pi}\mathrm{Im}\, G(\mathbf{k},\omega - i0^+) = Z_\mathbf{k}\delta(\omega - \epsilon_\mathbf{k}) + \text{continumm},} \tag{8.9}$$

where $\epsilon_\mathbf{k} = E_\mathbf{k} - \mu$, $Z_\mathbf{k}$ is the wave-function renormalization strength, which also holds the interpretation of the residue of the single nucleon pole in the exact propagator. We can prove that $Z_\mathbf{k}$ is inversely proportional to the nucleon effective mass. See Fig. M for a sketch of the spectral function; in a free Fermi gas, the spectral function is a sharp delta function at $\epsilon_\mathbf{k}$ (left panel) while in an interacting Fermi liquid the quasi-particle forms a broadened peak of width $\Gamma_\mathbf{k}$ at $\epsilon_\mathbf{k}$ (right panel), see expression (7.58). At the Fermi momentum, this peak becomes infinitely sharp, corresponding to a long-lived quasi-particle on the Fermi surface. The weight in the quasi-particle peak could be shown as is $Z_\mathbf{k}^{-1} \sim M^*$, where M^* is the effective mass of the nucleon (which could also be extracted from experiments). Then the nucleon momentum distribution function becomes

$$\boxed{n_\mathbf{k} = Z_\mathbf{k}\Theta(-\epsilon_\mathbf{k}) + \text{smooth background}.} \tag{8.10}$$

We find while finite temperature can induce a continuous high momentum tail (HMT) in the momentum distribution function (left panel of Fig. N), the interactions (at zero temperature) can similarly induce an jumped HMT (right panel of Fig. N). Although interactions do smear the momentum distribution, the jump continues to survive in reduced form so long as the Landau Fermi-liquid is intact. This jump is often called Migdal–Luttinger jump. Besides the HMT, we often call the low momentum below k_F in $n_\mathbf{k}$ the depletion. In the Landau Fermi-liquid, the Fermi surface volume measures the particle density. Since the Fermi surfaces of the quasi-particles and of the unrenormalized particles coincide, it follows that the Fermi surface volume must be an adiabatic invariant when the interactions are turned on, and this is called the Luttinger theorem (Luttinger sum rule).

The smooth background part of the momentum distribution function also contains much interesting information. Particularly, both theoretical and experimental investigations indicate that a $|\mathbf{k}|^{-4} = k^{-4}$ form of the HMT exists. Let us

[7] Notice that in units with $\hbar = 1$, we have $\mathbf{p} = \mathbf{k}$. Moreover, we also suppress other degrees of freedom such as spin σ, therefore $n_\mathbf{k} \to n_{\mathbf{k}\sigma}$.

calculate the kinetic energy via the general single-nucleon momentum distribution function with a k^{-4} HMT,

$$n_{\mathbf{k}}=\begin{cases}A, & 0<|\mathbf{k}|<k_{\rm F},\\ C_\infty/|\mathbf{k}|^4, & k_{\rm F}<|\mathbf{k}|<\lambda k_{\rm F}^0,\\ 0, & \text{others},\end{cases}\tag{8.11}$$

where C_∞ is the strength of the HMT and λ the cutoff. Under the normalization condition, one has $[1/(2\pi)^3]\int_0^\infty g n_{\mathbf{k}}\mathrm{d}\mathbf{k}=1$, here the degenerate factor $g=2\times 2=4$ for nuclear matter. We calculate the following quantity,

$$\langle k^j\rangle\equiv\langle|\mathbf{k}|^j\rangle=\frac{1}{(2\pi)^3}\int_0^\infty g k^j n_{\mathbf{k}}\mathrm{d}\mathbf{k}\Big/\frac{1}{(2\pi)^3}\int_0^\infty g n_{\mathbf{k}}\mathrm{d}\mathbf{k}\equiv\frac{1}{(2\pi)^3}\int_0^\infty g k^j n_{\mathbf{k}}\mathrm{d}\mathbf{k},\tag{8.12}$$

where $j\geq 2$ is an integer. Considering that (normalization condition),

$$\frac{4\pi g}{(2\pi)^3}\left[\int_0^{k_{\rm F}}Ak^2\mathrm{d}k+\int_{k_{\rm F}}^{\lambda k_{\rm F}^0}\frac{C_\infty}{k^4}k^2\mathrm{d}k\right]=1,\tag{8.13}$$

we have

$$\begin{aligned}A=&\frac{3}{k_{\rm F}^3}\left[\frac{2\pi^2}{g}-C_\infty\left(\frac{1}{k_{\rm F}}-\frac{1}{\lambda k_{\rm F}^0}\right)\right]=\frac{3\pi^2}{k_{\rm F}^3}\left[\frac{2}{g}-\frac{C_\infty}{\pi^2}\left(\frac{1}{k_{\rm F}}-\frac{1}{\lambda k_{\rm F}^0}\right)\right]\\ =&\frac{3\pi^2}{k_{\rm F}^{0,3}}\frac{k_{\rm F}^{0,3}}{k_{\rm F}^3}\left[\frac{2}{g}-\frac{C_\infty}{\pi^2}\left(\frac{1}{k_{\rm F}}-\frac{1}{\lambda k_{\rm F}^0}\right)\right]=\frac{3\pi^2}{k_{\rm F}^{0,3}}\frac{\rho_0}{\rho}\left[\frac{2}{g}-\frac{c_0}{\pi^2}\left(1-\frac{1}{\lambda}\left(\frac{\rho}{\rho_0}\right)^{1/3}\right)\right],\end{aligned}\tag{8.14}$$

and consequently,

$$\boxed{\begin{aligned}\langle k^j\rangle=&\frac{g}{2\pi^2}\left[\int_0^{k_{\rm F}}Ak^{j+2}\mathrm{d}k+\int_{k_{\rm F}}^{\lambda k_{\rm F}^0}\frac{C_\infty}{k^4}k^{j+2}\mathrm{d}k\right]=\frac{g}{2\pi^2}\left[\frac{Ak_{\rm F}^{j+3}}{j+3}+\frac{C_\infty}{j-1}\left((\lambda k_{\rm F}^0)^{j-1}-k_{\rm F}^{j-1}\right)\right]\\ =&\frac{g}{2\pi^2}\left[\frac{k_{\rm F}^{j+3}}{j+3}\cdot\frac{3\pi^2}{k_{\rm F}^3}\left(\frac{2}{g}-\frac{c_0}{\pi^2}\left(1-\frac{1}{\lambda}\left(\frac{\rho}{\rho_0}\right)^{1/3}\right)\right)+\frac{c_0k_{\rm F}}{j-1}\left(\lambda^{j-1}k_{\rm F}^{0,j-1}-k_{\rm F}^{j-1}\right)\right]\\ =&\frac{3k_{\rm F}^j}{j+3}-\frac{gc_0k_{\rm F}^j}{2\pi^2}\left[\frac{4j}{j^2+2j-3}-\frac{1}{\lambda}\frac{3}{j+3}\left(\frac{\rho}{\rho_0}\right)^{1/3}-\frac{\lambda^{j-1}}{j-1}\left(\frac{\rho_0}{\rho}\right)^{j/3-1/3}\right].\end{aligned}}\tag{8.15}$$

where $C_\infty=c_0k_{\rm F},c_0$ is a constant. According to this expression, we have

(a) In the free Fermi gas model, $\lambda=(\rho/\rho_0)^{1/3}$, A depends on g but the physical quantity $\langle k^j\rangle$ does not depend on g.

(b) In the presence of the HMT, both A and $\langle k^j\rangle$ depend on g, and in this situation a correct g is relevant. This phenomenon originates from the fact that the momentum scaling forms of the low momentum part ($|\mathbf{k}|\leq k_{\rm F}$) and that of the high momentum part is different, i.e., if $|\mathbf{k}|>k_{\rm F}$ one has $|\mathbf{k}|^{-4}$, while on the other hand if $|\mathbf{k}|<k_{\rm F}$ one has $|\mathbf{k}|^0$. Actually $\langle k^j\rangle$ is a physical quantity but A not.

One can use the parabolic approximation to estimate the kinetic symmetry energy, see **EXERCISE 41**.

EXERCISE 40: Denote $E_J=T+U_J$ as the single nucleon energy in asymmetric nucleonic matter with density $\rho=\sum_{J=\rm n,p}\rho_J$ and isospin asymmetry $\delta=(\rho_{\rm n}-\rho_{\rm p})/(\rho_{\rm n}+\rho_{\rm p})$, here $T=\mathbf{k}^2/2M$ is the kinetic energy with M the static mass of nucleons, and $U_J=U_J(\rho,\delta,\mathbf{k})$ is the single nucleon potential. The density ρ_J and the momentum $\mathbf{k}$ is connected via the Fermi relation as $k_{\rm F}^J=(3\pi^2\rho_J)^{1/3}$ where $k_{\rm F}^J$ is the Fermi momentum for nucleon J. The value of E_J at the Fermi momentum is the chemical potential and is denoted as μ_J which is function of ρ and δ (and not of momentum $\mathbf{k}$). Thermodynamic relation tells that $\mu_J=\partial[\rho E(\rho,\delta)]/\partial\rho_J$ where $E(\rho,\delta)\approx E_0(\rho)+E_{\rm sym}(\rho)\delta^2+\cdots$ is the equation of state of the system and $E_{\rm sym}(\rho)$ is the symmetry energy. Derive using the integration form of the perturbative method the expressions for $E_{\rm sym}(\rho)$ and $L(\rho)=3\rho\mathrm{d}E_{\rm sym}(\rho)/\mathrm{d}\rho$ in terms of $U_0,U_{\rm sym}$ and $U_{\rm sym,2}$, with them defined via $U_J(\rho,\delta,\mathbf{k})=U_0(\rho,\mathbf{k})+U_{\rm sym}(\rho,\mathbf{k})\tau_3^J\delta+U_{\rm sym,2}(\rho,\mathbf{k})\delta^2$ under the convention $\tau_3^{\rm n}=+1$ (neutron) and $\tau_3^{\rm p}=-1$ (proton).

EXERCISE 41: If one adopts the momentum distribution (8.11) and the parabolic approximation, show that the kinetic symmetry energy could be obtained as

$$E_{\rm sym}^{\rm kin}(\rho)=\underbrace{\left(2^{2/3}-1\right)\cdot\frac{3k_{\rm F}^2}{10M}}_{E_{\rm sym}^{\rm kin,FFG}(\rho)}-\frac{c_0}{\pi^2}\frac{k_{\rm F}^2}{2M}\left[\frac{6}{5}\frac{1}{\lambda}\left(\frac{\rho}{\rho_0}\right)^{1/3}+2\lambda\left(\frac{\rho_0}{\rho}\right)^{1/3}-\frac{16}{5}\right],\tag{8.16}$$

here the nucleons in pure neutron matter are assumed to have no HMT.

EXERCISE 42: Assume that the single nucleon momentum distribution function in an asymmetric nuclear matter is

$$n_{\mathbf{k}}^{J}(\rho,\delta)\equiv n_{J}(\rho,|\mathbf{k}|,\delta)=\begin{cases}\Delta_{J}+\beta_{J}I\left(|\mathbf{k}|/k_{\mathrm{F}}^{J}\right), & 0<|\mathbf{k}|<k_{\mathrm{F}}^{J},\\ C_{J}\left(k_{\mathrm{F}}^{J}/|\mathbf{k}|\right)^{4}, & k_{\mathrm{F}}^{J}<|\mathbf{k}|<\phi_{J}k_{\mathrm{F}}^{J}.\end{cases}\tag{8.17}$$

Here, the Δ_J is the depletion of the Fermi sphere at zero momentum with respect to the FFG model prediction while the β_J characterizes the strength of the momentum dependence $I(|\mathbf{k}|/k_{\mathrm{F}}^{J})$ of the depletion near (and at) the nucleon Fermi surface. Show that the relation between the contact C_J and cutoff coefficient ϕ_J relating the fraction of nucleons in the HMT as

$$x_{J}^{\mathrm{HMT}}=\int_{k_{\mathrm{F}}^{J}}^{\phi_{J}k_{\mathrm{F}}^{J}}n_{\mathbf{k}}^{J}\mathrm{d}\mathbf{k}\Big/\int_{0}^{\phi_{J}k_{\mathrm{F}}^{J}}n_{\mathbf{k}}^{J}\mathrm{d}\mathbf{k}=3C_{J}\left(1-\frac{1}{\phi_{J}}\right).\tag{8.18}$$

The normalization condition

$$\frac{2}{(2\pi)^{3}}\int_{0}^{\infty}n_{\mathbf{k}}^{J}(\rho,\delta)\mathrm{d}\mathbf{k}=\rho_{J}=\frac{(k_{\mathrm{F}}^{J})^{3}}{3\pi^{2}}\tag{8.19}$$

requires that only three of the four parameters, i.e., β_J, C_J, ϕ_J and Δ_J, are independent. show that this gives Δ_J as

$$\Delta_{J}=1-\frac{3\beta_{J}}{(k_{\mathrm{F}}^{J})^{3}}\int_{0}^{k_{\mathrm{F}}^{J}}I\left(\frac{k}{k_{\mathrm{F}}^{J}}\right)k^{2}\mathrm{d}k-3C_{J}\left(1-\frac{1}{\phi_{J}}\right).\tag{8.20}$$

Moreover, we assume that all of the four parameters in the distribution Eq. (8.17) take the form of $Y_J=Y_0(1+Y_1^J\delta)$. Physically the odd order terms of the kinetic part of the EOS of ANM should be zero considering the isospin symmetry between neutrons and protons, indicating that the first order of the kinetic energy

$$E^{\mathrm{kin}}(\rho,\delta)=\frac{1}{\rho}\frac{2}{(2\pi)^{3}}\sum_{J=\mathrm{n,p}}\int_{0}^{\phi_{J}k_{\mathrm{F}}^{J}}\frac{\mathbf{k}^{2}}{2M}n_{\mathbf{k}}^{J}(\rho,\delta)\mathrm{d}\mathbf{k},\tag{8.21}$$

should be zero. Based on the distribution Eq. (8.17), the $E^{\mathrm{kin}}(\rho,\delta)$ acquires a linear term in isospin asymmetry δ with a coefficient of

$$E_{1}^{\mathrm{kin}}(\rho)\equiv\left.\frac{\partial E^{\mathrm{kin}}(\rho,\delta)}{\partial\delta}\right|_{\delta=0}=\frac{3}{5}\frac{k_{\mathrm{F}}^{2}}{2M}\left[\frac{5}{2}C_{0}\phi_{0}(\phi_{1}^{\mathrm{n}}+\phi_{1}^{\mathrm{p}})+\frac{5}{2}C_{0}(\phi_{0}-1)(C_{1}^{\mathrm{n}}+C_{1}^{\mathrm{p}})+\frac{1}{2}\Delta_{0}(\Delta_{1}^{\mathrm{n}}+\Delta_{1}^{\mathrm{p}})+\frac{5\beta_{0}(\beta_{1}^{\mathrm{n}}+\beta_{1}^{\mathrm{p}})}{2k_{\mathrm{F}}^{5}}\int_{0}^{k_{\mathrm{F}}}I\left(\frac{k}{k_{\mathrm{F}}}\right)k^{4}\mathrm{d}k\right].\tag{8.22}$$

To enforce the neutron-proton exchange symmetry of EOS, by setting the $E_1^{\mathrm{kin}}(\rho)$ to zero gives $Y_J=Y_0(1+Y_1\tau_3^J\delta)$.

EXERCISE 43: Assume that the $I(x)$ function in Eq. (8.17) takes the form $I(|\mathbf{k}|/k_{\mathrm{F}}^{J})=(|\mathbf{k}|/k_{\mathrm{F}}^{J})^{2}$, with the parameters β_0 and β_1 appeared in $\beta_J=\beta_0(1+\tau_3^J\beta_1\delta)$ used in the $n_{\mathbf{k}}^{J}(\rho,\delta)$ of Eq. (8.17) being constrained about $\beta_0\approx-0.27\pm0.08$ and $-1\leq\beta_1\leq1$. Calculate the correction to the EOS of SNM, the kinetic symmetry energy and the kinetic fourth-order symmetry energy. How the nucleon effective mass modifies in the presence of β_J?

EXERCISE 44: The depletion of the Fermi surface is defined as

$$\kappa_{J}=1-\Delta_{J}-\frac{1}{k_{\mathrm{F}}^{J}}\int_{0}^{k_{\mathrm{F}}^{J}}I\left(\frac{|\mathbf{k}|}{k_{\mathrm{F}}^{J}}\right)\mathrm{d}k.\tag{8.23}$$

Calculate κ_0 and its isospin splitting to order δ^3.

Comments. The experimental finding that there exists more high momentum protons (neutrons) than neutrons (protons) in neutron-rich (poor) is believed originating from the tensor correlations between nucleons in finite nuclei. Moreover, the analysis based on electron-nucleus scattering experiments and predictions by nuclear many body theories strongly indicate that the sizable HMT of the single-nucleon momentum distribution function in finite nuclei/infinite nucleonic matter scales k^{-4}. Exploring the physics of the NN-SRCs and/or the tensor correlations are and will be one of the continuing physical aims of several facilities around the world. For instance, the determination of the magnitude of the SRCs in nuclei is very important to the final solution of the EMC puzzle. More interestingly, the k^{-4} form of the HMT in nucleonic matter was also found to be very similar with that from the ultra-cold atomic Fermi gases although the densities of the two systems are different by 25 orders of magnitude. Physically, the strength of the HMT characterized by $C(k_{\mathrm{F}}/k)^4$ for large k represents the short-ranged two-body contact interaction. Moreover, a k^{-4} form of the HMT was also found recently in a Bose system both theoretically ad experimentally, indicating the very generality of the HMT shared by the quantum many-body systems in the unitary region. Owing to the Efimov effect existed in a unitary Bose gas, a three-body contact C' emerges, i.e., $n(k)k^4\to C+f(k)C'$ at large k, where $f(k)$ characterizes the Efimov physics. Current research interests on the contact physics both in nuclei/nucleonic matter and ultra-cold atomic gases are mainly focused on these systems with large (even infinite) s-wave scattering length a (s-wave resonant interaction). However, very recent studies showed that systems with a p-wave resonant interaction also display several universal relations, and the momentum distribution at large k was found to scale as $n(k)\sim C_{\mathrm{p}}/k^2$ where C_{p} is the p-wave contact. Finally, we would like to point out that experimental techniques in other systems, like the angle-resolved photoemission

spectroscopy (ARPES), which directly probes the electronic structure in momentum space, has played a central role in the discovery, characterization, and understanding of quantum materials ranging from strongly correlated states of matter to those exhibiting nontrivial topology. See the related reference given in the start of this section.

I Real-time Green's Functions, Random Phase Approximation

RELEVANT REFERENCE:

- L. Kadanoff and G. Baym, *Quantum Statistical Mechanics*, Westview Press, 1962, Chapters 6 and 7.
- G. Stefanucci and R. van Leeuwen, *Nonequilibrium Many-body Theory of Quantum Systems: a Modern Introduction*, Cambridge University Press, 2013, Chapters 1-9.
- G. Baym and L. Kadanoff, *Conservation Laws and Correlation Functions*, Phys. Rev. **124**, 287 (1961).
- P. Danielewicz, *Quantum Theory of Nonequilibrium Processes. I*, Ann. Phys. **152**, 239 (1984).

We introduce the real-time Green's functions, as a companion of Section G, through the viewpoint of transport theories. The problem posed by transport theory, be it quantum or classical, is to calculate the space- and time-dependent responses induced in a system by external space- and time-dependent disturbances. We shall consider only disturbances of the form

$$\boxed{H'(t) = \int \mathrm{d}\mathbf{x} U(\mathbf{x},t) n(\mathbf{x},t), \quad n(\mathbf{x},t) = \psi^\dagger(\mathbf{x},t)\psi(\mathbf{x},t).} \tag{9.1}$$

We then want to calculate the expectation values of physical operators, as they develop in time when the system is influenced by U. In the Heisenberg representation, any operator, $X(\mathbf{X},T)$, develops in time according to the equation,

$$i\frac{\partial}{\partial T} X_U(\mathbf{X},T) = \left[X_U(\mathbf{X},T), H_U(T) + \int \mathrm{d}\mathbf{X}' n_U(\mathbf{x}',T) U(\mathbf{x}',T) \right]. \tag{9.2}$$

Here $H_U(T)$ is the Hamiltonian (7.2) of the system. It now depends on time because there is an external time-dependent perturbation. The subscript U on the operators indicates the time development is given by (9.2) and thus depends on U.

Suppose that at a very early time to, before U is turned on, the system is in a definite eigenstate, $|i,t_0\rangle$ of H. The t_0 in the designation of the state means that,

$$H(T)|i,t_0\rangle = E_i|i,t_0\rangle, \quad T < t_0. \tag{9.3}$$

In the Heisenberg picture, the system always remains in this state, and only the operators change in time ((9.3) fails to hold as soon as T becomes later than the time when U is turned on). The expectation of X at the time T and point $\mathbf{X}$ is,

$$\langle X(\mathbf{X},T)\rangle_U = \langle i,t_0|X_U(\mathbf{X},T)|i,t_0\rangle. \tag{9.4}$$

In an actual experiment, the system is not in a definite eigenstate of the Hamiltonian at time t_0, but is rather at a definite temperature. We start with a system in thermal equilibrium at a definite temperature (and chemical potential) when we begin the experiment, and then observe how the system develops in time. We need to average (9.4) over a grand-canonical ensemble of eigenstates of the system at time t_0. The expectation value becomes,

$$\langle X(\mathbf{X},T)\rangle_U = \frac{\sum_i e^{-\beta(E_i-\mu N_i)}\langle i,t_0|X_U(\mathbf{X},T)|i,t_0\rangle}{\sum_i e^{-\beta(E_i-\mu N_i)}}. \tag{9.5}$$

The ensemble can still be represented by a trace, but we must be careful to specify, by writing $H(t_0)$, the time at which the ensemble was prepared. Actually, (9.5) is independent of t as long as t is before the time that U is turned on. The number operator is independent of time, since an external potential does not change the number of particles.

Next notice that we can solve (9.2), at least formally, by going to the interaction representation. In this representation the operators develop in time according to

$$i\partial X(\mathbf{X},T)/\partial T = [X(\mathbf{X},T), H(T)]. \tag{9.6}$$

The transformation between the interaction and Heisenberg pictures is given by,

$$X_U(\mathbf{X},T) = \mathcal{U}^{-1}(T) X(\mathbf{X},T)\mathcal{U}(T), \quad \mathcal{U}(t) = \mathrm{T}\left[\exp\left(-i\int_{t_0}^{t}\mathrm{d}t'\int \mathrm{d}\mathbf{x}' n(\mathbf{x}',t')U(\mathbf{x}',t')\right)\right]. \tag{9.7}$$

EXERCISE 45: Check (9.7) by explicit differentation with respect to t_0.

The problem of calculating the expectation value of an operator in the presence of U is then reduced to,

$$\boxed{\langle X_U(\mathbf{X},T)=\langle X(\mathbf{X},T)\rangle_U=\frac{\mathrm{tr}[e^{-\beta[H(t_0)-\mu N]}\mathcal{U}^{-1}(T)X(\mathbf{X},T)\mathcal{U}(T)]}{\mathrm{tr}[e^{-\beta[H(t_0)-\mu N]}]}.} \tag{9.8}$$

Since we are in the interaction representation, $H(t_0)$ is independent of time so that we can drop the t_0 in $H(t_0)$. Since t_0 can be any time before the disturbance is turned on, (9.8) does not depend on t_0. Then we can write,

$$\boxed{\langle X(\mathbf{X},T)\rangle_U=\langle\mathcal{U}^{-1}(T)X(\mathbf{X},T)\mathcal{U}(T)\rangle,\ \ \mathcal{U}(T)=\mathrm{T}\left[\exp\left[-i\int_{-\infty}^{t}\mathrm{d}t'\mathrm{d}\mathbf{x}'n(\mathbf{x}',t')U(\mathbf{x}',t')\right]\right],} \tag{9.9}$$

where the expectation written without U denotes the equilibrium value. Eq. (9.9) is in a certain sense the solution to the problem of transport, since all the operators develop as they would in the equilibrium ensemble. All the dependence on the external field U is explicit in (9.9). Our program for determining quantities like (9.9) will be to write equations of motion for the generalized Green's functions in terms of which quantities like (9.9) can be expressed. These equations of motion will bear a strong resemblance to Boltzmann equations.

Using the Heisenberg representation creation and annihilation operators, we define the Green's functions,

$$\boxed{\begin{aligned} g(1,1';U)&=\frac{1}{i}\langle\mathrm{T}(\psi_U(1)\psi_U^\dagger(1'))\rangle, &(9.10)\\ g_2(12,1'2';U)&=\left(\frac{1}{i}\right)^2\langle\mathrm{T}(\psi_U(1)\psi_U(2)\psi_U^\dagger(2')\psi_U^\dagger(1'))\rangle, &(9.11)\\ g^{>}(1,1';U)&=\frac{1}{i}\langle\psi_U(1)\psi_U^\dagger(1')\rangle, &(9.12)\\ g^{<}(1,1';U)&=\pm\frac{1}{i}\langle\mathrm{T}(\psi_U^\dagger(1')\psi_U(1))\rangle. &(9.13)\end{aligned}}$$

In terms of these Green's functions, one may describe the response of a system initially in thermodynamic equilibrium to the applied disturbance U. For example, the average density and current at the point $\mathbf{X},T$ are given by,

$$\langle n(\mathbf{X},T)\rangle_U=\langle\psi_U^\dagger(\mathbf{X},T)\psi_U(\mathbf{X},T)\rangle=\pm ig^{<}(\mathbf{X}T,\mathbf{X}T;U),\ \ \langle\mathbf{j}(\mathbf{X},T)\rangle_U=\left[\frac{\nabla-\nabla'}{2im}\left[\pm ig^{<}(\mathbf{X}T,\mathbf{X}'T;U)\right]\right]_{\mathbf{X}'=\mathbf{X}}. \tag{9.14}$$

The lowercase letter "g" is used to distinguish these physical response functions which are defined for real times, from their imaginary-time counterparts, $G(U),G_2(U)$. There is a close connection between these two different sets of Green's functions. To derive these we notice from (9.2) that,

$$i\frac{\partial}{\partial t}\psi_U(\mathbf{x},t)=-\frac{\nabla^2}{2m}\psi_U(\mathbf{x},t)+U(\mathbf{x},t)\psi_U(\mathbf{x},t)+\int\mathrm{d}\mathbf{x}'v(\mathbf{x}-\mathbf{x}')\psi_U^\dagger(\mathbf{x}',t)\psi_U(\mathbf{x}',t)\psi_U(\mathbf{x},t), \tag{9.15}$$

so that

$$\boxed{\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-U(1)\right]g(1,1';U)=\delta(1-1')\pm i\int_{-\infty}^{+\infty}\mathrm{d}t_2\mathrm{d}\mathbf{x}_2V(1-2)g_2(12,1'2^+;U).} \tag{9.16}$$

Similarly,

$$\boxed{\left[-i\frac{\partial}{\partial t_{1'}}+\frac{\nabla_{1'}^2}{2m}-U(1')\right]g(1,1';U)=\delta(1-1')\pm i\int_{-\infty}^{+\infty}\mathrm{d}t_2\mathrm{d}\mathbf{x}_2V(1'-2)g_2(12^-,1'2;U),} \tag{9.17}$$

here $V(1-2)=v(\mathbf{x}_1-\mathbf{x}_2)\delta(t_1-t_2)$. As in the case of the equilibrium Green's functions, we shall construct approximations for $g(U)$ by substituting an approximation for $g_2(U)$ into these equations of motion.

When a system is disturbed from equilibrium, the first thing that happens is that the collisions force the system to a situation that is close to local thermodynamic equilibrium. This happens in a comparatively short time. After this rapid decay has occurred, there is a much slower return to all-over equilibrium. During this latter stage the behavior of the system is dominated by the conservation laws. These laws very strongly limit the ways in which the system can return to full equilibrium. For example, if there is an excess of energy in one portion of the system, this energy cannot just disappear; it must slowly spread itself out over the entire system. This slow spreading out is the transport process known as heat conduction. Therefore, in order to predict even the existence of transport phenomena—like heat

conduction or sound propagation—it is absolutely essential that we include the effects of the conservation laws. We must be sure that any approximate calculation leads to an $\langle n(\mathbf{X},T)\rangle$ and $\langle \mathbf{j}(\mathbf{X},T)\rangle$, which satisfy the equation,

$$\frac{\partial}{\partial T}\langle n(\mathbf{X},T)\rangle_U + \nabla_{\mathbf{X}}\cdot\langle \mathbf{j}(\mathbf{X},T)\rangle_U = 0. \tag{9.18}$$

This conservation law becomes a restriction on $g(U)$. In particular, by using (9.14), one can express this restriction as,

$$\boxed{\left[\left(i\frac{\partial}{\partial t_1}+i\frac{\partial}{\partial t_{1'}}\right)g(1,1';U)\right]_{1'=1^+}+(\nabla_1+\nabla_{1'})\cdot\left[\frac{\nabla_1-\nabla_{1'}}{2m}g(1,1';0)\right]_{1'=1^+}=0,} \tag{9.19}$$

where $1'=1^+$ means $\mathbf{x}_{1'}=\mathbf{x}_1, t_{1'}=t_1^+$.

It is straightforward to state criteria which will guarantee that an approximation for $g(U)$ is conserving, i.e., that it satisfies the restrictions imposed by the number-, momentum-, and energy-conservation laws. We get an approximation for $g(U)$ by substituting an approximation for $g_2(U)$ into (9.16) and (9.17). This procedure really defines two different approximations for $g(U)$, one given by (9.16) and the other by (9.17). We shall show that the differential number-conservation law is equivalent to the requirement on the approximation:

$$\boxed{\text{criterion I: } g(U) \text{ satisfies both (9.16) and (9.17).}} \tag{9.20}$$

To derive the number-conservation law from criterion I, it is only necessary to subtract (9.17) from (9.16) to find,

$$\left[i\frac{\partial}{\partial t_1}+i\frac{\partial}{\partial t_{1'}}+(\nabla_1+\nabla_{1'})\cdot\frac{\nabla_1-\nabla_{1'}}{2m}-U(1)+U(1')\right]g(1,1';U)=\pm i\int \mathrm{d}2[V(1-2)-V(1'-2)]g_2(12^-;1'2^+;U). \tag{9.21}$$

Setting $1'=1^+$ in (9.21) gives (9.19), so that the approximation indeed satisfies the differential number-conservation law exactly. We shall not write differential momentum- or energy-conservation laws analogous to (9.21). Instead we employ the integrated forms of these conservation laws. For example, the conservation law for the total momentum is,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{p}(t)\rangle_U = -\int \mathrm{d}\mathbf{x}[\nabla U(\mathbf{x},t)]\langle n(\mathbf{x},t)\rangle_U, \tag{9.22}$$

which states that the time derivative of the total momentum is equal to the total force acting on the system. In order to have an approximation which conserves the total momentum, we place one more restriction on the approximate $g_2(U)$ to be substituted into (9.16), etc.,

$$\boxed{\text{criterion II: } g_2(12;1^+2^+;U)=g_2(21;2^+1^+;U).} \tag{9.23}$$

In order to see that this additional restriction is sufficient to obtain a momentum-conserving approximation, we construct the time derivative of the total momentum in the system by applying $(\nabla_1-\nabla_{1'})/2i$ to (9.15), setting $1'=1^+$ and integrating over all $\mathbf{x}_1$. In this way, we find,

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t_1}\left[\int \mathrm{d}\mathbf{x}_1\left[\frac{\nabla_1-\nabla_{1'}}{2i}ig^<(1,1';U)\right]_{1'=1^+}\right]+\int \mathrm{d}\mathbf{x}_1\nabla_1\cdot\left[\frac{\nabla_1-\nabla_{1'}}{2i}\frac{\nabla_1-\nabla_{1'}}{2m}g^<(1,1';U)\right]_{1'=1}\\ &=\pm\int \mathrm{d}\mathbf{x}_1\mathrm{d}\mathbf{x}_2[\nabla_{\mathbf{x}_1}v(|\mathbf{x}_1-\mathbf{x}_2|)]g_2(\mathbf{x}_1t_1,\mathbf{x}_2t_1;\mathbf{x}_1t_1^+,\mathbf{x}_2t_1^+;U)-i\int \mathrm{d}\mathbf{x}_1[\nabla U(\mathbf{x}_1)]g^<(\mathbf{x}_1t_1,\mathbf{x}_1t_1;U).\end{aligned} \tag{9.24}$$

The term proportional to a divergence on the left side of (9.24) vanishes after integration over all $\mathbf{x}_1$. The term proportional to g_2 vanishes in this equation because criterion II implies that this term changes sign when the labels $\mathbf{x}_1$ and $\mathbf{x}_2$ are interchanged. Therefore, this term must be zero. Equation (9.24) then becomes

$$i\frac{\mathrm{d}}{\mathrm{d}t_1}\int \mathrm{d}\mathbf{x}_1\left[\frac{\nabla_1-\nabla_{1'}}{2i}g^<(1,1';U)\right]_{1'=1}=-i\int \mathrm{d}\mathbf{x}_1 g^<(1,1;U)\nabla U(\mathbf{x}_1), \tag{9.25}$$

this is just the momentum-conservation law that we wished to build into our approximations.

The discussion of the energy-conservation law is no more complicated in principle but it involves some algebraic complexities. By using the same device as discussed in the section on equilibrium properties of (7.42) we can express the energy density in terms of U and of differential operators acting upon $\psi_U^\dagger(1')\psi_U(1)$. Then, with the aid of (9.21), we can construct the time derivative of the total energy. After a bit of algebraic manipulation which employs only criteria I and II, we find,

$$\frac{\mathrm{d}}{\mathrm{d}T}\langle H(T)\rangle_U = -\int \mathrm{d}\mathbf{X}[\nabla U(\mathbf{X},T)]\cdot\langle \mathbf{j}(\mathbf{X},T)\rangle_U, \tag{9.26}$$

which says that the time derivative of the total energy in the system is equal to the total power fed into the system by the external disturbance. As a summary, any approximation that satisfies criteria I and II must automatically agree with the differential number-conservation law and the integral conservation laws for energy and momentum. Therefore, we may expect that these conserving approximations for $g(U)$ lead to fitting descriptions of transport phenomena.

The Green's function theory of transport is logically independent of the Boltzmann equation approach. However, it will be interesting for us to make contact between the two theories. For this purpose, we write down the Boltzmann equation,

$$\boxed{\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}-[\nabla U(\mathbf{X},T)]\cdot\nabla_{\mathbf{p}}\right]f(\mathbf{p},\mathbf{X},T)=\left(\frac{\partial f}{\partial T}\right)_{\text{collision}},} \tag{9.27}$$

where, in terms of Born approximation collision cross sections,

$$\begin{aligned}\boxed{\left(\frac{\partial f}{\partial T}\right)_{\text{collision}}}&=\int\frac{\mathrm{d}\mathbf{p}'}{(2\pi)^3}\frac{\mathrm{d}\overline{\mathbf{p}}}{(2\pi)^3}\frac{\mathrm{d}\overline{\mathbf{p}}'}{(2\pi)^3}\frac{1}{2}\left[v(\mathbf{p}-\overline{\mathbf{p}})\pm v(\mathbf{p}-\overline{\mathbf{p}}')\right]^2\times(2\pi)^3\delta(\mathbf{p}+\mathbf{p}'-\overline{\mathbf{p}}-\overline{\mathbf{p}}')\\&\quad\times 2\pi\delta\left(\frac{\mathbf{p}^2}{2m}+\frac{\mathbf{p}'^2}{2m}-\frac{\overline{\mathbf{p}}^2}{2m}-\frac{\overline{\mathbf{p}}'^2}{2m}\right)\times\left[(1\pm f)(1\pm f')\overline{f}\,\overline{f}'-ff'(1\pm\overline{f})(1\pm\overline{f}')\right].\end{aligned} \tag{9.28}$$

Here $f=f(\mathbf{p},\mathbf{X},T), f'=f(\mathbf{p}',\mathbf{X},T)$, etc. This Boltzmann equation is appropriate only for systems with weak, short-ranged forces. It is necessary to indicate the connection between the distribution function $f(\mathbf{p},\mathbf{X},T)$ and the Green's function $g(U)$. Notice that $f(\mathbf{p},\mathbf{X},T)$ has no well-defined quantum mechanical meaning. Therefore, the best that we can do is to define an f (in terms of g) that has many properties analogous to those of the classical distribution function. To do this we write the real-time Green's function, $\pm ig^<(1,1';U)$, in terms of the variables, $\mathbf{x}=\mathbf{x}_1-\mathbf{x}_{1'}, t=t_1-t_{1'}, \mathbf{X}=(\mathbf{x}_1+\mathbf{x}_{1'})/2$ and $T=(t_1+t_{1'})/2$. Then we define,

$$\boxed{g^<(\mathbf{p},\omega;\mathbf{X},T;U)=\int\mathrm{d}\mathbf{x}\int_{-\infty}^{+\infty}\mathrm{d}t e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}[\pm ig^<(\mathbf{x},t;\mathbf{X},T;U)].} \tag{9.29}$$

This function may be thought of as the density of particles with momentum $\mathbf{p}$ and energy ω at the space time point $\mathbf{X},T$ at least in the limit in which g varies slowly in $\mathbf{X}$ and T. Hence, $f(\mathbf{p},\mathbf{X},T)$ can be defined as,

$$\boxed{f(\mathbf{p},\mathbf{X},T)=\int\frac{\mathrm{d}\omega}{2\pi}g^<(\mathbf{p},\omega;\mathbf{X},T;U)=\int\mathrm{d}\mathbf{x}e^{-i\mathbf{p}\cdot\mathbf{x}}\left\langle\psi_U^\dagger\left(\mathbf{X}-\frac{\mathbf{x}}{2},T\right)\psi_U\left(\mathbf{X}+\frac{\mathbf{x}}{2},T\right)\right\rangle,} \tag{9.30}$$

which originally due to Wigner, and is thus called Winger function.

The function f has many similarities to the classical distribution function. When it is integrated over all momenta, it gives the density at $\mathbf{X},T$, that is,

$$\boxed{\int\frac{\mathrm{d}\mathbf{p}}{(2\pi)^3}f(\mathbf{p},\mathbf{X},T)=\langle\psi_U^\dagger(\mathbf{X},T)\psi_U(\mathbf{X},T)\rangle=\langle n(\mathbf{X},T)\rangle_U.} \tag{9.31}$$

When it is integrated over all $\mathbf{X}$, it gives the number of particles with momentum $\mathbf{p}$ at time T since,

$$\boxed{\int\mathrm{d}\mathbf{X}f(\mathbf{p},\mathbf{X},T)=\int\mathrm{d}\mathbf{x}_1\mathrm{d}\mathbf{x}_{1'}e^{-i\mathbf{p}\cdot\mathbf{x}_1}e^{i\mathbf{p}\cdot\mathbf{x}_{1'}}\langle\psi_U^\dagger(\mathbf{x}_{1'},T)\psi_U(\mathbf{x}_1,T)=\langle\psi_U^\dagger(\mathbf{p},T)\psi_U(\mathbf{p},T)\rangle.} \tag{9.32}$$

Just as in the classical case, the particle current is,

$$\langle\mathbf{j}(\mathbf{X},T)\rangle_U=\int\frac{\mathrm{d}\mathbf{p}}{(2\pi)^3}\frac{\mathbf{p}}{m}f(\mathbf{p},\mathbf{X},T). \tag{9.33}$$

This identification of the distribution function f will enable us to see the relationship between the Green's function transport equations and the Boltzmann equation.

Our general procedure for describing transport phenomena will be based on approximations in which the $g(U)$ that appears in the equation of motion for $g(U)$ is expanded in terms of $g(U)$. Hartree approximation is the simplest,

$$\boxed{g_2(12,1'2';U)=g(1,1';U)g(2,2';U),} \tag{9.34}$$

The two particles added to the system are taken to propagate completely independently of each other. They feel the effects of the applied potential U as they propagate through the medium, and hence their propagation is described by

$g(U)$. When (9.34) is substituted in the equations of motion (9.16) and (9.17) these become,

$$\boxed{\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-U_{\rm eff}(1)\right]g(1,1';U)=\delta(1-1'),\quad \left[-i\frac{\partial}{\partial t_{1'}}+\frac{\nabla_{1'}^2}{2m}-U_{\rm eff}(1')\right]g(1,1';U)=\delta(1-1'),} \tag{9.35}$$

where

$$U_{\rm eff}(\mathbf{X},T)=U(\mathbf{X},T)\pm i\int {\rm d}\mathbf{X}'v(\mathbf{X}-\mathbf{X}')g^<(\mathbf{X}'T,\mathbf{X}'T). \tag{9.36}$$

Equations of (9.35) describe the propagation of free particles through the effective potential field $U_{\rm eff}(\mathbf{X},T)$. This potential is the sum of the applied potential U and the average potential produced by all the particles in the system. It is the potential that would be felt by a test charge added to the medium. When the particles have internal degrees of freedom, such as spin, or there is more than one kind of particle in the system, one must sum the last term in (9.36).

Before going further, we show that the approximation is conserving. From (9.34) we see that the criterion II, the symmetry of $g_2(12,1'2';U)$ under the interchange $1\leftrightarrow 2,1'\leftrightarrow 2'$ is trivially satisfied, i.e., $g_2(21,1'2';U)=g(2,2';U)g(1,1';U)=g(1,1';U)g(2,2';U)=g_2(12,1'2';U)$. Criterion I states that equations of (9.35) are consistent with one another. In order to check this, we construct,

$$\Lambda=\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-U_{\rm eff}(1)\right]\times\left[-i\frac{\partial}{\partial t_{1'}}+\frac{\nabla_{1'}^2}{2m}-U_{\rm eff}(1')\right]g(1,1';U) \tag{9.37}$$

in two ways. First, by multiplying the first of (9.35) by "$-i\partial/\partial t_{1'}+\nabla_{1'}^2/2m-U_{\rm eff}(1')$", and then multiplying the second of (9.35) by "$i\partial/\partial t_1+\nabla_1^2/2m-U_{\rm eff}(1)$". These two operations imply that,

$$\begin{aligned}\Lambda&=\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-U_{\rm eff}(1)\right]\delta(1-1')=i\frac{\partial}{\partial t_1}\delta(1-1')+\frac{\nabla_1\cdot\nabla_1}{2m}\delta(1-1')-U_{\rm eff}(1)\delta(1-1')\\&=-i\frac{\partial}{\partial t_{1'}}\delta(1-1')+\frac{(-\nabla_{1'})\cdot(-\nabla_{1'})}{2m}\delta(1-1')-U_{\rm eff}(1')\delta(1'-1)=\left[-i\frac{\partial}{\partial t_{1'}}+\frac{\nabla_{1'}^2}{2m}-U_{\rm eff}(1')\right]\delta(1-1').\end{aligned} \tag{9.38}$$

Therefore both of (9.35) lead to the same differential equation for g. When supplemented by suitable boundary conditions they will therefore both determine the same function g. Thus Hartree approximation is conserving.

If we take the difference of the two mutually consistent equations of (9.35) we find that,

$$\left[i\left(\frac{\partial}{\partial t_1}+\frac{\partial}{\partial t_{1'}}\right)+(\nabla_1+\nabla_{1'})\cdot\frac{\nabla_1-\nabla_{1'}}{2m}-[U_{\rm eff}(1)-U_{\rm eff}(1')]\right]g(1,1';U)=0. \tag{9.39}$$

We now set $t_{1'}=t_{1^+}=T$, then

$$\boxed{\left[i\frac{\partial}{\partial T}+(\nabla_1+\nabla_{1'})\cdot\frac{\nabla_1-\nabla_{1'}}{2m}-[U_{\rm eff}(1)-U_{\rm eff}(1')]\right]g(1,1';U)=0.} \tag{9.40}$$

By setting $t=t_1-t_{1'},T=(t_1+t_{1'})/2=t_{1^+}=t_{1'}$, we obtain

$$\frac{\partial}{\partial t_1}+\frac{\partial}{\partial t_{1'}}=\left(\frac{\partial t}{\partial t_1}+\frac{\partial t}{\partial t_{1'}}\right)\frac{\partial}{\partial t}+\left(\frac{\partial T}{\partial t_1}+\frac{\partial T}{\partial t_{1'}}\right)\frac{\partial}{\partial T}=\frac{\partial}{\partial T}=\frac{\partial}{\partial t_{1'}}=\frac{\partial}{\partial t_{1^+}}. \tag{9.41}$$

Similarly, we can rewrite the equation (9.19) in the form of,

$$\left[i\frac{\partial}{\partial T}g(1,1';U)\right]_{1'=1^+}+\nabla_1\cdot\left[\frac{\nabla_1-\nabla_{1'}}{2m}g(1,1';U)\right]_{1'=1^+}=0, \tag{9.42}$$

which is the conservation law of particle number,

$$\partial\langle n(\mathbf{X},T)\rangle_U/\partial T+\nabla_{\mathbf{X}}\cdot\langle\mathbf{j}(\mathbf{X},T)\rangle_U=0. \tag{9.43}$$

In the limit in which $U_{\rm eff}(\mathbf{X},T)$ varies slowly in space, (9.40) is equivalent to the collisionless Boltzmann equation. We now derive the collisionless Boltzmann equation from (9.40). When (9.40) is expressed in terms of the variables $\mathbf{x}=\mathbf{x}_1-\mathbf{x}_{1'}$ and $\mathbf{X}=(1/2)(\mathbf{x}_1+\mathbf{x}_{1'})$, and since $\nabla_1+\nabla_{1'}=\nabla_{\mathbf{X}}$ and $\nabla_1-\nabla_{1'}=2\nabla_{\mathbf{x}}$, we obtain,

$$\pm\left[\frac{\partial}{\partial T}+\frac{\nabla_{\mathbf{X}}\cdot\nabla_{\mathbf{x}}}{2im}-\frac{1}{i}\left[U_{\rm eff}\left(\mathbf{X}+\frac{\mathbf{x}}{2},T\right)-U_{\rm eff}\left(\mathbf{X}-\frac{\mathbf{x}}{2},T\right)\right]\right]\times\int\frac{{\rm d}\mathbf{p}'}{(2\pi)^3}e^{i\mathbf{p}'\cdot\mathbf{x}}f(\mathbf{p}',\mathbf{X},T)=0, \tag{9.44}$$

where

$$f(\mathbf{p},\mathbf{X},T)=\int d\mathbf{x}e^{-i\mathbf{p}\cdot\mathbf{x}}\left\langle\psi_U^\dagger\left(\mathbf{X}-\frac{\mathbf{x}}{2},T\right)\psi\left(\mathbf{X}+\frac{\mathbf{x}}{2},T\right)\right\rangle. \tag{9.45}$$

By multiplying (9.44) by $e^{-i\mathbf{p}\cdot\mathbf{x}}$ and integrating over all $\mathbf{x}$, (9.44) becomes (also multiplying both sides by "±"),

$$\boxed{\left(\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}\right)f(\mathbf{p},\mathbf{X},T)=\frac{1}{i}\int d\mathbf{x}\int\frac{d\mathbf{p}'}{(2\pi)^3}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}}\times\left[U_{\text{eff}}\left(\mathbf{X}+\frac{\mathbf{x}}{2},T\right)-U_{\text{eff}}\left(\mathbf{X}-\frac{\mathbf{x}}{2},T\right)\right]\times f(\mathbf{p},\mathbf{X},T).} \tag{9.46}$$

This equation is an exact consequence of the Hartree approximation (9.34).

EXERCISE 46: Derive the second term appearing on the left side, i.e., $[\mathbf{p}\cdot\nabla_{\mathbf{X}}/m]f(\mathbf{p},\mathbf{X},T)$.

Suppose that $U_{\text{eff}}(\mathbf{X},T)$ varies slowly in $\mathbf{X}$. In the integrand above we may therefore expand $U_{\text{eff}}(\mathbf{X}\pm\mathbf{x}/2,T)$ as,

$$U_{\text{eff}}\left(\mathbf{X}\pm\frac{\mathbf{x}}{2},T\right)\approx U_{\text{eff}}(\mathbf{X},T)\pm\frac{\mathbf{x}}{2}\cdot\nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)+\mathcal{O}(|\mathbf{x}|^2),\quad U_{\text{eff}}\left(\mathbf{X}+\frac{\mathbf{x}}{2},T\right)-U_{\text{eff}}\left(\mathbf{X}-\frac{\mathbf{x}}{2},T\right)\approx\mathbf{x}\cdot\nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T). \tag{9.47}$$

So that,

$$\left(\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}\right)f(\mathbf{p},\mathbf{X},T)=\nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)\cdot\int\frac{d\mathbf{p}'d\mathbf{x}}{(2\pi)^3}f(\mathbf{p}',\mathbf{X},T)\times\left[-\nabla_{\mathbf{p}'}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}}\right], \tag{9.48}$$

where

$$-f(\mathbf{p}',\mathbf{X},T)\nabla_{\mathbf{p}'}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}}=\left[\nabla_{\mathbf{p}'}f(\mathbf{p}',\mathbf{X},T)\right]e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}}-\nabla_{\mathbf{p}'}\left[f(\mathbf{p}',\mathbf{X},T)e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}}\right]. \tag{9.49}$$

According to the formula $\int\nabla k d\mathbf{x}=\int_S k\mathbf{n}(\mathbf{x})dS_{\mathbf{x}}$ where $\mathbf{n}(\mathbf{x})$ is the unit normal vector outside to the surface S, we can transform the second term into an integration over surface which is zero by considering that the physical quantity W is zero on the boundary. Consequently, we have

$$\boxed{\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}}{m}\cdot\nabla_{\mathbf{X}}-\nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}}\right]f(\mathbf{p},\mathbf{X},T)=0,} \tag{9.50}$$

which is the collisionless Boltzmann equation, where the effective potential U_{eff} is,

$$\boxed{U_{\text{eff}}(\mathbf{X},T)=U(\mathbf{X},T)+\int d\mathbf{X}'v(\mathbf{X}-\mathbf{X}')\int\frac{d\mathbf{p}'}{(2\pi)^3}f(\mathbf{p}',\mathbf{X}',T),\quad\int\frac{d\mathbf{p}'}{(2\pi)^3}f(\mathbf{p}',\mathbf{X}',T)=\langle\psi_U^\dagger(\mathbf{X}',T)\psi_U(\mathbf{X}',T)\rangle=\langle n(\mathbf{X}',T)\rangle_U.} \tag{9.51}$$

We may solve (9.40), or equivalently (9.46), exactly in the limit in which the potential $U(\mathbf{X},T)$ is small. We consider only disturbances that vanish as $T\to-\infty$. The boundary condition on (9.46) is an initial condition which states that at $T=-\infty$, the system is in equilibrium, i.e., that $f(\mathbf{p},\mathbf{X},T)$ is given by the equilibrium value of $\int[d\omega/2\pi]G^<(\mathbf{p},\omega)$, evaluated in the Hartree approximation. Thus,

$$\lim_{T\to-\infty}f(\mathbf{p},\mathbf{X},T)=\frac{1}{e^{\beta(E(\mathbf{p})-\mu)}\mp1}=f(E(\mathbf{p})),\quad E(\mathbf{p})=\frac{\mathbf{p}^2}{2m}+n\int d\mathbf{x}v(\mathbf{x}). \tag{9.52}$$

From the definition (9.13) of $g^<(U)$, we see that $f(\mathbf{p},\mathbf{X},T)$ depends on the values of $U(\mathbf{X}',T')$ only for times T' earlier than time T (causality). We may therefore write, to first order in U, that

$$\boxed{f(\mathbf{p},\mathbf{X},T)=f(E(\mathbf{p}))+\delta f(\mathbf{p},\mathbf{X},T),\quad\delta f(\mathbf{p},\mathbf{X},T)=\int_{-\infty}^{T}dT'\int d\mathbf{X}'\frac{\delta f}{\delta U}(\mathbf{X}-\mathbf{X}',T-T')U(\mathbf{X}',T').} \tag{9.53}$$

This equation defines the linear response function, $\delta f/\delta U$, in the real time domain. It is closely related to the functional derivative in the imaginary-time domain. Owing to the smallness of U, one may write (9.46) and (9.51) linearly as

$$\boxed{\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}\right]\delta f(\mathbf{p},\mathbf{X},T)=\frac{1}{i}\int\frac{d\mathbf{x}d\mathbf{p}'}{(2\pi)^3}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}}f(E(\mathbf{p}'))\times\left[\delta U_{\text{eff}}\left(\mathbf{X}+\frac{\mathbf{x}}{2},T\right)-U_{\text{eff}}\left(\mathbf{X}-\frac{\mathbf{x}}{2},T\right)\right],} \tag{9.54}$$

where,

$$\boxed{\delta U_{\text{eff}}(\mathbf{X},T)=U(\mathbf{X},T)+\int d\mathbf{X}'v(\mathbf{X}-\mathbf{X}')\int\frac{d\mathbf{p}'}{(2\pi)^3}\delta f(\mathbf{p}',\mathbf{X}',T).} \tag{9.55}$$

The Hartree approximation, when linearized in the external field, is known as the "random phase approximation" (abbreviated as RPA). Equations (9.54) and (9.55) are just one of many equivalent statements of such approximation.

To solve these equations, we consider the case in which $U(\mathbf{X},T)$ is of the form,

$$U(\mathbf{X},T) = U(\mathbf{k},\Omega)e^{i\mathbf{k}\cdot\mathbf{X}-i\Omega T}, \tag{9.56}$$

where Ω is a complex frequency such that $\mathrm{Im}\,\Omega > 0$, then $U(\mathbf{X},T)$ vanishes as $T \to -\infty$. We see from (9.53) that,

$$\delta f(\mathbf{p},\mathbf{X},T) = e^{i\mathbf{k}\cdot\mathbf{X}-i\Omega T}\delta f(\mathbf{p},\mathbf{k},\Omega),\quad \delta f(\mathbf{p},\mathbf{k},\Omega) = \int_{-\infty}^{0} dT' \int d\mathbf{X}' e^{-i\Omega T'+i\mathbf{k}\cdot\mathbf{X}'}\frac{\delta f}{\delta U}(\mathbf{p},-\mathbf{X}',-T')U(\mathbf{k},\Omega). \tag{9.57}$$

Since

$$\frac{\partial}{\partial T}\delta f(\mathbf{p},\mathbf{X},\Omega) = -i\Omega e^{i\mathbf{k}\cdot\mathbf{X}-i\Omega T}\delta f(\mathbf{p},\mathbf{k},\Omega),\quad \mathbf{p}\cdot\nabla_{\mathbf{X}}\delta f(\mathbf{p},\mathbf{X},T) = i\mathbf{k}\cdot\mathbf{p}e^{i\mathbf{k}\cdot\mathbf{X}-i\Omega T}\delta f(\mathbf{p},\mathbf{k},\Omega), \tag{9.58}$$

we have

$$\left[\frac{\partial}{\partial T} + \frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}\right]\delta f(\mathbf{p},\mathbf{X},T) = -i\left[\Omega - \frac{\mathbf{k}\cdot\mathbf{p}}{m}\right]e^{i\mathbf{k}\cdot\mathbf{X}-i\Omega T}\delta f(\mathbf{p},\mathbf{k},\Omega). \tag{9.59}$$

EXERCISE 47: Show that the two terms on the right side of Eq. (9.54) are given as,

$$\int \frac{d\mathbf{x}d\mathbf{p}'}{(2\pi)^3}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}}f(E(\mathbf{p}'))\delta U_{\mathrm{eff}}\left(\mathbf{X}\pm\frac{\mathbf{x}}{2},T\right) = \left[U(\mathbf{k},\Omega) + v(\mathbf{k})\int\frac{d\mathbf{p}''}{(2\pi)^3}\delta f(\mathbf{p}'',\mathbf{k},\Omega)\right]\times f(E(\mathbf{p}\mp\mathbf{k}/2))e^{i\mathbf{k}\cdot\mathbf{X}-i\Omega T}. \tag{9.60}$$

The second term in δU_{eff} contains certain complicated aspects.

Then Eq. (9.54) becomes,

$$\boxed{\left(\Omega - \frac{\mathbf{k}\cdot\mathbf{p}}{m}\right)\delta f(\mathbf{p},\mathbf{k},\Omega) = \left[f(E(\mathbf{p}-\mathbf{k}/2)) - f(E(\mathbf{p}+\mathbf{k}/2))\right]\delta U_{\mathrm{eff}}(\mathbf{k},\Omega),} \tag{9.61}$$

$$\boxed{\delta U_{\mathrm{eff}}(\mathbf{k},\Omega) = U(\mathbf{k},\Omega) + v(\mathbf{k})\int\frac{d\mathbf{p}'}{(2\pi)^3}\delta f(\mathbf{p}',\mathbf{k},\Omega),} \tag{9.62}$$

where $v(\mathbf{k}) = \int d\mathbf{x}e^{-i\mathbf{k}\cdot\mathbf{x}}v(\mathbf{x})$ is the Fourier transform of the potential $v(\mathbf{x})$. We readily find,

$$\boxed{\delta f(\mathbf{p},\mathbf{k},\Omega) = \frac{f(E(\mathbf{p}-\mathbf{k}/2)) - f(E(\mathbf{p}+\mathbf{k}/2))}{\Omega - \mathbf{k}\cdot\mathbf{p}/m}\delta U_{\mathrm{eff}}(\mathbf{k},\Omega),} \tag{9.63}$$

$$\begin{aligned}\boxed{\delta U_{\mathrm{eff}}(\mathbf{k},\Omega) &= U(\mathbf{k},\Omega) + v(\mathbf{k})\int\frac{d\mathbf{p}'}{(2\pi)^3}\times\frac{f(E(\mathbf{p}'-\mathbf{k}/2)) - f(E((\mathbf{p}'+\mathbf{k}/2))}{\Omega-\mathbf{k}\cdot\mathbf{p}'/m}\delta U_{\mathrm{eff}}(\mathbf{k},\Omega)\\ &= U(\mathbf{k},\Omega)\times\left[1 - v(\mathbf{k})\int\frac{d\mathbf{p}'}{(2\pi)^3}\frac{f(E(\mathbf{p}'-\mathbf{k}/2)) - f(E((\mathbf{p}'+\mathbf{k}/2))}{\Omega-\mathbf{k}\cdot\mathbf{p}'/m}\right]^{-1}.}\end{aligned} \tag{9.64}$$

First consider the change in density. Let

$$\left(\frac{\delta n}{\delta U}\right)_0(\mathbf{k},\Omega) = \int\frac{d\mathbf{p}}{(2\pi)^3}\frac{f(E(\mathbf{p}-\mathbf{k}/2)) - f(E(\mathbf{p}+\mathbf{k}/2))}{\Omega-\mathbf{k}\cdot\mathbf{p}/m}, \tag{9.65}$$

this is the density response of a system of free particles, with single-particle energies $E(\mathbf{p})$, to the applied field. Then δn is given by,

$$\boxed{\delta n(\mathbf{k},\Omega) = \int\frac{d\mathbf{p}}{(2\pi)^3}\delta f(\mathbf{p},\mathbf{k},\Omega) = \frac{(\delta n/\delta U)_0(\mathbf{k},\Omega)}{1 - v(\mathbf{k})(\delta n/\delta U)_0(\mathbf{k},\Omega)}U(\mathbf{k},\Omega).} \tag{9.66}$$

Another interesting function of importance is the dynamic dielectric response function K. This function, defined by,

$$\boxed{\delta U_{\mathrm{eff}}(\mathbf{X},T) = \int_{-\infty}^{T} dT' \int d\mathbf{X}' K(\mathbf{X}-\mathbf{X}',T-T')U(\mathbf{X}',T'),\ \text{ or }\ K(\mathbf{X}-\mathbf{X}',T-T') = \frac{\delta U_{\mathrm{eff}}(\mathbf{X},T)}{U(\mathbf{X}',T')},} \tag{9.67}$$

gives the change in the effective potential when one changes the externally applied potential. It is a generalization of the ordinary (inverse) dielectric constant to the case in which the external potential depends on space and time. When $U(\mathbf{X}',T')$ is of the form (9.56), it follows that,

$$\delta U_{\mathrm{eff}}(\mathbf{X},T) = e^{i\mathbf{k}\cdot\mathbf{X}-i\Omega T}K(\mathbf{k},\Omega)U(\mathbf{k},\Omega),\quad K(\mathbf{k},\Omega) = \int_{-\infty}^{0} dT' \int d\mathbf{X}' e^{i\mathbf{k}\cdot\mathbf{X}'-i\Omega T'}K(-\mathbf{X}',-\mathbf{T}'). \tag{9.68}$$

In the limit $\Omega=0,\mathbf{k}\to\infty$, $K^{-1}(\mathbf{k},\Omega)$ becomes the ordinary static dielectric constant ϵ. It is clear from (9.64) that in the random phase approximation,

$$\boxed{K(\mathbf{k},\Omega)=\frac{1}{1-v(\mathbf{k})(\delta n/\delta U)_0(\mathbf{k},\Omega)}.} \tag{9.69}$$

EXERCISE 48: Solve the RPA equation in the Coulomb potential $v(\mathbf{X})=e^2/|\mathbf{X}|$. Especially, derive the effective potential

$$U_{\text{eff}}(\mathbf{X},T)=C\frac{e^{-|\mathbf{X}|/r_{\text{D}}}}{|\mathbf{X}|}, \tag{9.70}$$

where r_{D} is the Debye shielding distance. What is its expression? The result tells that the total field produced by a point charge drops off with exponential rapidity, with a range equal to the shielding radius r_{D}.

In a low-temperature and highly degenerate Fermi system, the evaluation of $(\delta n/\delta U)_0$ in (9.65) is particularly simple. In the long-wavelength limit, as $\beta\mu\to-\infty$,

$$f(E(\mathbf{p}-\mathbf{k}/2))-f(E(\mathbf{p}+\mathbf{k}/2))=\frac{\mathbf{k}\cdot\mathbf{p}}{m}\delta\left(\frac{\mathbf{p}^2}{2m}+nv-\mu\right). \tag{9.71}$$

Therefore (9.65) becomes,

$$\left(\frac{\delta n}{\delta U}\right)_0(\mathbf{k},\Omega)=\frac{1}{4\pi^2}\int_0^\infty p^2\mathrm{d}p\int_{-1}^1\mathrm{d}u\,\frac{kpu/m}{\Omega-kpu/m}\delta\left(\frac{\mathbf{p}^2}{2m}-\frac{p_{\text{F}}^2}{2m}\right)=\rho(E)\int_{-1}^1\frac{\mathrm{d}u}{2}\frac{kp_{\text{F}}u/m}{\Omega-kp_{\text{F}}u/m}, \tag{9.72}$$

where the Fermi momentum p_{F} is defined by $p_{\text{F}}^2/2m=\mu-nv=\mu-n\int\mathrm{d}\mathbf{x}v(\mathbf{x})$, and u is the direction cosine between $\mathbf{k}$ and $\mathbf{p}$, i.e., $u=\cos(\widehat{\mathbf{k},\mathbf{p}})$. Moreover, $\rho(E)=mp_{\text{F}}/2\pi^2$ is the density of energy states at the top of the Fermi sea,

$$\frac{\mathrm{d}\mathbf{p}}{(2\pi)^3}=\frac{1}{2}\rho(E)\mathrm{d}E\mathrm{d}u. \tag{9.73}$$

By introducing the transform $-t=\Omega-x$, we have

$$\int_{-kp_{\text{F}}/m}^{kp_{\text{F}}/m}\frac{x\mathrm{d}x}{\Omega-x}=\int_{-kp_{\text{F}}/m-\Omega}^{kp_{\text{F}}/m-\Omega}\frac{(\Omega+t)\mathrm{d}t}{-t}=\Omega\int_{kp_{\text{F}}/m-\Omega}^{-kp_{\text{F}}/m-\Omega}\frac{\mathrm{d}t}{t}+\int_{kp_{\text{F}}/m-\Omega}^{-kp_{\text{F}}/m-\Omega}\mathrm{d}t=-\Omega\int_{-kp_{\text{F}}/m}^{kp_{\text{F}}/m}\frac{\mathrm{d}t}{t-\Omega}-\frac{2kp_{\text{F}}}{m}, \tag{9.74}$$

and that,

$$\boxed{\left(\frac{\delta n}{\delta U}\right)_0(\mathbf{k},\Omega)=-\rho(E)\left(1+\frac{m\Omega}{2kp_{\text{F}}}\int_{-kp_{\text{F}}/m}^{kp_{\text{F}}/m}\frac{\mathrm{d}x}{x-\Omega}\right).} \tag{9.75}$$

The inverse of the response function K is thus given by,

$$K^{-1}(\mathbf{k},\Omega)=1+v(\mathbf{k})\rho(E)\left(1+\frac{m\Omega}{2kp_{\text{F}}}\int_{-kp_{\text{F}}/m}^{kp_{\text{F}}/m}\frac{\mathrm{d}x}{x-\Omega}\right). \tag{9.76}$$

Letting $\Omega=\omega+i\epsilon$, where ω is a real positive frequency and, $\epsilon=0^+$, $\int_{-kp_{\text{F}}/m}^{kp_{\text{F}}/m}$ has the form of the principal integration, we find explicitly,

$$\boxed{K^{-1}(\mathbf{k},\Omega)=1+v(\mathbf{k})\rho(E)\left[1+\frac{m\omega}{2kp_{\text{F}}}\left[\ln\left|\frac{kp_{\text{F}}/m-\omega}{kp_{\text{F}}/m+\omega}\right|+\pi i\Theta\left(\frac{kp_{\text{F}}}{m}-\omega\right)\right]\right].} \tag{9.77}$$

If the interaction is sufficiently weak, so that the dimensionless parameter $v(\mathbf{k})\rho(E)$ is much less than unity, then K will be very close to unity except when the logarithm is very large, and this happens when $\omega\approx kp_{\text{F}}/m$. In this case,

$$\begin{aligned}K^{-1}(\mathbf{k},\omega+i\epsilon)&=1+v(\mathbf{k})\rho(E)\left[1+\frac{1}{2}\ln\frac{1}{2}\left|1-\frac{m\omega}{kp_{\text{F}}}\right|+\pi i\Theta\left(\frac{kp_{\text{F}}}{m}-\omega\right)\right]\\&\approx 1+\frac{v(\mathbf{k})\rho(E)}{2}\left[1+\ln\frac{1}{2}\left|1-\frac{m\omega}{kp_{\text{F}}}\right|+\pi i\Theta\left(\frac{kp_{\text{F}}}{m}-\omega\right)\right].\end{aligned} \tag{9.78}$$

When the interaction is attractive, $v(\mathbf{k})<0$, a very special condensation occurs in a low-temperature Fermi system: The transition to the superconducting state. This condensation leads to new physical effects which completely invalidate the Hartree approximation. In (9.78) all we see is that K becomes very small in the neighborhood of $\omega=kp_{\text{F}}/m$, indicating that a disturbance with this frequency and wave number would be screened out.

On the other hand, when the interaction is repulsive, $v(\mathbf{k})$ is positive, the real part of the response function $\mathrm{Re}K(\mathbf{k},\omega+i0^+)$ is given by

$$\frac{1+\frac{v(\mathbf{k})\rho(E)}{2}\left(1+\ln\frac{1}{2}\left|1-\frac{m\omega}{kp_\mathrm{F}}\right|\right)}{\left[1+\frac{v(\mathbf{k})\rho(E)}{2}\left(1+\ln\frac{1}{2}\left|1-\frac{m\omega}{kp_\mathrm{F}}\right|\right)\right]^2+\left[\frac{v(\mathbf{k})\rho(E)}{2}\pi\Theta\left(\frac{kp_\mathrm{F}}{m}-\omega\right)\right]^2}. \tag{9.79}$$

For $\omega > kp_\mathrm{F}/m, \Theta(kp_\mathrm{F}/m-\omega)=0$,

$$\mathrm{Re}K(\mathbf{k},\omega+i0^+)=\left[1+\frac{v(\mathbf{k})\rho(E)}{2}\left(1+\ln\frac{1}{2}\left|1-\frac{m\omega}{kp_\mathrm{F}}\right|\right)\right]^{-1}. \tag{9.80}$$

The sharp resonance is located at,

$$\boxed{1+\frac{v(\mathbf{k})\rho(E)}{2}\left(1+\ln\frac{1}{2}\left|1-\frac{m\omega}{kp_\mathrm{F}}\right|\right)=0,\ \ \omega_\mathrm{R}=\frac{kp_\mathrm{F}}{m}\left[1+2\exp\left(-\frac{2+2v(\mathbf{k})\rho(E)}{v(\mathbf{k})\rho(E)}\right)\right].} \tag{9.81}$$

For $\omega=\omega_0=kp_\mathrm{F}/m$, we have $\omega_\mathrm{R}>\omega_0$. This corresponds to a resonant phenomena in the system which is called zero sound. It is characterized by the sound velocity, $c_0=\omega/k\approx p_\mathrm{F}/m=v_\mathrm{F}$. An analogue of zero sound is observed in the giant dipole resonance of nuclei. It is instructive to compare the zero sound with the ordinary sound in a high-degenerate Fermi system. The ordinary sound is given by $c_\mathrm{s}^2=p_\mathrm{F}^2/3m^2=c_0^2/3$, i.e., $c_\mathrm{s}=v_\mathrm{F}/\sqrt{3}$. The dispersion relation for the zero sound is $\omega=v_\mathrm{F}k$, while that for the ordinary sound is $\omega=(v_\mathrm{F}/\sqrt{3})k$. For the latter, one can show that

$$\boxed{\delta f(\mathbf{p},\mathbf{k},\Omega)\approx\left[\mathbf{p}\cdot\mathbf{v}(\mathbf{k},\Omega)-\delta\mu(\mathbf{k},\Omega)\right]\frac{\partial f(E(\mathbf{p}))}{\partial(\mathbf{p}^2/2m)}.} \tag{9.82}$$

On the other hand, (9.63) implies that for zero sound,

$$\boxed{\delta f(\mathbf{p},\mathbf{k},\Omega)=\frac{\mathbf{k}\cdot\mathbf{p}/m}{\mathbf{k}\cdot\mathbf{p}/m-\Omega}\frac{\partial f(E(\mathbf{p}))}{\partial(\mathbf{p}^2/2m)}\delta U_\mathrm{eff}(\mathbf{k},\Omega)=\frac{\mathbf{k}\cdot\mathbf{p}/m}{\mathbf{k}\cdot\mathbf{p}/m-\Omega}\frac{\partial f(E(\mathbf{p}))}{\partial(\mathbf{p}^2/2m)}\times\frac{U(\mathbf{k},\Omega)}{1-v(\mathbf{k})\int\frac{\mathrm{d}\mathbf{q}}{(2\pi)^3}\frac{\mathbf{k}\cdot\mathbf{q}/m}{\mathbf{k}\cdot\mathbf{q}/m-\Omega}\frac{\partial f(E(\mathbf{q}))}{\partial(\mathbf{q}^2/2m)}}.} \tag{9.83}$$

This is clearly not a form for local equilibrium phenomena. Ordinary sound is just an oscillating translation and an oscillating expansion of the Fermi sphere, but its shape remains spherical. Zero sound is a complex oscillation of the surface of the Fermi sphere. More vividly, at a particular instant the Fermi surface is considerably elongated in the forward direction of propagation and slightly shortened in the backward direction (like an egg), but half a cycle later it is slightly elongated in the backwards direction and considerably shortened in the forward direction, the amplitude of oscillation being greater at the forward pole than at the backward pole. Finally, the change in density for zero sound is,

$$\boxed{\delta n(\mathbf{k},\Omega)=\rho(E)v_\mathrm{F}^2\mathbf{k}^2\int_{-1}^{1}\frac{\mathrm{d}u}{2}\frac{u^2}{\Omega^2-v_\mathrm{F}^2\mathbf{k}^2u^2}\delta U_\mathrm{eff}(\mathbf{k},\Omega),} \tag{9.84}$$

whereas, in ordinary sound it is

$$\boxed{\delta n(\mathbf{k},\Omega)=\frac{\rho(E)c_\mathrm{s}^2k}{\Omega^2-c_\mathrm{s}^2\mathbf{k}^2}\delta U_\mathrm{eff}(\mathbf{k},\Omega).} \tag{9.85}$$

Zero sound is certainly a more complex phenomena. Compare (9.85) with **EXERCISE 32** on the response function.

EXERCISE 49: Discuss under which circumstance the RPA approximation may break down.

J Kadanoff–Baym Equations: General Nonequilibrium Cases

Relevant Reference:

- L. Kadanoff and G. Baym, *Quantum Statistical Mechanics*, Westview Press, 1962, Chapters 5 and 8.
- G. Stefanucci and R. van Leeuwen, *Nonequilibrium Many-body Theory of Quantum Systems: a Modern Introduction*, Cambridge University Press, 2013, Chapters 1-9.
- P. Danielewicz, *Quantum Theory of Nonequilibrium Processes. I*, Ann. Phys. **152**, 239 (1984).

In the last section we used the Hartree approximation to describe nonequilibrium phenomena. We cannot further directly write more complicated approximations in the real-time domain because we have no simple boundary conditions that can act as a guide in determining $g_2(U)$. Therefore, we have at this stage no complete theory for determining the physical response function $g(U)$. Simple physical arguments do not suffice to determine approximations for the two-particle Green's function, it is necessary to use the boundary conditions to determine the range of the time integrations. We discuss in this section the close relationship between $g(U)$, the physical response function, $G(U)$, and the imaginary-time response function. Therefore we first develop a few imaginary-time results.

As a purely formal device, we define a generalization of the one-particle Green's function in the time interval $[0,-i\beta]$,

$$\boxed{G(1,1';U)=\frac{1}{i}\frac{\langle \mathrm{T}[S\psi(1)\psi^\dagger(1')]\rangle}{\langle \mathrm{T}[S]\rangle},\quad S=\exp\left(-i\int_0^{-i\beta}\mathrm{d}2U(2)n(2)\right),} \tag{10.1}$$

where T means imaginary-time ordering and $n(2)=\psi^\dagger(2)\psi(2)$, $U(2)$ is a function of space and times in the interval $[0,-i\beta]$. We may regard $G(1,1';U)$ as a one-particle Green's function, written in the interaction representation, for the system developing in imaginary time in the presence of the scalar potential U. This potential is represented by adding a term $\int \mathrm{d}\mathbf{x}U(\mathbf{x},t)n(\mathbf{x},t)$ to the Hamiltonian. In the interaction picture, all the U-dependence is explicit in the S factor, and the field operators are the same as in the absence of the potential. One reason that the Green's function (10.1) is convenient to use is that it satisfies the same boundary condition,

$$G(1,1';U)|_{t_1=0}=\pm e^{\beta\mu}G(1,1';U)|_{t_1=-i\beta}. \tag{10.2}$$

EXERCISE 50: Prove the boundary condition (10.2).

Another reason this Green's function is convenient is that it obeys equations of motion quite similar to those obeyed by the equilibrium function G. These are

$$\left(i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-U(1)\right)G(1,1';U)=\delta(1-1')\pm i\int \mathrm{d}\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)G_2(12,1'2^+;U)|_{t_2=t_1}, \tag{10.3}$$

$$\left(-i\frac{\partial}{\partial t_{1'}}+\frac{\nabla_{1'}^2}{2m}-U(1')\right)G(1,1';U)=\delta(1-1')\mp i\int \mathrm{d}\mathbf{x}_2 v(\mathbf{x}_2-\mathbf{x}_{1'})G_2(12^-,1'2;U)|_{t_2=t_1}, \tag{10.4}$$

where

$$G_2(12,1'2';U)=\left(\frac{1}{i}\right)^2\frac{\langle \mathrm{T}[S\psi(1)\psi(2)\psi^\dagger(2')\psi^\dagger(1')]\rangle}{\langle \mathrm{T}[S]\rangle}. \tag{10.5}$$

We can derive (10.3) and (10.4) in exactly the same way as the equations of motion for the equilibrium function $G(1-1')$. The new feature is the appearance of UG. To see the origin of these terms, consider, for example,

$$\mathrm{T}[S\psi(1)]=\mathrm{T}\left[\exp\left(-i\int_{t_1}^{-i\beta}\mathrm{d}2U(2)n(2)\right)\right]\psi(1)\mathrm{T}\left[\exp\left(-i\int_0^{t_1}\mathrm{d}2U(2)n(2)\right)\right]. \tag{10.6}$$

Then,

$$\begin{aligned}
i\frac{\partial}{\partial t_1}\mathrm{T}[S\psi(1)]=&\mathrm{T}\left[i^2\int \mathrm{d}\mathbf{x}_2U(2)n(2)\exp\left(-i\int_{t_1}^{-i\beta}\mathrm{d}2U(2)n(2)\right)\right]\psi(1)\times\mathrm{T}\left[\exp\left(-i\int_0^{t_1}\mathrm{d}2U(2)n(2)\right)\right]\\
&+\mathrm{T}\left[\exp\left(-i\int_{t_1}^{-i\beta}\mathrm{d}2U(2)n(2)\right)\right]\left(i\frac{\partial\psi(1)}{\partial t}\right)\times\mathrm{T}\left[\exp\left(-i\int_0^{t_1}\mathrm{d}2U(2)n(2)\right)\right]\\
&+\mathrm{T}\left[\exp\left(-i\int_{t_1}^{-i\beta}\mathrm{d}2U(2)n(2)\right)\right]\psi(1)\times\mathrm{T}\left[-i^2\int \mathrm{d}\mathbf{x}_2U(2)n(2)\exp\left(-i\int_0^{t_1}\mathrm{d}2U(2)n(2)\right)\right]\\
=&\mathrm{T}\left[\exp\left(-i\int_{t_1}^{-i\beta}\mathrm{d}2U(2)n(2)\right)\right]\left[i\frac{\partial\psi(1)}{\partial t_1}+\int \mathrm{d}\mathbf{x}_2U(\mathbf{x}_2,t_1)[\psi(1),n(\mathbf{x}_2,t_1)]\right]\mathrm{T}\left[\exp\left(-i\int_0^{t_1}\mathrm{d}2U(2)n(2)\right)\right].
\end{aligned} \tag{10.7}$$

When calculating the integration, one can move the factor $\pm i^2\int \mathrm{d}\mathbf{x}_2U(n)n(2)$ as it is independent of the time t_1. Since $[\psi(\mathbf{x}_1,t_1),n(\mathbf{x}_2,t_1)]=\delta(\mathbf{x}_1-\mathbf{x}_2)\psi(\mathbf{x}_1,t_1)$, it follows that,

$$i\frac{\partial}{\partial t_1}\mathrm{T}[S\psi(1)]=\mathrm{T}\left[Si\frac{\partial\psi(1)}{\partial t_1}\right]+\mathrm{T}[S\psi(1)]U(1). \tag{10.8}$$

Such a calculation is the source of the UG term in (10.3).

We can learn something by considering the change in $G(U)$ resulting from an infinitesimal change in U by letting $U(2) \to U(2) + \delta U(2)$. The change in G resulting from this change in U is,

$$\delta G(1,1';U) = \delta\left[\frac{1}{i}\frac{\langle \mathrm{T}[S\psi(1)\psi^\dagger(1')]\rangle}{\langle \mathrm{T}[S]\rangle}\right] = \frac{1}{i}\left[\frac{\langle \mathrm{T}[\delta S\psi(1)\psi^\dagger(1')]\rangle}{\langle \mathrm{T}[S]\rangle} - \frac{\langle \mathrm{T}[\delta S]\rangle}{\langle \mathrm{T}[S]\rangle}\frac{\langle \mathrm{T}[S\psi(1)\psi^\dagger(1')]\rangle}{\langle \mathrm{T}[S]\rangle}\right]. \tag{10.9}$$

When δS appears in a time-ordered product, it can be evaluated as

$$\delta S = \delta\left[\exp\left(-i\int_0^{-i\beta} \mathrm{d}2U(2)n(2)\right)\right] = S\left[\frac{1}{i}\int_0^{-i\beta} \mathrm{d}2\delta U(2)n(2)\right], \tag{10.10}$$

since the T's automatically provide the proper (imaginary) time ordering. On substituting (10.10) into (10.9) we find,

$$\begin{aligned}\delta G(1,1';U) &= \int_0^{-i\beta} \mathrm{d}2\delta U(2) \times \left[\frac{\langle \mathrm{T}[S\psi(1)\psi^\dagger(1')n(2)]\rangle}{i^2\langle \mathrm{T}[S]\rangle} - \frac{\langle \mathrm{T}[S\psi(1)\psi^\dagger(1')]\rangle}{i\langle \mathrm{T}[S]\rangle}\frac{\langle \mathrm{T}[Sn(2)]\rangle}{i\langle \mathrm{T}[S]\rangle}\right] \\ &= \pm\int_0^{-i\beta} \mathrm{d}2[G_2(12,1'2^+;U) - G(1,1';U)G(2,2^+;U)]\delta U(2).\end{aligned} \tag{10.11}$$

Since this calculation of δG is just a generalization of the method by which one obtains an ordinary derivative, we call the coefficient of $\delta U(2)$ in (10.11) the functional derivative, or variational derivative, of $G(1,1';U)$ with respect to $U(2)$. It is denoted by $\delta G(1,1';U)/\delta U(2)$, so that

$$\boxed{\frac{\delta G(1,1';U)}{\delta U(2)} = \pm[G_2(12,1'2^+;U) - G(1,1';U)G(2,2^+;U)],} \tag{10.12}$$

and $G_2(12,1'2^+;U) = \pm\delta G(1,1';U)/\delta U(2) + G(1,1';U)G(2,2^+;U)$.

Based on (10.12), we define

$$L(1-2) = \pm i\left[\frac{\delta G(1,1^+;U)}{\delta U(2)}\right]_{U=0} = \frac{1}{i}\langle \mathrm{T}[(n(1)-\langle n\rangle)(n(2)-\langle n\rangle)]\rangle. \tag{10.13}$$

Notice that $L(1-2)$ is quite analogous in structure to the one-particle Green's function. Just as $G(1-1')$ is composed of the two analytic functions of time $G^>(1-1')$ and $G^<(1-1')$, so

$$L(1-2) = \begin{cases} L^>(1-2), & t_1 > t_2 \\ L^<(1-2), & t_1 < t_2 \end{cases}, \tag{10.14}$$

where,

$$\boxed{L^>(1-2) = \frac{1}{i}\langle[n(1)-\langle n\rangle][n(2)-\langle n\rangle]\rangle,\ \ L^<(1-2) = \frac{1}{i}\langle[n(2)-\langle n\rangle][n(1)-\langle n\rangle]\rangle.} \tag{10.15}$$

As G satisfies the boundary condition $G(1-1')|_{t_1=0} = \pm e^{\beta\mu}G(1-1')|_{t_1=-i\beta}$, so $L(1-2)$ satisfies the boundary condition $L(1-2)|_{t_1=0} = L(1-2)|_{t_1=-i\beta}$. Therefore, L can also be written in terms of a Fourier series as,

$$L(1-2) = \frac{1}{-i\beta}\sum_\nu \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} L(\mathbf{k},\Omega_\nu)e^{i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)-i\Omega_\nu(t_1-t_2)}, \tag{10.16}$$

where $\Omega_\nu = \pi\nu/(-i\beta)$, with ν being even. In exactly the same way as we establish that the Fourier coefficient for $G(1-1')$ we find that,

$$\boxed{L(\mathbf{k},\Omega) = \int \frac{\mathrm{d}\omega'}{2\pi}\frac{L^>(\mathbf{k},\omega') - L^<(\mathbf{k},\omega')}{\Omega-\omega'},\ \ L^{>}_{<}(\mathbf{k},\omega) = \int \mathrm{d}\mathbf{x}_1 \int_{-\infty}^{\infty} \mathrm{d}t_1 e^{-i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)+i\omega(t_1-t_2)} \times iL^{>}_{<}(\mathbf{x}_1-\mathbf{x}_2,t_1-t_2).} \tag{10.17}$$

The function $L(\mathbf{k},\Omega)$ is the quantity that is most directly evaluated by a Green's function analysis in the imaginary-time domain. The linear response of the density to a physical disturbance can be easily expressed in terms of $L(\mathbf{k},\Omega)$. The physical response is given as:

$$\langle n(1)\rangle_U = \langle \mathcal{U}^\dagger(t_1)n(1)\mathcal{U}(t_1)\rangle,\ \ \mathcal{U}(t_1) = \mathrm{T}\left[\exp\left(-i\int_{-\infty}^{t_1} \mathrm{d}2U(2)n(2)\right)\right], \tag{10.18}$$

and all the times are real. Hence, the linear response of $\langle n(1)\rangle_U$ to U is,

$$\begin{aligned}\delta[\pm ig(1,1^+;U)] =& \delta\langle n(1)\rangle_U = \langle \delta\mathcal{U}^\dagger(t_1)n(1)\mathcal{U}(t_1)\rangle + \langle \mathcal{U}^\dagger(t_1)n(1)\delta\mathcal{U}(t_1)\rangle \\ =& \left\langle i\int_{-\infty}^{t_1} \mathrm{d}2U(2)n(2)\mathrm{T}\left[\exp\left(-i\int_{-\infty}^{t_1}\mathrm{d}2U(2)n(2)\right)\right] n(1)\mathcal{U}(t_1)\right\rangle \\ &+ \left\langle \mathcal{U}^\dagger(t_1)n(1)(-i)\int_{-\infty}^{t_1}\mathrm{d}2U(2)n(2)\mathrm{T}\left[\exp\left(-i\int_{-\infty}^{t_1}\mathrm{d}2U(2)n(2)\right)\right]\right\rangle \\ =& i\int_{-\infty}^{t_1}\mathrm{d}2\left\langle \mathcal{U}^\dagger(t_1)[n(2),n(1)]\mathcal{U}(t_1)\right\rangle U(2) = \int_{-\infty}^{t_1}\mathrm{d}2[L^>(1-2)-L^<(1-2)]U(2),\end{aligned} \tag{10.19}$$

where

$$\begin{aligned}L^>(1-2)-L^<(1-2) =& \frac{1}{i}\langle[n(1)-\langle n\rangle][n(2)-\langle n\rangle]\rangle - \frac{1}{i}\langle[n(2)-\langle n\rangle][n(1)-\langle n\rangle]\rangle \\ =& \frac{1}{i}\langle n(1)n(2)-n(2)n(1)\rangle = \frac{1}{i}\langle[n(1),n(2)]\rangle.\end{aligned} \tag{10.20}$$

If the external field takes the form $U(\mathbf{X},T) = U_0 e^{i\mathbf{k}\cdot\mathbf{X}-i\Omega T}$, then $\delta\langle n(1)\rangle_U = (\delta n/\delta U)(\mathbf{k},\Omega)U(\mathbf{X},T)$, where

$$\left(\frac{\delta n}{\delta U}\right)(\mathbf{k},\Omega) = \int_{-\infty}^{t_1}\mathrm{d}2[L^>(1-2)-L^<(1-2)]U(2)\frac{e^{-i\mathbf{k}\cdot\mathbf{x}_1+i\Omega T_1}}{U_0} = \int\frac{\mathrm{d}\omega'}{2\pi}\frac{L^>(\mathbf{k},\omega')-L^<(\mathbf{k},\omega')}{\Omega-\omega'}. \tag{10.21}$$

However, we can recognize this last expression as just $L(\mathbf{k},\Omega)$, so that,

$$\boxed{(\delta n/\delta U)(\mathbf{k},\Omega) = L(\mathbf{k},\Omega).} \tag{10.22}$$

Therefore, the Fourier coefficient function $L(\mathbf{k},\Omega)$ is exactly the linear response of $\langle n(1)\rangle_U$ to a disturbance with wave number $\mathbf{k}$ and frequency Ω in the upper half-plane.

We determine this Fourier coefficient by the Hartree approximation in the complex time domain. We certainly expect that this approximation has the same physical content as the real-time Hartree approximation. Therefore, we anticipate that the linear response $L(\mathbf{k},\Omega)$ computed from this approximation for $G(U)$ should be identical to the $(\delta n/\delta U)(\mathbf{k},\Omega)$ that we computed in the last section by means of RPA. In the imaginary-time domain, the Hartree approximation is,

$$G^{-1}(1,1';U) = \left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{\mathrm{eff}}(1)\right]\delta(1-1') = \left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(1) \mp i\int_0^{-i\beta}\mathrm{d}2V(1-2)G^<(2,2^+;U)\right]\delta(1-1'). \tag{10.23}$$

We can compute (considering that $\delta G = -G\delta G^{-1}G$),

$$\begin{aligned}\frac{\delta G(1,1';U)}{\delta U(2)} =& -\int_0^{-i\beta}\mathrm{d}3\mathrm{d}3' G(1,3;U)\frac{\delta G^{-1}(3,3';U)}{\delta U(2)}G(3',1';U) = \int_0^{-i\beta}\mathrm{d}3 G(1,3;U)\frac{\delta U_{\mathrm{eff}}(3)}{\delta U(2)}G(3',1';U) \\ =& G(1,2;U)G(2,1';U) \pm i\int_0^{-i\beta}\mathrm{d}3\mathrm{d}4 G(1,3;U)G(3,1';U)V(3-4)\times\frac{\delta G(4,4^+;U)}{\delta U(2)},\end{aligned} \tag{10.24}$$

$$L(1-2) \equiv \pm i\left[\frac{\delta G(1,1^+;U)}{\delta U(2)}\right]_{U=0} = \pm iG(1-2)G(2-1) + \int_0^{-i\beta}\mathrm{d}3\mathrm{d}4[\pm iG(1-3)G(3-1)]V(3-4)L(4-2). \tag{10.25}$$

If we define,

$$\boxed{L_0(1-2) = \pm iG(1-2)G(2-1),} \tag{10.26}$$

then,

$$\boxed{L(1-2) = L_0(1-2) + \int_0^{-i\beta}\mathrm{d}3\mathrm{d}4 L_0(1-3)V(3-4)L(4-2).} \tag{10.27}$$

By employing the boundary conditions on G, namely $G(1-2)|_{t_1=0} = \pm e^{\beta\mu}G(1-2)|_{t_1=-i\beta}$ and $G(1-2)|_{t_2=0} = \pm e^{-\beta\mu}G(1-2)|_{t_2=-i\beta}$, we find that L_0 satisfies the same boundary condition as L. Thus, L_0 may also be expanded in a Fourier series of the form (10.16), with a Fourier coefficient $L_0(\mathbf{k},\Omega)$. From (10.26) it follows that,

$$L_0^>(1-2) = \pm iG^>(1-2)G^<(2-1),\quad L_0^<(1-2) = \pm iG^<(1-2)G^>(2-1), \tag{10.28}$$

$$L_0^{>}_{<}(\mathbf{k},\omega) = \int\frac{\mathrm{d}\mathbf{p}'}{(2\pi)^3}\frac{\mathrm{d}\omega'}{2\pi}G^{>}_{<}\left(\mathbf{p}'+\frac{\mathbf{k}}{2},\omega'+\frac{\omega}{2}\right)G^{<}_{>}\left(\mathbf{p}'-\frac{\mathbf{k}}{2},\omega'-\frac{\omega}{2}\right). \tag{10.29}$$

Consequently,

$$L_0^>(\mathbf{k},\Omega)-L_0^<(\mathbf{k},\Omega)=\int\frac{\mathrm{d}\mathbf{p}'}{(2\pi)^3}\frac{\mathrm{d}\omega'}{2\pi}A\left(\mathbf{p}'+\frac{\mathbf{k}}{2},\omega'+\frac{\omega}{2}\right)A\left(\mathbf{p}'-\frac{\mathbf{k}}{2},\omega'-\frac{\omega}{2}\right)$$
$$\times\left[\left[1\pm f\left(\omega'+\frac{\omega}{2}\right)\right]\times f\left(\omega'-\frac{\omega}{2}\right)-f\left(\omega'+\frac{\omega}{2}\right)\times\left[1\pm f\left(\omega'-\frac{\omega}{2}\right)\right]\right]. \tag{10.30}$$

Because (10.27) is derived by differentiating the Hartree approximation, the G's that appear in (10.26) must be the Hartree Green's functions, and for these, $A(\mathbf{p},\omega)=2\pi\delta(\omega-E(\mathbf{p}))=2\pi\delta(\omega-\mathbf{p}^2/2m-nv)$. Therefore $L_0^>-L_0^<$ has the form,

$$L_0^>(\mathbf{k},\omega)-L_0^<(\mathbf{k},\omega)=\int\frac{\mathrm{d}\mathbf{p}}{(2\pi)^3}\times 2\pi\delta\left(\omega-E\left(\mathbf{p}+\frac{\mathbf{k}}{2}\right)+E\left(\mathbf{p}-\frac{\mathbf{k}}{2}\right)\right)\times\left[f(E(\mathbf{p}-\mathbf{k}/2))-f(E(\mathbf{p}+\mathbf{k}/2))\right], \tag{10.31}$$

from which one can obtain the coefficient $L_0(\mathbf{k},\Omega)$ as,

$$L_0(\mathbf{k},\Omega)=\int\frac{\mathrm{d}\omega'}{2\pi}\frac{L_0^>(\mathbf{k},\omega')-L_0^<(\mathbf{k},\omega')}{\Omega-\omega'}=\int\frac{\mathrm{d}\mathbf{p}}{(2\pi)^3}\frac{f(E(\mathbf{p}-\mathbf{k}/2))-f(E(\mathbf{p}+\mathbf{k}/2))}{\Omega-\mathbf{k}\cdot\mathbf{p}/m}. \tag{10.32}$$

If we compare (10.32) with (9.65), we see that

$$\boxed{L_0(\mathbf{k},\Omega)=\left(\frac{\delta n}{\delta U}\right)_0(\mathbf{k},\Omega),} \tag{10.33}$$

the latter function is the quantity that appears in the solution of the real-time Hartree approximation.

It is trivial to solve (10.27) by transforming. We multiply it by $e^{-i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)+i\Omega_\nu(t_1-t_2)}$ and integrate over all $\mathbf{x}_1$ and all t_1 between 0 and $-i\beta$. The left hand side gives,

$$\int_0^{-i\beta}e^{-i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)+i\Omega_\nu(t_1-t_2)}L(1-2)\mathrm{d}\mathbf{x}_1\mathrm{d}t_1=L(\mathbf{k},\Omega_\nu), \tag{10.34}$$

where we use the identity $\int_0^{-i\beta}e^{i\Omega_\nu t}\mathrm{d}t=-i\beta\delta_{\nu,0}$. The first term on the right side gives $L_0(\mathbf{k},\Omega)$, and the second term is,

$$\int_0^{-i\beta}\mathrm{d}3\mathrm{d}4L_0(1-3)V(3-4)L(4-2)e^{-i\mathbf{k}\cdot(\mathbf{x}_1-\mathbf{x}_2)+i\Omega_\nu(t_1-t_2)}\mathrm{d}\mathbf{x}_1\mathrm{d}t_1=L_0(\mathbf{k},\Omega_\nu)v(\mathbf{k})L(\mathbf{k},\Omega_\nu), \tag{10.35}$$

so that $L(\mathbf{k},\Omega_\nu)=L_0(\mathbf{k},\Omega_\nu)[1+v(\mathbf{k})L(\mathbf{k},\Omega_\nu)]$. After the analytical continuation, we have

$$\boxed{L(\mathbf{k},\Omega)=L_0(\mathbf{k},\Omega)[1+v(\mathbf{k})L(\mathbf{k},\Omega)],\quad L(\mathbf{k},\Omega)=\frac{L_0(\mathbf{k},\Omega)}{1-v(\mathbf{k})L_0(\mathbf{k},\Omega)}=\frac{(\delta n/\delta U)_0(\mathbf{k},\Omega)}{1-v(\mathbf{k})(\delta n/\delta U)_0(\mathbf{k},\Omega)}.} \tag{10.36}$$

We recognize this expression for $L(\mathbf{k},\Omega)$ is exactly as the one derived for $(\delta n/\delta U)(\mathbf{k},\Omega)$ in RPA (see (9.66)). Therefore, $(\delta n/\delta U)(\mathbf{k},\Omega)$ can be determined equally well from the imaginary-time theory. One just has to solve for $L(\mathbf{k},\Omega)$, using an approximation for $G(U)$, to find the physical response $(\delta n/\delta U)(\mathbf{k},\Omega)$. Unfortunately, this procedure for determining the physical response from the imaginary-time response is very difficult to employ for approximations fancier than the Hartree approximation. It is only for this approximation that we can solve exactly for the response and hence obtain an exact solution for the Fourier coefficient. In other situations, we cannot obtain an explicit form for $L(\mathbf{k},\Omega)$ from the imaginary-time Green's functions, and hence we cannot employ the simple analysis that we have developed here.

EXERCISE 51: Prove the relations (10.34) and (10.35).

Instead of working with $g_2(U)$ directly, we shall show how $g_2(U)$ may be derived from $G_2(U)$. We begin this analysis by introducing an essentially trivial generalization of $G(U)$ and $G_2(U)$. These functions were originally defined as for pure imaginary times in the interval $0<it,it'<\beta$. However, there is nothing very special about the time zero. We could just as well define Green's functions in the interval $[t_0,t_0-i\beta]$, i.e., $0<i(t-t_0)<\beta, t_0\in\mathrm{R}$. For times in this interval, we write,

$$G(1,1';U;t_0)=\frac{1}{i}\frac{\langle\mathrm{T}[S\psi(1)\psi^\dagger(1')]\rangle}{\langle\mathrm{T}[S]\rangle},\quad S=\exp\left(-i\int_{t_0}^{t_0-i\beta}\mathrm{d}2U(2)n(2)\right). \tag{10.37}$$

Here T orders according to the size of $i(t-t_0)$; operators with larger values of $i(t-t_0)$ appear on the left. When $t_0=0$, the $G(U;t_0)$ defined by (10.37) reduces to the $G(U)$ discussed previously in this section. The theory of $G(U;t_0)$ is identical to the theory of $G(U)$. This generalized response function satisfies the boundary condition, $G(1,1';U;t_0)|_{t_1=t_0}=\pm e^{\beta\mu}G(1,1';U;t_0)|_{t_1=t_0-i\beta}$, instead of $G(1,1';U)|_{t_1=t_0}=\pm e^{\beta\mu}G(1,1';U)|_{t_1=t_0-i\beta}$. Therefore, the only change that has to be made in the previous formulas is to make them apply to $G(U;t_0)$ is to replace all time integrals over the interval $[0,-i\beta]$

by integrals over $[t_0, t_0 - i\beta]$. In particular, $G(U;t_0)$ satisfies the equations of motion:

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(1)\right] G(1,1';U;t_0) - \int_{t_0}^{t_0-i\beta} \mathrm{d}\bar{1}\Sigma(1,\bar{1};U;t_0)G(\bar{1},1';U;t_0) = \delta(1-1'), \tag{10.38}$$

$$\left[-i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} - U(1')\right] G(1,1';U;t_0) - \int_{t_0}^{t_0-i\beta} \mathrm{d}\bar{1}G(1,\bar{1};U;t_0)\Sigma(\bar{1},1';U;t_0) = \delta(1-1'), \tag{10.39}$$

here Σ is the self-energy, which is defined by in the equilibrium case as,

$$\boxed{\left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right) G(1-1') - \int_0^{-i\beta} \mathrm{d}\bar{1}\Sigma(1-\bar{1})G(\bar{1}-1') = \delta(1-1').} \tag{10.40}$$

In the presence of U we define Σ by the equation,

$$\boxed{\int_0^{-i\beta} \mathrm{d}\bar{1}[G_0^{-1}(1,\bar{1};U) - \Sigma(1,\bar{1};U)]G(\bar{1},1';U) = \delta(1-1').} \tag{10.41}$$

If we define the matrix inverse of G by $\int_0^{-i\beta} \mathrm{d}\bar{1}G^{-1}(1,\bar{1};U)G(\bar{1},1';U) = \delta(1-1')$, we obtain Dyson's equation:

$$\boxed{G^{-1}(1,1';U) = G_0^{-1}(1,1';U) - \Sigma(1,1';U).} \tag{10.42}$$

Let's establish a relationship between $G(U;t_0)$ and $g(U)$ in order that we may convert (10.38) and (10.39) into equations of motion for $g(U)$. To do this, we consider the case $i(t_1 - t_0) < i(t_{1'} - t_0)$. Then,

$$\begin{aligned} G(1,1';U;t_0) = G^<(1,1';U;t_0) &= \pm\frac{1}{i}\frac{\langle \mathrm{T}[S\psi(1)\psi^\dagger(1')]\rangle}{\langle \mathrm{T}[S]\rangle} \\ &= \pm\frac{1}{i}\frac{\langle \mathcal{U}(t_0,t_0-i\beta)[\mathcal{U}^\dagger(t_0,t_{1'})\psi^\dagger(1')\mathcal{U}(t_0,t_{1'})][\mathcal{U}^\dagger(t_0,t_1)\psi(1)\mathcal{U}(t_0,t_1)]\rangle}{\langle \mathcal{U}(t_0,t_0-i\beta)\rangle}, \end{aligned} \tag{10.43}$$

where,

$$\mathcal{U}(t_0,t_1) = \mathrm{T}\left[\exp\left(-i\int_{t_0}^{t_1} \mathrm{d}2U(2)n(2)\right)\right]. \tag{10.44}$$

For comparison we also write out the physical response function, which is defined for real times. For example,

$$g^<(1,1';U) = \pm\frac{1}{i}\langle\psi_U^\dagger(1')\psi_U(1)\rangle = \pm\frac{1}{i}\langle[\mathcal{U}^\dagger(t_{1'})\psi^\dagger(1')\mathcal{U}(t_{1'})]\times[\mathcal{U}^\dagger(t_1)\psi(1)\mathcal{U}(t_1)]\rangle, \tag{10.45}$$

with

$$\mathcal{U}(t_1) = \mathrm{T}\left[\exp\left(-i\int_{-\infty}^{t_1} \mathrm{d}2U(2)n(2)\right)\right]. \tag{10.46}$$

We consider the case in which $U(1)$ is an analytic function of t_1, for $0 > \mathrm{Im}\, t_1 > -\beta$, which satisfies

$$\lim_{\mathrm{Re}\, t_1 \to -\infty} U(t_1) = 0. \tag{10.47}$$

For example, $U(\mathbf{X},T)$ might be $U(\mathbf{X},T) = U_0 e^{i\mathbf{k}\cdot\mathbf{x} - i\Omega T}$ where $\mathrm{Im}\,\Omega > 0$. If $U(\mathbf{X},T)$ is an analytic function of the time, then $\mathcal{U}(t_0,t_1)$ and $\mathcal{U}(t_0)$ are analytic functions of their time variables in the sense that every matrix element of each term in their power-series expansions is analytic. If all sums converge uniformly, as we shall assume, $G^<(1,1';U;t_0)$ and $g^<(1;1,';U)$ are then each analytic functions of their time arguments. The analytic functions $\mathcal{U}(t_0,t_1)$ and $\mathcal{U}(t_0)$ can also be defined by

$$\boxed{i\frac{\partial}{\partial t_1}\mathcal{U}(t_1) = \int \mathrm{d}\mathbf{x}_1 n(1)U(1)\mathcal{U}(t_1);\ \ \mathcal{U}(-\infty) = 1,\ \ i\frac{\partial}{\partial t_1}\mathcal{U}(t_0,t_1) = \int \mathrm{d}\mathbf{x}_1 n(1)U(1)\mathcal{U}(t_0,t_1),\ \ \mathcal{U}(t_0,t_0) = 1.} \tag{10.48}$$

Because of this analyticity it follows that $\lim_{t_0\to-\infty}\mathcal{U}(t_0,t_1) = \mathcal{U}(t_1)$, and because of (10.47), $\lim_{t_0\to-\infty}\mathcal{U}(t_0,t_0-i\beta) = 1$. Therefore, the imaginary- and real-time analytic functions are connected by

$$\boxed{\lim_{t_0\to-\infty} G^<(1,1';U;t_0) = g^<(1,1';U),\quad \lim_{t_0\to-\infty} G^>(1,1';U;t_0) = g^>(1,1';U).} \tag{10.49}$$

In order to have a simple confirmation of the result that we have just obtained, let us compute $\pm iG^<(1,1';U;t_0)$ and $\pm ig^<(1,t;U)$ to first order in U. These are,

$$\begin{aligned}\pm iG^<(1,1';U;t_0) &= \langle n\rangle + \int_{t_0}^{t_0-i\beta} \mathrm{d}2\frac{1}{i}\langle \mathrm{T}\{[n(1)-\langle n\rangle][n(2)-\langle n\rangle]\}\rangle \\ &= \langle n\rangle + \int_{t_0}^{t_1} \mathrm{d}2\frac{1}{i}\langle [n(1)-\langle n\rangle][n(2)-\langle n\rangle]\rangle U(2) - \int_{t_0-i\beta}^{t_1} \mathrm{d}2\frac{1}{i}\langle [n(2)-\langle n\rangle][n(1)-\langle n\rangle]\rangle U(2) \\ &= \langle n\rangle + \int_{t_0}^{t_1} \mathrm{d}2L^>(1-2)U(2) - \int_{t_0-i\beta}^{t_1} \mathrm{d}2L^<(1-2)U(2). \end{aligned} \tag{10.50}$$

Since $L^>$ and $L^<$ are analytic functions of their time variables, when U is also analytic, the right side of (10.50) is clearly an analytic function of t_1 and t_0. If we take the limit $t_0 \to -\infty$, (10.50) becomes,

$$\boxed{\lim_{t_0\to-\infty}[\pm iG^<(1,1';U;t_0)] = \langle n\rangle + \int_{-\infty}^{t_1} \mathrm{d}2[L^>(1-2)-L^<(1-2)]U(2),} \tag{10.51}$$

and this should be compared with (10.19), which indicates that the physical response is,

$$\langle n(1)\rangle_U = \pm ig^<(1,1';U) = \langle n\rangle + \int_{-\infty}^{t_1} \mathrm{d}2[L^>(1-2)-L^<(1-2)]U(2). \tag{10.52}$$

This is, of course, the same as (10.51).

We now describe how approximate equations of motion for $G(U;t_0)$ may be continued into equations of motion for the physical response function $g(U)$. In the Hartree approximation (10.38) is

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{\mathrm{eff}}(1;t_0)\right] G^<(1,1';U;t_0) = \delta(1-1'), U_{\mathrm{eff}}(\mathbf{X},T;t_0) = U(\mathbf{X},T) \pm i\int \mathrm{d}\mathbf{X}' v(\mathbf{X}-\mathbf{X}')G^<(\mathbf{X}'T,\mathbf{X}'T;U;t_0). \tag{10.53}$$

We consider the case in which $i(t_1-t_0) < i(t_{1'}-t_0)$. Then,

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{\mathrm{eff}}(1;t_0)\right] G^<(1,1';U;t_0) = 0. \tag{10.54}$$

Using the analyticity of $U(\mathbf{X},T)$, we take the limit $t_0 \to -\infty$ to find,

$$U_{\mathrm{eff}}(\mathbf{X},T;-\infty) = U(\mathbf{X},T) \pm i\int \mathrm{d}\mathbf{X}' v(\mathbf{X}-\mathbf{X}')g^<(\mathbf{X}'T,\mathbf{X}'T;U), \quad \left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{\mathrm{eff}}(1;-\infty)\right] g^<(1,1';U) = 0. \tag{10.55}$$

These equations hold for all complex values of t_1 and $t_{1'}$ such that $\beta > \mathrm{Im}(t_1-t_{1'}) \geq 0$. When they are specialized to the case of real values of the time variables they become just the familiar statement of the real-time Hartree approximation.

The original derivation of the Hartree approximation depends in no way on the analytic properties of $U(\mathbf{X},T)$. In fact, the validity of the equations for $g(U)$ that we shall derive does not depend on the analyticity of U. The analytic continuation device is a convenient way of handling boundary conditions on the real-time response functions. It also gives a particularly way of seeing the connection between the imaginary-time $G(U)$ and the physical response function $g(U)$. This can be applied in a much more general discussion of the equations of motion for $g(U)$.

The self-energy $\Sigma(1,1';U;t_0)$ splits as $\Sigma(1,1';U;t_0) = \Sigma_{\mathrm{HF}}(1,1';U;t_0) + \Sigma_{\mathrm{C}}(1,1';U;t_0)$, where the Hartree–Fock term is

$$\Sigma_{\mathrm{HF}}(1,1';U;t_0) = \delta(t_1-t_{1'})\left[\pm i\delta(\mathbf{x}_1-\mathbf{x}_{1'})\int \mathrm{d}\mathbf{x}_2 v(\mathbf{x}_1-\mathbf{x}_2)G^<(\mathbf{x}_2t_1,\mathbf{x}_2t_1;U;t_0) + iv(\mathbf{x}_1-\mathbf{x}_{1'})G^<(1,1';U;t_0)\right], \tag{10.56}$$

and the collisional part of Σ is composed of two analytic functions of the time variables $\Sigma^>$ and $\Sigma^<$,

$$\Sigma_{\mathrm{C}}(1,1';U;t_0) = \begin{cases} \Sigma^>(1,1';U;t_0), & i(t_1-t_{1'}) > 0, \\ \Sigma^<(1,1';U;t_0), & i(t_1-t_{1'}) < 0. \end{cases} \tag{10.57}$$

In the Born collision approximation, we have

$$\begin{aligned}\Sigma_{\mathrm{C}}(1,1';U;t_0) = \pm i^2\int \mathrm{d}\mathbf{x}_2\mathrm{d}\mathbf{x}_{2'} v(\mathbf{x}_1-\mathbf{x}_2)v(\mathbf{x}_{1'}-\mathbf{x}_{2'}) \times \Big[&G(1,1';U;t_0)G(2,2';U;t_0)G(2',2;U;t_0) \\ &\pm G(1,2';U;t_0)G(2,1';U;t_0)G(2',2;U;t_0)\Big]_{t_2=t_1,t_{2'}=t_{1'}},\end{aligned} \tag{10.58}$$

where $\Sigma^{>}$ and $\Sigma^{<}$ are,

$$\Sigma^{>}_{<}(1,1';U;t_0) = \pm i^2 \int d\mathbf{x}_2 d\mathbf{x}_{2'} v(\mathbf{x}_1-\mathbf{x}_2)v(\mathbf{x}_{1'}-\mathbf{x}_{2'}) \times \Big[G^{>}_{<}(1,1';U;t_0)G^{>}_{<}(2,2';U;t_0)G^{<}_{>}(2',2;U;t_0) \\ \pm G^{>}_{<}(1,2';U;t_0)G^{>}_{<}(2,1';U;t_0)G^{<}_{>}(2',2;U;t_0)\Big]_{t_2=t_1,t_{2'}=t_{1'}}. \tag{10.59}$$

Since the $G^{>}$ and $G^{<}$ are analytic functions of their time variables, so is $\Sigma^{>}_{<}$. For the sake of simplicity in writing, we temporally drop the exchange term in $\Sigma_{\rm HF}$, i.e., the term proportional to $v(\mathbf{x}_1-\mathbf{x}_{1'})$, in (10.56). Then (10.38) becomes,

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{\rm eff}(1;t_0)\right] G(1,1';U';t_0) = \delta(1-1') + \int_{t_0}^{t_0-i\beta} d\bar{1}\Sigma_{\rm C}(1,\bar{1};U;t_0)G(\bar{1},1';U;t_0). \tag{10.60}$$

For the case, $i(t_1-t_0) < i(t_{1'}-t_0)$, this gives

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{\rm eff}(1;t_0)\right] G(1,1';U';t_0) \\ = \int_{t_0}^{t_1} d\bar{1}\Sigma^{>}(1,\bar{1};U;t_0)G^{<}(\bar{1},1';U;t_0) + \int_{t_1}^{t_{1'}} d\bar{1}\Sigma^{<}(1,\bar{1};U;t_0)G^{<}(\bar{1},1';U;t_0) + \int_{t_{1'}}^{t_0-i\beta} d\bar{1}\Sigma^{<}(1,\bar{1};U;t_0)G^{>}(\bar{1},1';U;t_0). \tag{10.61}$$

If we now take the limit $t_0 \to -\infty$, we find that $g^{<}(U)$ obeys,

$$\boxed{\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{\rm eff}(1)\right] g^{<}(1,1';U) \\ = \int_{-\infty}^{t_1} d\bar{1}[\Sigma^{>}(1,\bar{1};U) - \Sigma^{<}(1,\bar{1};U)]g^{<}(\bar{1},1';U) - \int_{-\infty}^{t_{1'}} d\bar{1}\Sigma^{<}(1,\bar{1};U)[g^{>}(\bar{1},1';U) - g^{<}(\bar{1},1';U)],} \tag{10.62}$$

where the following relations are adopted when doing the derivation,

$$\int_{t_1}^{t_{1'}} d\bar{1}\cdots = -\int_{t_0}^{t_1} d\bar{1}\cdots + \int_{t_0}^{t_1} d\bar{1}\cdots + \int_{t_1}^{t_{1'}} d\bar{1}\cdots = -\int_{t_0}^{t_1} d\bar{1}\cdots + \int_{t_0}^{t_{1'}} d\bar{1}\cdots, \tag{10.63}$$

and

$$U_{\rm eff}(1) = U_{\rm eff}(1;-\infty), \quad \Sigma^{>}_{<}(1,1';U) = \Sigma^{>}_{<}(1,1';U;-\infty). \tag{10.64}$$

Applying the same arguments (10.38) in the case $i(t_1-t_0) > i(t_{1'}-t_0)$, we find,

$$\boxed{\left[i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U_{\rm eff}(1)\right] g^{>}(1,1';U) \\ = \int_{-\infty}^{t_1} d\bar{1}[\Sigma^{>}(1,\bar{1};U) - \Sigma^{<}(1,\bar{1};U)]g^{>}(\bar{1},1';U) - \int_{-\infty}^{t_{1'}} d\bar{1}\Sigma^{>}(1,\bar{1};U)[g^{>}(\bar{1},1';U) - g^{<}(\bar{1},1';U)].} \tag{10.65}$$

Similarly, equation (10.39) implies,

$$\boxed{\left[-i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} - U_{\rm eff}(1')\right] g^{<}(1,1';U) \\ = \int_{-\infty}^{t_1} d\bar{1}[g^{>}(1,\bar{1};U) - g^{<}(1,\bar{1};U)]\Sigma^{<}(\bar{1},1';U) - \int_{-\infty}^{t_{1'}} d\bar{1}g^{<}(1,\bar{1};U)[\Sigma^{>}(\bar{1},1';U) - \Sigma^{<}(\bar{1},1';U)],} \tag{10.66}$$

and,

$$\boxed{\left[-i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_{1'}^2}{2m} - U_{\rm eff}(1')\right] g^{>}(1,1';U) \\ = \int_{-\infty}^{t_1} d\bar{1}[g^{>}(1,\bar{1};U) - g^{<}(1,\bar{1};U)]\Sigma^{>}(\bar{1},1';U) - \int_{-\infty}^{t_{1'}} d\bar{1}g^{>}(1,\bar{1};U)[\Sigma^{>}(\bar{1},1';U) - \Sigma^{<}(\bar{1},1';U)].} \tag{10.67}$$

When $\Sigma^{>}_{<}(U;t_0=-\infty)$ is expressed in terms of $g^{>}_{<}(U)$, (10.62), (10.65), (10.66) and (10.67) can be used to determine the real-time response functions $g^{>}(U)$ and $g^{<}(U)$, e.g., the Born collision approximation for $g(U)$ is derived by using (10.58)

to find,

$$\boxed{\begin{aligned}\Sigma^{>}_{<}(1,1';U) \equiv & \Sigma^{>}_{<}(1,1';U;t_0=-\infty) \\ & = \pm i^2 \int d\mathbf{x}_2 d\mathbf{x}_{2'} v(\mathbf{x}_1-\mathbf{x}_2) v(\mathbf{x}_{1'}-\mathbf{x}_{2'}) \\ & \quad \times \left[g^{>}_{<}(1,1';U) g^{>}_{<}(2,2';U) g^{<}_{>}(2'2;U) \pm g^{>}_{<}(1,2';U) g^{<}_{>}(2,1';U) g^{<}_{>}(2',2;U) \right]_{t_2=t_1, t_{2'}=t_{1'}}.\end{aligned}} \tag{10.68}$$

Eqs (10.62), (10.65), (10.66) and (10.67) are exact, except for the trivial omission of exchange term in $\Sigma_{\rm HF}$, they are called the Kadanoff–Baym equations. In the next section we shall discuss how these equations may be used to describe transport problems. In particular, we use the approximation (10.68) to derive a generalization of the Boltzmann equation.

EXERCISE 52: Write down the Kadanoff–Baym equations by including the exchange term in $\Sigma_{\rm HF}$.

K Generalized Boltzmann Equations, Normal Fermi Liquid

Eauations(10.62), (10.65), (10.66), (10.67), and (10.68) are, in general extremely complicated, and they become much simpler in the limit in which $U(\mathbf{X},T)$ varies slowly in space and time. This is exactly the situation in which simple transport processes occur. When U varies slowly, $g^{>}(1,1';U)$ and $g^{<}(1,1';U)$ are slowly varying functions of the coordinates,

$$\mathbf{X} = (\mathbf{x}_1 + \mathbf{x}_{1'})//2, \quad T = (t_1 + t_{1'})/2, \tag{11.1}$$

but are sharply peaked about zero values of

$$\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_{1'}, \quad t = t_1 - t_{1'}. \tag{11.2}$$

The equilibrium Green's functions are sharply peaked about $\mathbf{x}=\mathbf{0}$ and $t=0$, e.g., the $G^{<}_0(\mathbf{x},t)$ at low densities is,

$$G^{<}_0(\mathbf{x},t) = \pm i \int \frac{d\mathbf{p}}{(2\pi)^3} \exp\left[-\beta\left(\frac{\mathbf{p}^2}{2m} - \mu\right) - \frac{i\mathbf{p}^2 t}{2m} + i\mathbf{p}\cdot\mathbf{x} \right] = \pm \left(\frac{m}{2\pi(\beta+it)}\right)^{3/2} \exp\left[\beta\mu - \frac{mr^2(\beta - it)}{2(\beta^2+t^2)} \right]. \tag{11.3}$$

This function has a spatial range on the order of a thermal wavelength, $\lambda_{\rm th} = \hbar\beta/2m$, and in time it decreases with a $t^{-3/2}$ dependence. Actually, if one included a lifetime, then $G^{<}_0$ would decay exponentially in time. We may expect then that external disturbances with wavelengths much longer than the thermal wavelength and frequencies much smaller than the single-particle collision rates will not change this sharp $\mathbf{x},t$ dependence of g.

It is therefore convenient to consider $g^{>}_{<}(1,1';U)$ as functions of the variables (11.1) and (11.2). We therefore write $g^{>}_{<}(1,1';U)$ as $g^{>}_{<}(\mathbf{x},t;\mathbf{X},T)$. Recall that $g^{<}(\mathbf{p},\omega;\mathbf{X},T) = \int d\mathbf{x} dt e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}[\pm i g^{<}(\mathbf{x},t;\mathbf{X},T)]$ can be interpreted as the density of particles with momentum $\mathbf{p}$ and energy ω at space time point $\mathbf{X},T$. Also, $g^{>}(\mathbf{p},\omega;\mathbf{X},T) = \int d\mathbf{x} dt e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t} i g^{>}(\mathbf{x},t;\mathbf{X},T)$ is essentially the density of states available to a particle that is added to the system at $\mathbf{X},T$ with momentum $\mathbf{p}$ and energy ω. We may derive an equation of motion for $g^{<}(\mathbf{p},\omega;\mathbf{X},T)$ by subtracting (10.66) from (10.62),

$$\boxed{\begin{aligned} & \left[i\frac{\partial}{\partial t_1} + i\frac{\partial}{\partial t_{1'}} + \frac{\nabla_1^2}{2m} - \frac{\nabla_{1'}^2}{2m} - U_{\rm eff}(1) + U_{\rm eff}(1') \right] g^{<}(1,1';U) \\ & = \int_{-\infty}^{t_1} d\bar{1} [\Sigma^{>}(1,\bar{1};U) - \Sigma^{<}(1,\bar{1};U)] g^{<}(\bar{1},1';U) + \int_{-\infty}^{t_{1'}} d\bar{1} g^{<}(1,\bar{1};U) [\Sigma^{>}(\bar{1},1';U) - \Sigma^{<}(\bar{1},1';U)] \\ & \quad - \int_{-\infty}^{t_{1'}} d\bar{1} \Sigma^{<}(1,\bar{1};U) [g^{>}(\bar{1},1';U) - g^{<}(\bar{1},1';U)] - \int_{-\infty}^{t_1} d\bar{1} [g^{>}(1,\bar{1};U) - g^{<}(1,\bar{1};U)] \Sigma^{<}(\bar{1},1';U). \end{aligned}} \tag{11.4}$$

We now rewrite (11.4) in terms of the variables $\mathbf{x},t;\mathbf{X},T$ by expressing the g's that appear in this equation in terms of these variables and also writing Σ as $\Sigma^{>}_{<}(1,1';U) = \Sigma^{>}_{<}(\mathbf{x},t;\mathbf{X},T)$. The left side of (11.4) becomes,

$$\left[i\frac{\partial}{\partial T} + \frac{\nabla_{\mathbf{X}}\cdot\nabla_{\mathbf{x}}}{m} - U_{\rm eff}\left(\mathbf{X}+\frac{\mathbf{x}}{2}, T+\frac{t}{2}\right) + U_{\rm eff}\left(\mathbf{X}-\frac{\mathbf{x}}{2}, T-\frac{t}{2}\right) \right] g^{<}(\mathbf{x},t;\mathbf{X},T). \tag{11.5}$$

Because $g^{<}(\mathbf{x},t;\mathbf{X},T)$ is very sharply peaked about $\mathbf{x}=\mathbf{0}, t=0$, we can consider $\mathbf{x}$ and t to be small in (11.5). Then we can expand the difference of $U_{\rm eff}$'s in powers of $\mathbf{x}$ and t, retaining only the lowest-order terms. In this way, we see that (11.5) may be approximately replaced by,

$$\left[i\frac{\partial}{\partial T} + \frac{\nabla_{\mathbf{X}}\cdot\nabla_{\mathbf{x}}}{m} - \left[\left(\mathbf{x}\cdot\nabla_{\mathbf{X}} + t\frac{\partial}{\partial T} \right) U_{\rm eff}(\mathbf{X},T) \right] \right] g^{<}(\mathbf{x},t;\mathbf{X},T). \tag{11.6}$$

In terms of the variables $\mathbf{x},t,\mathbf{X},T$, the first term on the right side of (11.4) may be written as,

$$\int_{-\infty}^{t} d\bar{t}d\bar{\mathbf{x}}\left[\Sigma^{>}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X}+\frac{\bar{\mathbf{x}}}{2},T+\frac{\bar{t}}{2}\right)-\Sigma^{<}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X}+\frac{\bar{\mathbf{x}}}{2},T+\frac{\bar{t}}{2}\right)\right]\times g^{<}\left(\bar{\mathbf{x}},\bar{t};\mathbf{X}-\frac{\mathbf{x}-\bar{\mathbf{x}}}{2},T-\frac{t-\bar{t}}{2}\right), \tag{11.7}$$

where we have made the change of variables, $\bar{\mathbf{x}}=\bar{\mathbf{x}}_1-\mathbf{x}_{1'}=\bar{\mathbf{x}}_1-(\mathbf{X}-\mathbf{x}/2), t=\bar{t}_1-t_{1'}=\bar{t}_1-(T-t/2)$. Because $\Sigma^{>}(\mathbf{x},t;\mathbf{X},T)$ and $g^{<}(\mathbf{x},t;\mathbf{X},T)$ are each sharply peaked about $\mathbf{x}=\mathbf{0}, t=0$, and slowly varying in $\mathbf{X},T$, we can neglect the necessarily small quantities added to $\mathbf{X}$ and T in (11.7). Then (11.7) becomes,

$$\int_{-\infty}^{t} d\bar{t}d\bar{\mathbf{x}}\left[\Sigma^{>}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)-\Sigma^{<}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)\right]g^{<}(\bar{\mathbf{x}},\bar{t};\mathbf{X},T). \tag{11.8}$$

The second term on the right side of (11.4) can be similarly analyzed to give,

$$\int_{t}^{\infty} d\bar{t}d\bar{\mathbf{x}}g^{<}(\bar{\mathbf{x}},\bar{t};\mathbf{X},T)\left[\Sigma^{>}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)-\Sigma^{<}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)\right]. \tag{11.9}$$

When (11.8) and (11.9) are added together, we see the first two terms on the right side of (11.4) is approximated by,

$$\boxed{\int_{-\infty}^{\infty} d\bar{t}\int d\bar{\mathbf{x}}g^{<}(\bar{\mathbf{x}},\bar{t};\mathbf{X},T)\left[\Sigma^{>}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)-\Sigma^{<}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)\right].} \tag{11.10}$$

Similarly, the remaining two terms in (11.4) can be evaluated as,

$$\boxed{-\int_{-\infty}^{\infty} d\bar{t}\int d\bar{\mathbf{x}}\left[g^{>}\left(\bar{\mathbf{x}},\bar{t};\mathbf{X},T\right)-g^{<}\left(\bar{\mathbf{x}},\bar{t};\mathbf{X},T\right)\right]\Sigma^{<}(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T).} \tag{11.11}$$

Consequently, (11.4) may be approximately replaced by,

$$\boxed{\begin{aligned}&\left[i\frac{\partial}{\partial T}+\frac{\nabla_{\mathbf{X}}\cdot\nabla_{\mathbf{x}}}{m}-\mathbf{x}\cdot\nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)-t\frac{\partial}{\partial T}U_{\text{eff}}(\mathbf{X},T)\right]g^{<}(\mathbf{x},t;\mathbf{X},T)\\&=\int d\bar{t}d\bar{\mathbf{x}}\Big[g^{<}(\bar{\mathbf{x}},\bar{t};\mathbf{X},T)\left[\Sigma^{>}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)-\Sigma^{<}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)\right]\\&\qquad-\left[g^{>}\left(\bar{\mathbf{x}},\bar{t};\mathbf{X},T\right)-g^{<}\left(\bar{\mathbf{x}},\bar{t};\mathbf{X},T\right)\right]\Sigma^{<}(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T)\Big]\\&=\int d\bar{t}d\bar{\mathbf{x}}\left[g^{<}(\bar{\mathbf{x}},\bar{t};\mathbf{X},T)\Sigma^{>}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)-g^{>}(\bar{\mathbf{x}},\bar{t};\mathbf{X},T)\Sigma^{<}\left(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T\right)\right].\end{aligned}} \tag{11.12}$$

To convert Eq. (11.12) into a more useful form, we multiply by $\pm e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}$ and integrate over $\mathbf{x}$ and t. The result is,

$$\boxed{\begin{aligned}&\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}-\nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}}+\frac{\partial U_{\text{eff}}(\mathbf{X},T)}{\partial T}\frac{\partial}{\partial\omega}\right]g^{<}(\mathbf{p},\omega;\mathbf{X},T)\\&\qquad=-g^{<}(\mathbf{p},\omega;\mathbf{X},T)\Sigma^{>}(\mathbf{p},\omega;\mathbf{X},T)+g^{>}(\mathbf{p},\omega;\mathbf{X},T)\Sigma^{<}(\mathbf{p},\omega;\mathbf{X},T),\end{aligned}} \tag{11.13}$$

$$\boxed{\Sigma^{>}(\mathbf{p},\omega;\mathbf{X},T)=\int d\mathbf{x}dt e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}i\Sigma^{>}(\mathbf{x},t;\mathbf{X},T),\quad \Sigma^{<}(\mathbf{p},\omega;\mathbf{X},T)=\int d\mathbf{x}dt e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}[\pm i\Sigma^{<}(\mathbf{x},t;\mathbf{X},T)].} \tag{11.14}$$

Doing the similar steps for the equations (10.65) and (10.67), one can obtain the equation for $g^{>}(\mathbf{p},\omega;\mathbf{X},T)$ as,

$$\boxed{\begin{aligned}&\pm\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}-\nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}}+\frac{\partial U_{\text{eff}}(\mathbf{X},T)}{\partial T}\frac{\partial}{\partial\omega}\right]g^{>}(\mathbf{p},\omega;\mathbf{X},T)\\&=-g^{<}(\mathbf{p},\omega;\mathbf{X},T)\Sigma^{>}(\mathbf{p},\omega;\mathbf{X},T)+g^{>}(\mathbf{p},\omega;\mathbf{X},T)\Sigma^{<}(\mathbf{p},\omega;\mathbf{X},T).\end{aligned}} \tag{11.15}$$

In order to gain some insight into the result we have just obtained, we consider the Born collision approximation in which $\Sigma^{>}_{<}$ are given by (10.68), where this equation is written in terms of the variables $\mathbf{x},t,\mathbf{X},T$,

$$\begin{aligned}\Sigma^{>}_{<}(\mathbf{x},t;\mathbf{X},T)=\pm i^2\int d\bar{\mathbf{X}}d\bar{\mathbf{x}}\times v\left(\mathbf{X}+\frac{\mathbf{x}}{2}-\bar{\mathbf{X}}-\frac{\bar{\mathbf{x}}}{2}\right)v\left(\mathbf{X}-\frac{\mathbf{x}}{2}-\bar{\mathbf{X}}+\frac{\bar{\mathbf{x}}}{2}\right)\times g^{<}_{>}(-\bar{\mathbf{x}},-t;\bar{\mathbf{X}},T)\times\Big[g^{>}_{<}(\mathbf{x},t;\mathbf{X},T)g^{>}_{<}(\bar{\mathbf{x}},t;\bar{\mathbf{X}},T)\\\pm g^{>}_{<}\left(\bar{\mathbf{X}}+\frac{\bar{\mathbf{x}}}{2}-\mathbf{X}+\frac{\mathbf{x}}{2},t;\frac{\mathbf{X}+\bar{\mathbf{X}}}{2}+\frac{\bar{\mathbf{x}}-\mathbf{x}}{4},T\right)\times g^{>}_{<}\left(\mathbf{X}+\frac{\mathbf{x}}{2}-\bar{\mathbf{X}}+\frac{\bar{\mathbf{x}}}{2},t;\frac{\mathbf{X}+\bar{\mathbf{X}}}{2}+\frac{\mathbf{x}-\bar{\mathbf{x}}}{4},T\right)\Big]_{\mathbf{X}=\bar{\mathbf{X}},\mathbf{x}=\bar{\mathbf{x}}},\end{aligned} \tag{11.16}$$

where $\mathbf{x}_1 = \mathbf{X} + \mathbf{x}/2, \mathbf{x}_{1'} = \mathbf{X} - \mathbf{x}/2, \mathbf{x}_2 = \overline{\mathbf{X}} + \overline{\mathbf{x}}/2$ and $\mathbf{x}_{2'} = \overline{\mathbf{X}} - \overline{\mathbf{x}}/2$. If the disturbance varies very little within a distance on the order of the potential range, the second spatial argument of all the g's may be taken to be $\mathbf{X}$, i.e.,

$$\begin{aligned}\Sigma^{>}_{<}(\mathbf{x},t;\mathbf{X},T) = \pm i^2 \int \mathrm{d}\overline{\mathbf{X}}\mathrm{d}\overline{\mathbf{x}} \times v\left(\mathbf{X}+\frac{\mathbf{x}}{2}-\overline{\mathbf{X}}-\frac{\overline{\mathbf{x}}}{2}\right) v\left(\mathbf{X}-\frac{\mathbf{x}}{2}-\overline{\mathbf{X}}+\frac{\overline{\mathbf{x}}}{2}\right) \times g^{<}_{>}(-\overline{\mathbf{x}},-t;\overline{\mathbf{X}},T) \\ \times \left[g^{>}_{<}(\mathbf{x},t;\mathbf{X},T) g^{>}_{<}(\overline{\mathbf{x}},t;\overline{\mathbf{X}},T) \pm g^{>}_{<}\left(\overline{\mathbf{X}}+\frac{\overline{\mathbf{x}}}{2}-\mathbf{X}+\frac{\mathbf{x}}{2},t;\mathbf{X},T\right) g^{>}_{<}\left(\mathbf{X}+\frac{\mathbf{x}}{2}-\overline{\mathbf{X}}+\frac{\overline{\mathbf{x}}}{2},t;\mathbf{X},T\right)\right]_{\mathbf{X}=\overline{\mathbf{X}},\mathbf{x}=\overline{\mathbf{x}}}. \end{aligned} \tag{11.17}$$

Taking the Fourier transform of $\mathbf{x}, t$ gives,

$$\boxed{\begin{aligned}\Sigma^{>}_{<}(\mathbf{p},\omega;\mathbf{X},T) = \int \frac{\mathrm{d}\mathbf{p}'}{(2\pi)^3}\frac{\mathrm{d}\omega'}{2\pi}\frac{\mathrm{d}\overline{\mathbf{p}}}{(2\pi)^3}\frac{\mathrm{d}\overline{\omega}}{2\pi}\frac{\mathrm{d}\overline{\mathbf{p}}'}{(2\pi)^3}\frac{\mathrm{d}\overline{\omega}'}{2\pi} \times (2\pi)^4\delta(\mathbf{p}+\mathbf{p}'-\overline{\mathbf{p}}-\overline{\mathbf{p}}')\delta(\omega+\omega'-\overline{\omega}-\overline{\omega}') \\ \times \frac{1}{2}[v(\mathbf{p}-\overline{\mathbf{p}}) \pm v(\mathbf{p}-\overline{\mathbf{p}}')]^2 \times g^{<}_{>}(\mathbf{p}',\omega';\mathbf{X},T) g^{>}_{<}(\overline{\mathbf{p}},\overline{\omega};\mathbf{X},T) g^{>}_{<}(\overline{\mathbf{p}}',\overline{\omega}';\mathbf{X},T).\end{aligned}} \tag{11.18}$$

In interpreting Eq. (11.13) we should notice that $\Sigma^{>}(\mathbf{p},\omega;\mathbf{X},T)$ is the collision rate for a particle with momentum $\mathbf{p}$ and energy ω at $\mathbf{X},T$, while $\Sigma^{<}(\mathbf{p},\omega;\mathbf{X},T)$ is the rate of scattering into $\mathbf{p},\omega$ at the space time point $\mathbf{X},T$, assuming that the state is initially unoccupied. Therefore, the right-hand side of (11.13) is the net rate of change of the density of particles with momentum $\mathbf{p}$ and energy ω at $\mathbf{X},T$. The contributions $-\mathbf{p}\cdot\nabla_{\mathbf{X}} g^{<}$ and $\nabla_{\mathbf{X}} U_{\mathrm{eff}} \cdot \nabla_{\mathbf{p}} g^{<}$ to the rate of change of $g^{<}$ can also be recognized in the Boltzmann equation, see Eq. (9.27). They are, respectively, the result of the drift of particles into the volume element about $\mathbf{X}$ and the change in the momentum due to the average force acting on the particles at $\mathbf{X}$. The last term on the left-hand side of (11.13), $(\partial U_{\mathrm{eff}}/\partial T)\partial g^{<}/\partial\omega$, results from the change in the average energy of a particle at $\mathbf{X},T$ caused by the time variation of the potential field through which it moves. This term does not appear in the usual Boltzmann equation because this equation does not include the particle energy as an independent variable. Therefore, (11.13) has the same physical content as the usual Boltzmann equation. We subtract (11.13) from (11.15),

$$\left[\frac{\partial}{\partial T} + \frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m} - \nabla_{\mathbf{X}} U_{\mathrm{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}} + \frac{\partial U_{\mathrm{eff}}(\mathbf{X},T)}{\partial T}\frac{\partial}{\partial\omega}\right] \times [g^{>}(\mathbf{p},\omega;\mathbf{X},T) \mp g^{<}(\mathbf{p},\omega;\mathbf{X},T)] = 0. \tag{11.19}$$

Just as in the equilibrium case, we define a spectral function a by,

$$\boxed{a(\mathbf{p},\omega;\mathbf{X},T) = g^{>}(\mathbf{p},\omega;\mathbf{X},T) \mp g^{<}(\mathbf{p},\omega;\mathbf{X},T),} \tag{11.20}$$

thus one may write out the equation and the corresponding solution as,

$$\left[\frac{\partial}{\partial T} + \frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m} - \nabla_{\mathbf{X}} U_{\mathrm{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}} + \frac{\partial U_{\mathrm{eff}}(\mathbf{X},T)}{\partial T}\frac{\partial}{\partial\omega}\right] a(\mathbf{p},\omega;\mathbf{X},T) = 0, \quad a(\mathbf{p},\omega;\mathbf{X},T) = y\left(\omega - \frac{\mathbf{p}^2}{2m} - U_{\mathrm{eff}}(\mathbf{X},T)\right), \tag{11.21}$$

where y is an arbitrary function, since

$$\begin{aligned}&\frac{\partial y}{\partial T} + \frac{\partial U_{\mathrm{eff}}(\mathbf{X},T)}{\partial T}\frac{\partial y}{\partial\omega} + \frac{\mathbf{p}\cdot\nabla_{\mathbf{X}} y}{m} - \nabla_{\mathbf{X}} U_{\mathrm{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}} y \\ &= \frac{\partial y}{\partial W}\left[-\frac{\partial U_{\mathrm{eff}}(\mathbf{X},T)}{\partial T} + \frac{\partial U_{\mathrm{eff}}(\mathbf{X},T)}{\partial T} - \frac{\mathbf{p}\cdot\nabla_{\mathbf{X}} U_{\mathrm{eff}}(\mathbf{X},T)}{m} + \nabla_{\mathbf{X}} U_{\mathrm{eff}}(\mathbf{X},T)\cdot\frac{\mathbf{p}}{m}\right] = 0,\end{aligned} \tag{11.22}$$

where $W = \omega - \mathbf{p}^2/2m - U_{\mathrm{eff}}(\mathbf{X},T)$. To determine y one shall use the initial conditions and the equations of motion that as $T \to -\infty$ the functions $g^{<}(\mathbf{p},\omega;\mathbf{X},T)$ and $g^{>}(\mathbf{p},\omega;\mathbf{X},T)$ reduce to the equilibrium Green's functions $G^{>}(\mathbf{p},\omega)$ and $G^{<}(\mathbf{p},\omega)$.

Since (11.13), (11.15) and (11.18) are just extensions of the equilibrium Born collision approximation to a nonequilibrium situation, one must demand that as $T \to -\infty$, $a(\mathbf{p},\omega;\mathbf{X},T)$ reduce to the equilibrium $A(\mathbf{p},\omega)$, which emerges from the Born collision approximation. However, this equilibrium $A(\mathbf{p},\omega)$, which was discussed previously, is not a function only of $\omega - \mathbf{p}^2/2m$. Therefore, the $a(\mathbf{p},\omega;\mathbf{X},T)$ determined as a solution to (11.21) cannot possibly reduce to this $A(\mathbf{p},\omega)$ as $T \to -\infty$. Therefore, we must have made some mistake in our analysis, which would be corrected later. We do know one very simple $A(\mathbf{p},\omega)$, which is of the form of (11.21) or (7.54), namely the Hartree–Fock result:

$$A(\mathbf{p},\omega) = 2\pi\delta(\omega - E(\mathbf{p})), \quad E(\mathbf{p}) = \frac{\mathbf{p}^2}{2m} + nv. \tag{11.23}$$

If we take this to be the initial value of $a(\mathbf{p},\omega;\mathbf{X},T)$, we find from (11.21) that,

$$\boxed{a(\mathbf{p},\omega;\mathbf{X},T) = 2\pi\delta(\omega - E(\mathbf{p},\mathbf{X},T)), \quad E(\mathbf{p},\mathbf{X},T) = \frac{\mathbf{p}^2}{2m} + U_{\mathrm{eff}}(\mathbf{X},T).} \tag{11.24}$$

We now simplify the equation of motion (11.13) for $g^<(\mathbf{p},\omega;\mathbf{X},T)$ considerably. Assume that $g^<$ is of the form,

$$g^<(\mathbf{p},\omega;\mathbf{X},T) = a(\mathbf{p},\omega;\mathbf{X},T)f(\mathbf{p},\mathbf{X},T) = 2\pi\delta(\omega - E(\mathbf{p},\mathbf{X},T))f(\mathbf{p},\mathbf{X},T), \tag{11.25}$$

and therefore $g^>(\mathbf{p},\omega;\mathbf{X},T) = a(\mathbf{p},\omega;\mathbf{X},T)[1\pm f(\mathbf{p},\mathbf{X},T)]$. Here, $f(\mathbf{p},\mathbf{X},T)$ is the distribution function that appears in the Boltzmann equation, i.e., the density of particles with momentum $\mathbf{p}$ at $\mathbf{X},T$. The left side of (11.13) can be written,

$$\left[\frac{\partial}{\partial T} + \frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m} - \nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}} + \frac{\partial U_{\text{eff}}(\mathbf{X},T)}{\partial T}\frac{\partial}{\partial\omega}\right] a(\mathbf{p},\omega;\mathbf{X},T)f(\mathbf{p},\mathbf{X},T). \tag{11.26}$$

We have explicitly constructed $a(\mathbf{p},\omega;\mathbf{X},T)$ to commute with the differential operator appearing in (11.26). Therefore, (11.26) can just as well be written as,

$$a(\mathbf{p},\omega;\mathbf{X},T)\left[\frac{\partial}{\partial T} + \frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m} - \nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}}\right] f(\mathbf{p},\mathbf{X},T). \tag{11.27}$$

The right side of (11.13) is $a(\mathbf{p},\omega;\mathbf{X},T)\left[-f(\mathbf{p},\mathbf{X},T)\Sigma^>(\mathbf{p},\omega;\mathbf{X},T) + (1\pm f(\mathbf{p},\mathbf{X},T))\Sigma^<(\mathbf{p},\omega;\mathbf{X},T)\right]$. Therefore when we integrate (11.13) over all ω, it reduces to,

$$\begin{aligned}&\left[\frac{\partial}{\partial T} + \frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m} - \nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}}\right] f(\mathbf{p},\mathbf{X},T)\\ &- f(\mathbf{p},\mathbf{X},T)\Sigma^>(\mathbf{p},\omega = E(\mathbf{p},\mathbf{X},T);\mathbf{X},T) + [1\pm f(\mathbf{p},\mathbf{X},T)]\times\Sigma^<(\mathbf{p},\omega = E(\mathbf{p},\mathbf{X},T);\mathbf{X},T).\end{aligned} \tag{11.28}$$

By using the expressions (11.18), one obtains

$$\begin{aligned}&\left[\frac{\partial}{\partial T} + \frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m} - \nabla_{\mathbf{X}}U_{\text{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}}\right] f(\mathbf{p},\mathbf{X},T)\\ &= -\int\frac{d\mathbf{p}'}{(2\pi)^3}\frac{d\overline{\mathbf{p}}}{(2\pi)^3}\frac{d\overline{\mathbf{p}}'}{(2\pi)^3}\times(2\pi)^4\delta(\mathbf{p}+\mathbf{p}'-\overline{\mathbf{p}}-\overline{\mathbf{p}}')\times\delta\left(\frac{\mathbf{p}^2}{2m}+\frac{\mathbf{p}'^2}{2m}-\frac{\overline{\mathbf{p}}^2}{2m}-\frac{\overline{\mathbf{p}}'^2}{2m}\right)\\ &\times\frac{1}{2}[v(\mathbf{p}-\overline{\mathbf{p}})\mp v(\mathbf{p}-\overline{\mathbf{p}}')]^2\times\left[ff'(1\pm\overline{f})(1\pm\overline{f}') - (1\pm f)(1\pm f')\overline{f}\,\overline{f}'\right],\end{aligned} \tag{11.29}$$

where $f = f(\mathbf{p},\mathbf{X},T), f' = f(\mathbf{p}',\mathbf{X},T)$, etc. Except for the trivial substitution of U_{eff} for U, this is exactly the ordinary Boltzmann equation with Born approximation collision cross sections, see Eq. (9.27).

We derived a value for $a(\mathbf{p},\omega;\mathbf{X},T)$ previously that did not agree with the Born collision approximation from which we began. Since the Boltzmann equation purports to be nothing more than the extension of the Born collision approximation to the case in which there is a slowly varying external disturbance, this lack of agreement with the equilibrium analysis is indeed serious. We were trying to find an expansion of (11.4) that is valid in the limit in which all the functions involved vary slowly in the variables $\mathbf{X},T$. On the left side of (11.4) we held on to all terms of order $\partial/\partial T$ or $\nabla_{\mathbf{X}}$. However, in evaluating the right side of (11.4) we only considered terms that involved no space and time derivatives, we left out terms of order of $\partial/\partial T$ and $\nabla_{\mathbf{X}}$. This procedure is clearly inconsistent. The correct analysis would include all terms of order $\nabla_{\mathbf{X}}$ and $\partial/\partial T$ on both sides of (11.4). Let us reexamine the first two terms on the right side of (11.4). By employing exactly the same change of variables as we used earlier, we can write these terms as

$$\begin{aligned}&\int_{-\infty}^{t} d\bar{t}\,d\overline{\mathbf{x}}(\Sigma^> - \Sigma^<)\left(\mathbf{x}-\overline{\mathbf{x}},t-\bar{t};\mathbf{X}+\frac{\overline{\mathbf{x}}}{2},T+\frac{\bar{t}}{2}\right)\times g^<\left(\overline{\mathbf{x}},\bar{t};\mathbf{X}-\frac{\mathbf{x}-\overline{\mathbf{x}}}{2},T-\frac{t-\bar{t}}{2}\right)\\ &+\int_{t}^{\infty} d\bar{t}\,d\overline{\mathbf{x}}(\Sigma^> - \Sigma^<)\left(\mathbf{x}-\overline{\mathbf{x}},t-\bar{t};\mathbf{X}-\frac{\overline{\mathbf{x}}}{2},T-\frac{\bar{t}}{2}\right)\times g^<\left(\overline{\mathbf{x}},\bar{t};\mathbf{X}+\frac{\mathbf{x}-\overline{\mathbf{x}}}{2},T+\frac{t-\bar{t}}{2}\right),\end{aligned} \tag{11.30}$$

where $(\Sigma^> - \Sigma^<)(\mathbf{x},t;\mathbf{X},T) = \Sigma^>(\mathbf{x},t;\mathbf{X},T) - \Sigma^<(\mathbf{x},t;\mathbf{X},T)$. Because $\mathbf{x},\overline{\mathbf{x}}$ and $t,\bar{t}$ are small, compared to the characteristic distances and times over which the functions $g^<(\mathbf{p},\omega;\mathbf{X},T)$ and $\Sigma^<(\mathbf{p},\omega;\mathbf{X},T)$ vary, we can expand the various quantities that appear in the expression (11.30) as,

$$g^<\left(\overline{\mathbf{x}},\bar{t};\mathbf{X}-\frac{\mathbf{x}-\overline{\mathbf{x}}}{2},T-\frac{t-\bar{t}}{2}\right) \approx g^<\left(\overline{\mathbf{x}},\bar{t};\mathbf{X},T\right) - \left[\frac{\mathbf{x}-\overline{\mathbf{x}}}{2}\cdot\nabla_{\mathbf{X}} + \frac{t-\bar{t}}{2}\frac{\partial}{\partial T}\right] g^<\left(\overline{\mathbf{x}},\bar{t};\mathbf{X},T\right), \tag{11.31}$$

$$\begin{aligned}&\text{expression in (11.30) to order } \nabla_{\mathbf{X}} \text{ and } \partial/\partial T \text{ becomes} \approx \int_{-\infty}^{\infty} d\bar{t}\,d\overline{\mathbf{x}}(\Sigma^> - \Sigma^<)\left(\mathbf{x}-\overline{\mathbf{x}},t-\bar{t};\mathbf{X},T\right) g^<\left(\overline{\mathbf{x}},\bar{t};\mathbf{X},T\right)\\ &+\int_{-\infty}^{\infty} d\bar{t}\,d\overline{\mathbf{x}}\left[\left[\overline{\mathbf{x}}\cdot\nabla_{\mathbf{X}} + \bar{t}\frac{\partial}{\partial T} - (\mathbf{x}-\overline{\mathbf{x}})\cdot\nabla_{\mathbf{X}'} - (t-\bar{t})\frac{\partial}{\partial T'}\right]\times\sigma(\mathbf{x}-\overline{\mathbf{x}},t-\bar{t};\mathbf{X},T)g^<\left(\overline{\mathbf{x}},\bar{t};\mathbf{X}',T'\right)\right]_{\mathbf{X}=\mathbf{X}',T=T'},\end{aligned} \tag{11.32}$$

where,

$$\sigma(\mathbf{x},t;\mathbf{X},T)=\frac{1}{2}\frac{t}{|t|}(\Sigma^{>}-\Sigma^{<})(\mathbf{x},t;\mathbf{X},T). \tag{11.33}$$

The first integral in (11.30) was included in our earlier discussion; it appears on the right side of (11.12). The second integral was not included and it should be added to this right side. The last two terms in (11.4) also give an extra term:

$$-\int_{-\infty}^{\infty}\mathrm{d}\bar{t}\mathrm{d}\bar{\mathbf{x}}\left[\left[\bar{\mathbf{x}}\cdot\nabla_{\mathbf{X}}+\bar{t}\frac{\partial}{\partial T}-(\mathbf{x}-\bar{\mathbf{x}})\cdot\nabla_{\mathbf{X}'}-(t-\bar{t})\frac{\partial}{\partial T'}\right]\times b(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T)\Sigma^{<}\left(\bar{\mathbf{x}},\bar{t};\mathbf{X}',T'\right)\right]_{\mathbf{X}=\mathbf{X}',T=T'}, \tag{11.34}$$

where

$$b(\mathbf{x},t;\mathbf{X},T)=\frac{1}{2}\frac{t}{|t|}(g^{>}-g^{<})(\mathbf{x},t;\mathbf{X},T), \tag{11.35}$$

which also should be added to the right-hand side of (11.12). When these extra terms are included, this equation is correct to order $\nabla_{\mathbf{X}}$ and $\partial/\partial T$.

We derived the ordinary Boltzmann equation by taking the Fourier transform of (11.12) and hence finding (11.13). To obtain a generalized Boltzmann equation, we must add the Fourier transforms of these two extra terms to the right-hand side of (11.13). If we define $b(\mathbf{p},\omega;\mathbf{X},T)$ as the Fourier transform of $b(\mathbf{x},t;\mathbf{X},T)$ in the $\mathbf{x},t$ variables, we can write the transform of the term (11.34) as

$$\begin{aligned}
&-\int\mathrm{d}\mathbf{x}\mathrm{d}t\mathrm{d}\bar{\mathbf{x}}\mathrm{d}\bar{t}e^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}\left[\bar{\mathbf{x}}\cdot\nabla_{\mathbf{X}}+\bar{t}\frac{\partial}{\partial T}-(\mathbf{x}-\bar{\mathbf{x}})\cdot\nabla_{\mathbf{X}'}-(t-\bar{t})\frac{\partial}{\partial T'}\right]\\
&\times\underbrace{\int\frac{\mathrm{d}\mathbf{p}''}{(2\pi)^3}\frac{\mathrm{d}\omega''}{2\pi}e^{i\mathbf{p}''\cdot(\mathbf{x}-\bar{\mathbf{x}})-i\omega''(t-\bar{t})}b(\mathbf{p}'',\omega'';\mathbf{X},T)}_{=b(\mathbf{x}-\bar{\mathbf{x}},t-\bar{t};\mathbf{X},T)}\times\underbrace{\int\frac{\mathrm{d}\mathbf{p}'}{(2\pi)^3}\frac{\mathrm{d}\omega'}{2\pi}e^{i\mathbf{p}'\cdot\bar{\mathbf{x}}-i\omega'\bar{t}}\Sigma^{<}(\mathbf{p}',\omega';\mathbf{X}',T')}_{=\Sigma^{<}(\bar{\mathbf{x}},\bar{t};\mathbf{X}',T')}\\
&=\pm\left[-\nabla_{\mathbf{p}'}\cdot\nabla_{\mathbf{X}}+\frac{\partial}{\partial\omega'}\frac{\partial}{\partial T}+\nabla_{\mathbf{p}}\cdot\nabla_{\mathbf{X}'}-\frac{\partial}{\partial\omega}\frac{\partial}{\partial T'}\right]\times b(\mathbf{p},\omega;\mathbf{X},T)\Sigma^{<}(\mathbf{p}',\omega';\mathbf{X}',T')\Big|_{\mathbf{X}=\mathbf{X}',T=T',\mathbf{p}=\mathbf{p}',\omega=\omega'}.
\end{aligned} \tag{11.36}$$

In order to write expressions like this in a compact form, we define a generalized Poisson bracket,

$$\begin{aligned}
[X,Y]=&\frac{\partial X}{\partial\omega}(\mathbf{p},\omega;\mathbf{X},T)\frac{\partial Y}{\partial T}(\mathbf{p},\omega;\mathbf{X},T)-\frac{\partial X}{\partial T}(\mathbf{p},\omega;\mathbf{X},T)\frac{\partial Y}{\partial\omega}(\mathbf{p},\omega;\mathbf{X},T)\\
&-\nabla_{\mathbf{p}}X(\mathbf{p},\omega;\mathbf{X},T)\cdot\nabla_{\mathbf{X}}Y(\mathbf{p},\omega;\mathbf{X},T)+\nabla_{\mathbf{X}}X(\mathbf{p},\omega;\mathbf{X},T)\cdot\nabla_{\mathbf{p}}Y(\mathbf{p},\omega;\mathbf{X},T),
\end{aligned} \tag{11.37}$$

i.e.,

$$\boxed{[X,Y]=\frac{\partial X}{\partial\omega}\frac{\partial Y}{\partial T}-\frac{\partial X}{\partial T}\frac{\partial Y}{\partial\omega}-\nabla_{\mathbf{p}}X\cdot\nabla_{\mathbf{X}}Y+\nabla_{\mathbf{X}}X\cdot\nabla_{\mathbf{p}}Y.} \tag{11.38}$$

Using this Poisson bracket notation, we can write the Fourier transform of (11.34) as, $\mp[b,\Sigma^{<}]$. Similarly, the Fourier transform of the previously neglected term in (11.32) is $\pm[\sigma,g^{<}]$. By adding these extra two terms, we can correct (11.13) so that it includes all terms of order $\nabla_{\mathbf{X}}$ and $\partial/\partial T$, i.e.,

$$\boxed{\begin{aligned}
&\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}-\nabla_{\mathbf{X}}U_{\mathrm{eff}}(\mathbf{X},T)\cdot\nabla_{\mathbf{p}}+\frac{\partial U_{\mathrm{eff}}(\mathbf{X},T)}{\partial T}\frac{\partial}{\partial\omega}\right]g^{<}(\mathbf{p},\omega;\mathbf{X},T)-[\sigma,g^{<}]+[b,\Sigma^{<}]\\
&=-g^{<}(\mathbf{p},\omega;\mathbf{X},T)\Sigma^{>}(\mathbf{p},\omega;\mathbf{X},T)+g^{>}(\mathbf{p},\omega;\mathbf{X},T)\Sigma^{<}(\mathbf{p},\omega;\mathbf{X},T).
\end{aligned}} \tag{11.39}$$

Now, we have to evaluate the Fourier transforms $\sigma(\mathbf{p},\omega;\mathbf{X},T)$ and $b(\mathbf{p},\omega;\mathbf{X},T)$. The latter is given by,

$$\begin{aligned}
b(\mathbf{p},\omega;\mathbf{X},T)=&\int\mathrm{d}\mathbf{x}\mathrm{d}te^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}b(\mathbf{x},t;\mathbf{X},T)=\int\mathrm{d}\mathbf{x}\mathrm{d}te^{-i\mathbf{p}\cdot\mathbf{x}+i\omega t}\frac{t}{2|t|}[g^{>}(\mathbf{x},t;\mathbf{X},T)-g^{<}(\mathbf{x},t;\mathbf{X},T)]\\
=&\frac{1}{2i}\int\frac{\mathrm{d}\mathbf{x}\mathrm{d}t\mathrm{d}\mathbf{p}'\mathrm{d}\omega'}{(2\pi)^4}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}+i(\omega-\omega')t}a(\mathbf{p}',\omega';\mathbf{X},T)\frac{t}{|t|}=\frac{1}{2i}\int\frac{\mathrm{d}\omega'}{2\pi}e^{i(\omega-\omega')t}a(\mathbf{p},\omega';\mathbf{X},T)\frac{t}{|t|}.
\end{aligned} \tag{11.40}$$

Since the Fourier transform of $i[g^{>}-g^{<}]$ is $a(\mathbf{p},\omega;\mathbf{X},T)$, we can write,

$$b(\mathbf{p},\omega;\mathbf{X},T)=\frac{1}{2i}\int\frac{\mathrm{d}\omega'}{2\pi}a(\mathbf{p},\omega';\mathbf{X},T)\times\left[\int_0^{\infty}\mathrm{d}te^{i(\omega-\omega')t}-\int_{-\infty}^{0}\mathrm{d}te^{i(\omega-\omega')t}\right]=\mathcal{P}\int\frac{\mathrm{d}\omega'}{2\pi}\frac{a(\mathbf{p},\omega';\mathbf{X},T)}{\omega-\omega'}, \tag{11.41}$$

where $\mathcal{P}$ denotes the principal value integral.

Similar as in our discussion of the equilibrium Green's functions, we define,

$$g(\mathbf{p},z;\mathbf{X},T)=\mathcal{P}\int\frac{\mathrm{d}\omega'}{2\pi}\frac{a(\mathbf{p},\omega';\mathbf{X},T)}{z-\omega'},\tag{11.42}$$

i.e., $b(\mathbf{p},\omega;\mathbf{X},T)=\mathrm{Re}\,g(\mathbf{p},\omega;\mathbf{X},T)$. We also define an analogous nonequilibrium self-energy as

$$\Gamma(\mathbf{p},\omega;\mathbf{X},T)=\Sigma^{>}(\mathbf{p},\omega;\mathbf{X},T)\mp\Sigma^{<}(\mathbf{p},\omega;\mathbf{X},T),\quad \Sigma_{\mathrm{C}}(\mathbf{p},z;\mathbf{X},T)=\int\frac{\mathrm{d}\omega'}{2\pi}\frac{\Gamma(\mathbf{p},\omega';\mathbf{X},T)}{z-\omega'}.\tag{11.43}$$

By just the same argument we can see that $a(\mathbf{p},\omega;\mathbf{X},T)$, the Fourier transform of $[t/2|t|](\Sigma^{>}-\Sigma^{<})(\mathbf{x},t;\mathbf{X},T)$ is $\sigma(\mathbf{p},\omega;\mathbf{X},T)=\mathrm{Re}\,\Sigma_{\mathrm{C}}(\mathbf{p},\omega;\mathbf{X},T)$. Now, we can rewrite (11.39) in the form,

$$\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}-\nabla_{\mathbf{X}}U_{\mathrm{eff}}\cdot\nabla_{\mathbf{p}}+\frac{\partial U_{\mathrm{eff}}}{\partial T}\frac{\partial}{\partial\omega}\right]g^{<}-[\mathrm{Re}\,\Sigma_{\mathrm{C}},g^{<}]+[\mathrm{Re}\,g,\Sigma^{<}]=-\Sigma^{>}g^{<}+\Sigma^{<}g^{>}.\tag{11.44}$$

The last two terms on the left side of (11.44) are written in terms of the generalized Poisson bracket (11.37). This equation can be simplified in form a bit if we notice that the other terms on the left also form a Poisson bracket, i.e.,

$$\left[\frac{\partial}{\partial T}+\frac{\mathbf{p}\cdot\nabla_{\mathbf{X}}}{m}-\nabla_{\mathbf{X}}U_{\mathrm{eff}}\cdot\nabla_{\mathbf{p}}+\frac{\partial U_{\mathrm{eff}}}{\partial T}\frac{\partial}{\partial\omega}\right]g^{<}=\left[\omega-\frac{\mathbf{p}^2}{2m}-U_{\mathrm{eff}},g^{<}\right],\tag{11.45}$$

thus (11.44) becomes,

$$\boxed{\left[\omega-\frac{\mathbf{p}^2}{2m}-U_{\mathrm{eff}}-\mathrm{Re}\,\Sigma_{\mathrm{C}},g^{<}\right]+[\mathrm{Re}\,g,\Sigma^{<}]=-\Sigma^{>}g^{<}+\Sigma^{<}g^{>}.}\tag{11.46}$$

By exactly the same procedure we can derive the following equation of motion for $g^{>}$,

$$\boxed{\pm\left[\omega-\frac{\mathbf{p}^2}{2m}-U_{\mathrm{eff}}-\mathrm{Re}\,\Sigma_{\mathrm{C}},g^{>}\right]\pm[\mathrm{Re}\,g,\Sigma^{>}]=-\Sigma^{>}g^{<}+\Sigma^{<}g^{>}.}\tag{11.47}$$

Eqs. (11.46) and (11.47) are coupled integro-differential equations for the unknowns $g^{>}(\mathbf{p},\omega;\mathbf{X},T)$ and $g^{<}(\mathbf{p},\omega;\mathbf{X},T)$. The self-energies $\Sigma^{>}$ and $\Sigma^{<}$ are expressed in terms of $g^{>}$ and $g^{<}$ by the particular Green's function approximation being considered. Eqs. (11.46) and (11.47) are generally correct except for one rather trivial omission. So far, we have left the exchange term in Σ_{HF} out of our discussion. The direct (Hartree) term is included; it appears in $U_{\mathrm{eff}}(\mathbf{X},T)$. When $g^{<}(\mathbf{p},\omega;\mathbf{X},T)$ varies very little within distances of the order of the potential range, we can approximately evaluate as,

$$U_{\mathrm{eff}}(\mathbf{X},T)=U(\mathbf{X},T)+\int\frac{\mathrm{d}\mathbf{p}'}{(2\pi)^3}\frac{\mathrm{d}\omega'}{2\pi}\times\int\mathrm{d}\mathbf{X}'v(\mathbf{X}-\mathbf{X}')g^{<}(\mathbf{p}',\omega;\mathbf{X},T)=U(\mathbf{X},T)+\Sigma_{\mathrm{H}}(\mathbf{X},T).\tag{11.48}$$

With the inclusion of the exchange term in (11.46) and (11.47), $U_{\mathrm{eff}}(\mathbf{X},T)+\mathrm{Re}\,\Sigma_{\mathrm{C}}(\mathbf{p},\omega;\mathbf{X},T)\to U(\mathbf{X},T)+\mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T)$, where just as in the equilibrium case, the total self-energy is a sum of the Hartree–Fock and the collisional contribution,

$$\boxed{\begin{aligned}\mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T)&=\Sigma_{\mathrm{HF}}(\mathbf{p},\mathbf{X},T)+\mathrm{Re}\,\Sigma_{\mathrm{C}}(\mathbf{p},\omega;\mathbf{X},T)\\&=\int\frac{\mathrm{d}\mathbf{p}'}{(2\pi)^3}\frac{\mathrm{d}\omega'}{2\pi}[v\pm v(\mathbf{p}-\mathbf{p}')]g^{<}(\mathbf{p}',\omega';\mathbf{X},T)+\mathrm{Re}\,\Sigma_{\mathrm{C}}(\mathbf{p},\omega;\mathbf{X},T),\quad v=\int\mathrm{d}\mathbf{x}v(\mathbf{x}).\end{aligned}}\tag{11.49}$$

When (11.46) and (11.47) are modified via (11.49), they are exact for slowly varying disturbances.

The generalized Boltzmann equations can be integrated partially. Notice that the collision term on the right side of (11.47) is exactly the same as the collision term in (11.46). Therefore, when we subtract these two equations,

$$\left[\omega-\frac{\mathbf{p}^2}{2m}-U(\mathbf{X},T)-\mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T),a(\mathbf{p},\omega;\mathbf{X},T)\right]+[\mathrm{Re}\,g(\mathbf{p},\omega;\mathbf{X},T),\Gamma(\mathbf{p},\omega;\mathbf{X},T)]=0,\tag{11.50}$$

where $a=g^{>}\mp g^{<},\Gamma=\Sigma^{>}\mp\Sigma^{<}$. Equation (11.50) may be integrated simply. In fact, the solution to (11.50) gives almost exactly the same evaluation as in the equilibrium case. In equilibrium,

$$G(\mathbf{p},z)=\frac{1}{z-\mathbf{p}^2/2m-\Sigma(\mathbf{p},z)},\tag{11.51}$$

and therefore,

$$G(\mathbf{p},\omega-i0^{+})=\mathrm{Re}\,G(\mathbf{p},\omega)+\frac{i}{2}A(\mathbf{p},\omega)=\frac{1}{\mathrm{Re}\,G^{-1}(\mathbf{p},\omega)-i\Gamma(\mathbf{p},\omega)/2},\tag{11.52}$$

where $\mathrm{Re}G^{-1}$ is an abbreviation for $\omega - \mathbf{p}^2/2m - \Sigma(\mathbf{p},\omega)$. Also,

$$G(\mathbf{p},\omega+i0^+) = \mathrm{Re}G(\mathbf{p},\omega) - \frac{i}{2}A(\mathbf{p},\omega) = \frac{1}{\mathrm{Re}G^{-1}(\mathbf{p},\omega)+i\Gamma(\mathbf{p},\omega)/2}, \tag{11.53}$$

$$\mathrm{Re}G(\mathbf{p},\omega) = \frac{\mathrm{Re}G^{-1}(\mathbf{p},\omega)}{[\mathrm{Re}G^{-1}(\mathbf{p},\omega)]^2+[\Gamma(\mathbf{p},\omega)/2]^2}, \quad A(\mathbf{p},\omega) = \frac{\Gamma(\mathbf{p},\omega)}{[\mathrm{Re}G^{-1}(\mathbf{p},\omega)]^2+[\Gamma(\mathbf{p},\omega)/2]^2}. \tag{11.54}$$

Let us see whether there is a similar solution to (11.50) by trying

$$g(\mathbf{p},z;\mathbf{X},T) = \frac{1}{z-\mathbf{p}^2/2m-U(\mathbf{X},T)-\Sigma(\mathbf{p},z;\mathbf{X},T)}, \tag{11.55}$$

then,

$$\begin{aligned} a(\mathbf{p},\omega;\mathbf{X},T) &= \frac{1}{i}\left[\frac{1}{\mathrm{Re}\,g^{-1}(\mathbf{p},\omega;\mathbf{X},T)-(i/2)\Gamma(\mathbf{p},\omega;\mathbf{X},T)} - \frac{1}{\mathrm{Re}\,g^{-1}(\mathbf{p},\omega;\mathbf{X},T)+(i/2)\Gamma(\mathbf{p},\omega;\mathbf{X},T)}\right] \\ &= \frac{\Gamma(\mathbf{p},\omega;\mathbf{X},T)}{[\mathrm{Re}\,g^{-1}(\mathbf{p},\omega;\mathbf{X},T)]^2+[\Gamma(\mathbf{p},\omega;\mathbf{X},T)/2]^2}, \end{aligned} \tag{11.56}$$

$$\begin{aligned} \mathrm{Re}\,g(\mathbf{p},\omega;\mathbf{X},T) &= \frac{1}{2}\left[\frac{1}{\mathrm{Re}\,g^{-1}(\mathbf{p},\omega;\mathbf{X},T)-(i/2)\Gamma(\mathbf{p},\omega;\mathbf{X},T)} + \frac{1}{\mathrm{Re}\,g^{-1}(\mathbf{p},\omega;\mathbf{X},T)+(i/2)\Gamma(\mathbf{p},\omega;\mathbf{X},T)}\right] \\ &= \frac{\mathrm{Re}\,g^{-1}(\mathbf{p},\omega;\mathbf{X},T)}{[\mathrm{Re}\,g^{-1}(\mathbf{p},\omega;\mathbf{X},T)]^2+[\Gamma(\mathbf{p},\omega;\mathbf{X},T)/2]^2}, \end{aligned} \tag{11.57}$$

where

$$\mathrm{Re}\,g^{-1}(\mathbf{p},\omega;\mathbf{X},T) = \omega - \frac{\mathbf{p}^2}{2m} - U(\mathbf{X},T) - \Sigma(\mathbf{p},\omega;\mathbf{X},T). \tag{11.58}$$

The left side of (11.50) becomes,

$$\begin{aligned} [\mathrm{Re}\,g^{-1},a]+[\mathrm{Re}\,g,\Gamma] &= \frac{1}{i}\left[\mathrm{Re}\,g^{-1},\frac{1}{\mathrm{Re}\,g^{-1}-i\Gamma/2}\right] - \frac{1}{i}\left[\mathrm{Re}\,g^{-1},\frac{1}{\mathrm{Re}\,g^{-1}+i\Gamma/2}\right] \\ &\quad + \frac{1}{2}\left[\frac{1}{\mathrm{Re}\,g^{-1}-i\Gamma/2},\Gamma\right] + \frac{1}{2}\left[\frac{1}{\mathrm{Re}\,g^{-1}+i\Gamma/2},\Gamma\right]. \end{aligned} \tag{11.59}$$

Like the commutator, the Poisson bracket has the property $[A,B] = -[B,A]$. Hence expression (11.59) may be rearranged in the form,

$$\frac{1}{i}\left[\mathrm{Re}\,g^{-1}-\frac{i}{2}\Gamma,\frac{1}{\mathrm{Re}\,g^{-1}-i\Gamma/2}\right] - \frac{1}{i}\left[\mathrm{Re}\,g^{-1}+\frac{i}{2}\Gamma,\frac{1}{\mathrm{Re}\,g^{-1}+i\Gamma/2}\right]. \tag{11.60}$$

Therefore, expression (11.59) is in fact zero, proving that (11.55), (11.56), (11.57) and (11.58) together form a solution to (11.59). Since the solution (11.55) is of exactly the same form as the equilibrium solution, it must reduce to the equilibrium solution as $T \to -\infty$. Therefore, it satisfies the initial condition on the equation of motion.

To sum up, the equation of motion,

$$\boxed{\begin{aligned} &\left[\omega - \frac{\mathbf{p}^2}{2m} - U(\mathbf{X},T) - \mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T), g^<(\mathbf{p},\omega;\mathbf{X},T)\right] + [\mathrm{Re}\,g(\mathbf{p},\omega;\mathbf{X},T),\Sigma^<(\mathbf{p},\omega;\mathbf{X},T)] \\ &= -\Sigma^>(\mathbf{p},\omega;\mathbf{X},T)g^<(\mathbf{p},\omega;\mathbf{X},T) + \Sigma^<(\mathbf{p},\omega;\mathbf{X},T)g^>(\mathbf{p},\omega;\mathbf{X},T) \end{aligned}} \tag{11.61}$$

provides an exact description of the response to slowly varying disturbances. All the quantities appearing in this equation may be expressed in terms of $g^>$ and $g^<$. In particular, $\Sigma^>$ and $\Sigma^<$ are defined by a Green's function approximation that gives the self-energy in terms of $g^>$ and $g^<$. The lowest-order approximation of this kind is given by (11.14). Both $g^>$ and $g^<$ are related to g by,

$$\int \frac{\mathrm{d}\omega}{2\pi}\frac{g^>(\mathbf{p},\omega;\mathbf{X},T) \mp g^<(\mathbf{p},\omega;\mathbf{X},T)}{z-\omega} = g(\mathbf{p},z;\mathbf{X},T) = \frac{1}{z-\mathbf{p}^2/2m-U(\mathbf{X},T)-\Sigma(\mathbf{p},z;\mathbf{X},T)}, \tag{11.62}$$

which is exactly the same relation as defines the equilibrium Green's functions. To go from (11.61) back to the ordinary Boltzmann equation with Born approximation cross sections, we replace $\Sigma^>$ and $\Sigma^<$ on the right side of (11.61) by the approximations (11.18). On the left side of (11.61), however, we must employ the approximations $\Sigma^> = \Sigma^< = \Sigma = 0$. Since the left side of (11.61) determines the result (11.56) for a, we must therefore replace Σ and Γ in (11.62) by zero. Then we get $a = 2\pi\delta(\omega - \mathbf{p}^2/2m - U(\mathbf{X},T))$, this is the ordinary Boltzmann equation. The ordinary Boltzmann equation emerges then from an approximation in which the self-energies that appear on the left side of (11.61) are handled

differently from those which appear on the right. One can see that these two appearances of the self-energy Σ play a very different physical role in the description of transport phenomena. The $\Sigma^>$ and $\Sigma^<$ on the right side of (11.61) describe the dynamical effect of collisions, i.e., how the collisions transfer particles from one energy-momentum configuration to another. On the other hand, the Σ's on the left side of (11.61) describe the kinetic effects of the potential, i.e., how the potential changes the energy-momentum (dispersion) relation from that of free particles, $\omega = \mathbf{p}^2/2m + U$, to the more complex spectrum (11.62). Because these two effects of Σ are physically so different, we should not be surprised to find that we can independently approximate the kinetic effects of Σ and the dynamic effects of Σ. The more general equation (11.61) includes the effects of the potential on the motion of particles even between collisions. These effects arise from several different sources. When the system is fairly dense, the particles never get away from the other particles in the system. Therefore, we cannot ever really think of the particles as being "in between collisions". Quantum mechanically, the wave functions of the particles are sufficiently smeared out so that there is always some overlap of wave functions; the particle is always colliding. Also, the particle always retains some memory of the collisions it has experienced through its correlations with other particles in the system. This memory is also contained in its energy-momentum relation. Equations (11.61) and (11.62) can be used to describe all types of transport phenomena.

As the final example, we derive the transport equation for a Fermi liquid. The nonequilibrium theory described previously reduces to a particularly simple form for a system of Fermions very close to zero temperature. To see this, let us define a "local occupation number" $f(\mathbf{p},\omega;\mathbf{X},T)$ by writing

$$g^<(\mathbf{p},\omega;\mathbf{X},T) = a(\mathbf{p},\omega;\mathbf{X},T) f(\mathbf{p},\omega;\mathbf{X},T), \quad a(\mathbf{p},\omega;\mathbf{X},T) = g^>(\mathbf{p},\omega;\mathbf{X},T) \mp g^<(\mathbf{p},\omega;\mathbf{X},T). \tag{11.63}$$

In equilibrium, at zero temperature, $f(\mathbf{p},\omega;\mathbf{X},T) \to f(\omega) = \Theta(\mu-\omega)$. At very low temperatures f differs from 0 or 1 only for ω very near to μ. We assume that f still has this form at low temperatures, even in the presence of a disturbance. That is, we assume that there exists a $\mu(\mathbf{X},T)$ such that $f(\mathbf{p},\omega;\mathbf{X},T) = 0$ for ω appreciably greater than $\mu(\mathbf{X},T)$, and $f(\mathbf{p},\omega;\mathbf{X},T) = 1$ for ω appreciably less than μ. The only frequencies for which the local occupation number, $f(\mathbf{p},\omega;\mathbf{X},T)$, is different from zero or one are those within an infinitesimal range of $\mu(\mathbf{X},T)$. This dependence of f on ω is essentially what we mean by "low temperature" for a nonequilibrium system.

There is one simplification which makes this low-temperature system rather tractable: For ω near μ, the lifetime Γ becomes vanishingly small. At zero temperature in equilibrium, we have

$$\Sigma^>(\mathbf{p},\omega;\mathbf{X},T) = 0, \quad \omega < \mu(\mathbf{X},T); \quad \Sigma^<(\mathbf{p},\omega;\mathbf{X},T) = 0, \quad \omega > \mu(\mathbf{X},T), \tag{11.64}$$

when the system is very little excited from its zero-temperature state. Therefore, for situations near zero temperature, we shall take both $\Sigma^>$ and $\Sigma^<$ to be very small at those frequencies near μ, for which the occupation numbers $f(\mathbf{p},\omega;\mathbf{X},T)$ differ from 0 or 1. This approximation involves an assumption about the continuity of $\Sigma^>$ and $\Sigma^<$ at $\omega = \mu$. The continuity can be proved in all orders of perturbation theory, but it is not necessarily true for situations, such as the superconducting state, in which perturbation theory is not valid. Therefore, the discussion in the remainder of this section applies only to so-called "normal" Fermi systems and not to the superconductor. If $\Sigma^>$ and $\Sigma^<$ are both negligible for ω near μ, then in this region the Boltzmann equation (11.61) becomes,

$$\boxed{\left[\omega - \frac{\mathbf{p}^2}{2m} - U(\mathbf{X},T) - \mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T), a(\mathbf{p},\omega;\mathbf{X},T) f(\mathbf{p},\omega;\mathbf{X},T)\right] = 0, \quad \omega \approx \mu.} \tag{11.65}$$

We may verify that our assumptions about f for ω appreciably greater or less than $\mu(\mathbf{X},T)$ lead to a consistent solution of the Boltzmann equation. First if ω is appreciably less than μ, then from the assumption $f = 1$ we have,

$$\Sigma^> = 0, \quad \Sigma^< = \Gamma, \quad g^> = 0, \quad g^< = a. \tag{11.66}$$

When we substitute this solution into the Boltzmann equation (11.61), then Eq. (11.50) satisfied by a will be obtained, this means (11.66) is a consistent solution of (11.61) for ω appreciably less than μ. For ω appreciably greater than μ, the solution $g^< = \Sigma^< = 0$, which follows from the assumption $f = 0$, trivially satisfies (11.61). For all ω, $a(\mathbf{p},\omega;\mathbf{X},T)$ is given by (11.56). When ω is close to μ, we have $\Gamma(\mathbf{p},\omega;\mathbf{X},T) = \Sigma^>(\mathbf{p},\omega;\mathbf{X},T) \mp \Sigma^<(\mathbf{p},\omega;\mathbf{X},T) \to 0$, and a becomes

$$a(\mathbf{p},\omega;\mathbf{X},T) = 2\pi\delta\left(\omega - \frac{\mathbf{p}^2}{2m} - U(\mathbf{X},T) - \mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T)\right). \tag{11.67}$$

Note that at $\omega = \mu(\mathbf{X},T)$,

$$\frac{\partial}{\partial\omega}\mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T) = \frac{\partial}{\partial\omega}\int\frac{\mathrm{d}\omega'}{2\pi}\frac{\Gamma(\mathbf{p},\omega';\mathbf{X},T)}{\omega-\omega'} = -\int\frac{\mathrm{d}\omega'}{2\pi}\frac{\Gamma(\mathbf{p},\omega';\mathbf{X},T)}{(\mu-\omega')^2} < 0, \tag{11.68}$$

since Γ is a positive function. By continuity, $\partial\mathrm{Re}\,\Sigma/\partial\omega < 0$ for all ω near μ. Therefore, the argument of the delta function

in (11.67) is a monotonically increasing function of ω for all ω near μ. It follows then that for every $\mathbf{p},\mathbf{X},T$ there exists just one root of,

$$\omega = \frac{\mathbf{p}^2}{2m} + U(\mathbf{X},T) + \mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T). \tag{11.69}$$

Let us write this solution as $\omega = E(\mathbf{p},\mathbf{X},T) + U(\mathbf{X},T)$, where

$$\boxed{E(\mathbf{p},\mathbf{X},T) = \frac{\mathbf{p}^2}{2m} + \mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T)\Big|_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)}.} \tag{11.70}$$

In equilibrium states $E(\mathbf{p},\mathbf{X},T)$ reduces to $E(\mathbf{p})$. Because the response to the disturbance is primarily a change in the occupation of single particle levels with ω near μ, the response manifests itself mostly for momenta such that $E(\mathbf{p}) \approx \mu$. We know that there exists a unique momentum p_{F} (Fermi momentum) such that $E(p_{\mathrm{F}}) = \mu$. The two basic assumptions that go into this theory are the existence of a unique Fermi momentum and the smooth variation of $\Sigma^{>}$ and $\Sigma^{<}$ near $\omega = \mu$. Whenever these two assumptions are satisfied, the rest of our statements will hold for a Fermi system at sufficiently low temperatures, in which the disturbance varies very slowly in space and time. We can combine (11.65) and (11.67) into the form,

$$\boxed{\left[\omega - \frac{\mathbf{p}^2}{2m} - U - \mathrm{Re}\Sigma, 2\pi\delta\left(\omega - \frac{\mathbf{p}^2}{2m} - U - \mathrm{Re}\,\Sigma\right) f(\mathbf{p},\omega;\mathbf{X},T)\right] = 0, \quad \omega \approx \mu.} \tag{11.71}$$

Clearly one needs not consider the general $f(\mathbf{p},\omega;\mathbf{X},T)$ but only the simpler distribution function,

$$\boxed{n(\mathbf{p},\mathbf{X},T) = f(\mathbf{p},\omega;\mathbf{X},T)|_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)}.} \tag{11.72}$$

The symbol $n(\mathbf{p},\mathbf{X},T)$ for the quasi-particle distribution function, rather than $f(\mathbf{p},\mathbf{X},T)$, is conventional in the literature of low temperature Fermi systems.

We interpret $n(\mathbf{p},\mathbf{X},T)$ as the density of quasi-particles with momentum $\mathbf{p}$ at the space-time point $\mathbf{X},T$. As we proceed we shall find that these quasi-particles behave very much like a system of weakly interacting particles. For example, the quasi-particle distribution function obeys a simple Boltzmann equation. To derive this we use the fact that,

$$\left[\omega - \frac{\mathbf{p}^2}{2m} - U - \mathrm{Re}\,\Sigma, 2\pi\delta\left(\omega - \frac{\mathbf{p}^2}{2m} - U - \mathrm{Re}\,\Sigma\right)\right] = 0, \tag{11.73}$$

to rewrite (11.71) in the form,

$$2\pi\delta\left(\omega - \frac{\mathbf{p}^2}{2m} - U - \Sigma\right)\left[\omega - \frac{\mathbf{p}^2}{2m} - U - \Sigma, n\right] = 0. \tag{11.74}$$

Since we are assuming that $\Sigma(\mathbf{p},z;\mathbf{X},T)$ is real near $z = \mu$, we shall drop the "Re" in $\mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{X},T)$ henceforth. First notice that,

$$\delta\left(\omega - \frac{\mathbf{p}^2}{2m} - U - \Sigma\right) = \frac{\delta(\omega - U(\mathbf{X},T) - \Sigma(\mathbf{p},\mathbf{X},T))}{1 - \partial\Sigma(\mathbf{p},\omega;\mathbf{X},T)/\partial\omega}. \tag{11.75}$$

Thus,

$$\frac{2\pi\delta(\omega - U(\mathbf{X},T) - \Sigma(\mathbf{p},\mathbf{X},T))}{1 - \partial\Sigma(\mathbf{p},\omega;\mathbf{X},T)/\partial\omega}\left[\left[1 - \frac{\partial\Sigma(\mathbf{p},\omega;\mathbf{X},T)}{\partial\omega}\right]\frac{\partial n(\mathbf{p},\mathbf{X},T)}{\partial T} + \nabla_{\mathbf{p}}\left[\frac{\mathbf{p}^2}{2m} + U(\mathbf{X},T) + \Sigma(\mathbf{p},\omega;\mathbf{X},T)\right]\cdot\nabla_{\mathbf{X}} n(\mathbf{p},\mathbf{X},T)\right.$$
$$\left. - \nabla_{\mathbf{X}}\left[\frac{\mathbf{p}^2}{2m} + U(\mathbf{X},T) + \Sigma(\mathbf{p},\omega;\mathbf{X},T)\right]\cdot\nabla_{\mathbf{p}} n(\mathbf{p},\mathbf{X},T)\right] = 0, \tag{11.76}$$

where

$$\left[\nabla_{\mathbf{p}}\left[\frac{\mathbf{p}^2}{2m} + U(\mathbf{X},T) + \Sigma(\mathbf{p},\omega;\mathbf{X},T)\right]\right]_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)} = \left(\frac{\mathbf{p}}{m} + \frac{\partial\Sigma}{\partial\mathbf{p}}\right)_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)}. \tag{11.77}$$

Since,

$$E(\mathbf{p},\mathbf{X},T) = \frac{\mathbf{p}^2}{2m} + \Sigma(\mathbf{p},\underbrace{E(\mathbf{p},\mathbf{X},T) + U(\mathbf{X},T)}_{\omega};\mathbf{X},T), \tag{11.78}$$

we have

$$\frac{\partial E}{\partial\mathbf{p}} = \frac{\mathbf{p}}{m} + \frac{\partial\Sigma}{\partial\mathbf{p}} + \frac{\partial\Sigma}{\partial\omega}\frac{\partial\omega}{\partial\mathbf{p}}. \tag{11.79}$$

Consequently,

$$\left[\nabla_{\mathbf{p}}\left[\frac{\mathbf{p}^2}{2m}+U(\mathbf{X},T)+\Sigma(\mathbf{p},\omega;\mathbf{X},T)\right]\right]_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)}=\left(\frac{\partial E}{\partial\mathbf{p}}-\frac{\partial\Sigma}{\partial\mathbf{p}}-\frac{\partial\Sigma}{\partial\omega}\frac{\partial\omega}{\partial\mathbf{p}}+\frac{\partial\Sigma}{\partial\mathbf{p}}\right)_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)}$$
$$=\left(\frac{\partial E}{\partial\mathbf{p}}-\frac{\partial\Sigma}{\partial\omega}\frac{\partial\omega}{\partial\mathbf{p}}\right)_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)}=\nabla_{\mathbf{p}}E(\mathbf{p},\mathbf{X},T)-\nabla_{\mathbf{p}}E(\mathbf{p},\mathbf{X},T)\left.\frac{\partial\Sigma(\mathbf{p},\omega;\mathbf{X},T)}{\partial\omega}\right|_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)}. \tag{11.80}$$

Similarly,

$$\left[\nabla_{\mathbf{X}}\left[\frac{\mathbf{p}^2}{2m}+U(\mathbf{X},T)+\Sigma(\mathbf{p},\omega;\mathbf{X},T)\right]\right]_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)}$$
$$=\nabla_{\mathbf{X}}[E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)]\left[1-\left.\frac{\partial\Sigma(\mathbf{p},\omega;\mathbf{X},T)}{\partial\omega}\right]_{\omega=E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)}\right. . \tag{11.81}$$

Therefore, (11.76) can be written in the much simpler form for $\omega\approx\mu$,

$$2\pi\delta(\omega-E(\mathbf{p},\mathbf{X},T))\times\left[\frac{\partial n(\mathbf{p},\mathbf{X},T)}{\partial T}+\nabla_{\mathbf{p}}E(\mathbf{p},\mathbf{X},T)\cdot\nabla_{\mathbf{X}}n(\mathbf{p},\mathbf{X},T)-\nabla_{\mathbf{X}}[E(\mathbf{p},\mathbf{X},T)+U(\mathbf{X},T)]\cdot\nabla_{\mathbf{p}}n(\mathbf{p},\mathbf{X},T)\right]=0, \tag{11.82}$$

indicating that the quasi-particle distribution function satisfies the Boltzmann equation,

$$\boxed{\frac{\partial n}{\partial T}+\nabla_{\mathbf{p}}E\cdot\nabla_{\mathbf{X}}n-\nabla_{\mathbf{X}}E\cdot\nabla_{\mathbf{p}}n-\nabla_{\mathbf{X}}U\cdot\nabla_{\mathbf{p}}n=0.} \tag{11.83}$$

L Extension: Schwinger–Keldysh Contour

Relevant Reference:

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- L. Keldysh, *Diagram Technique for Nonequilibrium Processes*, Sov. Phys. JETP **20**, 1018 (1965).
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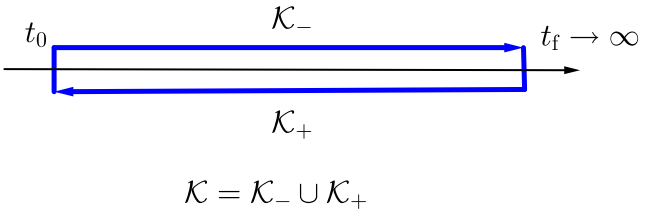

Fig. O: Closed-time paths (Schwinger–Keldysh contour).

The energy-momentum spectrum $\omega(\mathbf{p})$ in the Kadanoff–Baym equations is intrinsically non-relativistic. This introduces a potential drawback of the approach in situations where the relativistic effects are strong enough, e.g., in ultra-relativistic heavy ion collisions in nuclear physics.[8] An extension for the Kadanoff–Baym equations is the closed-time-path Green's function (CTPGF) field theory. Besides the well-behaved relativistic covariant energy-momentum in the CTPGF, it adopts similar analytical continuation as in the Kadanoff–Baym equations, see, e.g., Fig. O. Such contour is frequently called the Schwinger–Keldysh contour, and the technique is often abbreviated as the "in–in" formalism. Both Kadanoff–Baym equations and the CTPGF theories could be applied to problems far from equilibrium, they have also potential applications in issues like gauge/string duality and hydrodynamics,[9] the quantum open systems[10] and the non-Gaussian fluctuations/correlations[11] in early universe.

[8] See, e.g., O. Buss et al., *Transport-theoretical Description of Nuclear Reactions*, Phys. Rep. **1**, 124 (2012).
[9] J. Solana et al., *Gauge / String Duality, Hot QCD and Heavy Ion Collisions*, Cambridge University Press, 2014, Chapters 7 and 8.
[10] L. Sieberer, M. Buchhold, and S. Diehl, *Keldysh Field Theory for Driven Open Quantum Systems*, Rep. Prog. Phys. **79**, 096001 (2016).
[11] See, e.g., S. Weinberg, *Quantum Contributions to Cosmological Correlations*, Phys. Rev. D **72**, 043514 (2005).