Notes on Quantum many particle system

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This is largely a recap of the fantastic textbook *Quantum theory of many-particle systems*, by Alexandre L.Fetter and John Dirk Walecka. Therefore, by all means, please don't read this note, read the book instead.

This is still being updated.

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1 Second quantization

1.1 Degenerate electron gas

Let us consider an interacting electron gas with a uniformly distributed positive background. Let us assume the system to be a cubic box with sides of length L with periodic boundary conditions. Then the one partile eigenstates would be

$$\psi_{\boldsymbol{k}\sigma}(\boldsymbol{x}) = V^{-\frac{1}{2}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\eta_\sigma, \quad \boldsymbol{k} = \frac{2\pi\boldsymbol{n}}{L}, \boldsymbol{n} = (n_1, n_2, n_3) \in \mathbb{Z}^3, \quad \sigma \in \{\uparrow, \downarrow\} \tag{1.1}$$

Here $V = L^3$ is the volume of the box, η_σ is

$$\eta_\uparrow = (1,0)^T, \quad \eta_\uparrow = (0,1)^T$$

respresents the spin (up or down) of the electron.

The N-particle Hamiltonian would be

$$H = H_{el} + H_b + H_{el-b} \tag{1.2}$$

where H_{el} is the Hamiltonian for the electrons, H_b is the Hamiltonian for the background, H_{el-b} is the interaction energy between the electrons and the positive background:

$$H_{el} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2}e^2 \sum_{i\neq j}^{N} \frac{e^{-\mu|\boldsymbol{r}_i - \boldsymbol{r}_j|}}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} \tag{1.3}$$

$$H_b = \frac{1}{2}e^2 \iint d^3x d^3x' \frac{n(\boldsymbol{x}) n(\boldsymbol{x}') e^{-\mu|\boldsymbol{x}-\boldsymbol{x}'|}}{|\boldsymbol{x}-\boldsymbol{x}'|} \tag{1.4}$$

$$H_{el-b} = -e^2 \sum_{i=1}^{N} \int d^3x \frac{n(\boldsymbol{x}) e^{-\mu|\boldsymbol{x}-\boldsymbol{r}_i|}}{|\boldsymbol{x}-\boldsymbol{r}_i|} \tag{1.5}$$

We have inserted μ to gurantee the integral to be well-defined, and we will take $\mu \to 0$ in the end. We are interested in the following *thermodynamic limit*: what happens when $N \to \infty, V \to \infty$, but $n = N/V$ constant. The basic physical picture is that H_{el}, H_b, H_{el-b} all diverge in the above limit, but since the entire system is neutral, the sum of these three terms must remain meaningful in this limit. This has been mathematically rigorously justified in various mathematical literature. You'll also see this in a formal flavor in the following calculations.

Since we have $n(\boldsymbol{x}) = N/V$ being a constant, then we have

$$H_b = \frac{1}{2}\mathrm{e}^2 \left(\frac{N}{V}\right)^2 \iint \mathrm{d}^3x\mathrm{d}^3x' \frac{\mathrm{e}^{-\mu|\boldsymbol{x}-\boldsymbol{x}'|}}{|\boldsymbol{x}-\boldsymbol{x}'|} = \frac{1}{2}e^2 \left(\frac{N}{V}\right)^2 \int \mathrm{d}^3x \int \mathrm{d}^3z \frac{e^{-\mu z}}{z} = \frac{1}{2}e^2 \frac{N^2}{V}\frac{4\pi}{\mu^2} \tag{1.6}$$

and

$$H_{el-b} = -e^2 \sum_{i=1}^{N} \frac{N}{V} \int \mathrm{d}^3x \frac{e^{-\mu|\boldsymbol{x}-\boldsymbol{r}_i|}}{|\boldsymbol{x}-\boldsymbol{r}_i|} = -e^2 \sum_{i=1}^{N} \frac{N}{V} \int \mathrm{d}^3z \frac{e^{-\mu z}}{z} = -e^2 \frac{N^2}{V}\frac{4\pi}{\mu^2} \tag{1.7}$$

Using second quantization, one can derive that (left as an exercise)

$$\hat{H}_{el} = \sum_{\boldsymbol{k}\sigma} \frac{\hbar^2 k^2}{2m} a^\dagger_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} + \frac{e^2}{2V} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} \sum_{\sigma_1,\sigma_2} \frac{4\pi \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}}{|\boldsymbol{k}_1-\boldsymbol{k}_3|^2+\mu^2} a^\dagger_{\boldsymbol{k}_1\sigma_1} a^\dagger_{\boldsymbol{k}_2\sigma_2} a_{\boldsymbol{k}_4\sigma_2} a_{\boldsymbol{k}_3\sigma_1} \quad (1.8)$$

The requirement that $\boldsymbol{k}_1+\boldsymbol{k}_2=\boldsymbol{k}_3+\boldsymbol{k}_4$ implies the momentum conservation, and let us use the following change of variables:

$$\boldsymbol{k}_3 = \boldsymbol{k}_1+\boldsymbol{q}, \quad \boldsymbol{k}_4 = \boldsymbol{k}_2-\boldsymbol{q}$$

Then we have

$$\hat{H}_{el} = \sum_{\boldsymbol{k}\sigma} \frac{\hbar^2 k^2}{2m} a^\dagger_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} + \frac{e^2}{2V} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{q}} \sum_{\sigma_1,\sigma_2} \frac{4\pi}{|\boldsymbol{q}|^2+\mu^2} a^\dagger_{\boldsymbol{k}_1\sigma_1} a^\dagger_{\boldsymbol{k}_2\sigma_2} a_{\boldsymbol{k}_2-\boldsymbol{q},\sigma_2} a_{\boldsymbol{k}_1+\boldsymbol{q},\sigma_1} \quad (1.9)$$

Let us seperate the last term, i.e. the interacting Hamiltonian into two terms: $\boldsymbol{q}\neq 0$ and $\boldsymbol{q}=0$. For $\boldsymbol{q}=0$, summing up $\boldsymbol{k}_1,\boldsymbol{k}_2,\sigma_1,\sigma_2$, we have

$$\begin{aligned}
\frac{e^2}{2V}\frac{4\pi}{\mu^2} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_{\sigma_1,\sigma_2} a^\dagger_{\boldsymbol{k}_1\sigma_1} a^\dagger_{\boldsymbol{k}_2\sigma_2} a_{\boldsymbol{k}_2\sigma_2} a_{\boldsymbol{k}_1\sigma_1} &= -\frac{e^2}{2V}\frac{4\pi}{\mu^2} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_{\sigma_1,\sigma_2} a^\dagger_{\boldsymbol{k}_1\sigma_1} a^\dagger_{\boldsymbol{k}_2\sigma_2} a_{\boldsymbol{k}_1\sigma_1} a_{\boldsymbol{k}_2\sigma_2} \\
&= -\frac{e^2}{2V}\frac{4\pi}{\mu^2} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_{\sigma_1,\sigma_2} a^\dagger_{\boldsymbol{k}_1\sigma_1} (\delta_{\boldsymbol{k}_1\boldsymbol{k}_2}\delta_{\sigma_1\sigma_2} - a_{\boldsymbol{k}_1\sigma_1} a^\dagger_{\boldsymbol{k}_2\sigma_2}) a_{\boldsymbol{k}_2\sigma_2} = \frac{e^2}{2V}\frac{4\pi}{\mu^2}(\hat{N}^2-\hat{N})
\end{aligned}$$

Note that $\hat{N}=N$ since the electron number is fixed. Therefore $\frac{e^2}{2V}\frac{4\pi}{\mu^2}(\hat{N}^2)$ cancels $\hat{H}_{el}+\hat{H}_{el-b}$ and $-\frac{e^2}{2V}\frac{4\pi}{\mu^2}N$ gives an energy $-\frac{1}{2}\frac{4\pi e^2}{V\mu^2}$ per particle and claim it to vanish when first let $L\to\infty$ and then let $\mu\to 0$. This is not rigorous mathematically. Please find other places a mathematical justification.

In this way, the final Hamiltonian becomes

$$\hat{H} = \sum_{\boldsymbol{k}\sigma} \frac{\hbar^2 |\boldsymbol{k}|^2}{2m} a^\dagger_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} + \frac{e^2}{2V} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_{\boldsymbol{q}}{}' \sum_{\sigma_1,\sigma_2} \frac{4\pi}{|\boldsymbol{q}|^2} a^\dagger_{\boldsymbol{k}_1\sigma_1} a^\dagger_{\boldsymbol{k}_2\sigma_2} a_{\boldsymbol{k}_2-\boldsymbol{q},\sigma_2} a_{\boldsymbol{k}_1+\boldsymbol{q},\sigma_1} \quad (1.10)$$

where $\sum'_{\boldsymbol{q}} = \sum_{\boldsymbol{q}\neq\boldsymbol{0}}$. Let us define r_0 as the *effective radius* of a particle:

$$V = \frac{4}{3}\pi r_0^3 N$$

In atomic physics, we often use the Bohr radius $a_0 = \frac{\hbar^2}{me^2}$. Let $r_s = r_0/a_0$.

We want to use perturbation theory to study $\hat{H}$. Before that, let us first show that this is reasonable in the *high density limit*, i.e. $\hat{H}_1$ is somewhat small in the high density limit. Let us defnie the following dimensionless quantity:

$$\overline{V} = r_0^{-3}V, \quad \overline{\boldsymbol{k}} = r_0\boldsymbol{k}, \quad \overline{\boldsymbol{p}} = r_0\boldsymbol{p}, \quad \overline{\boldsymbol{q}} = r_0\boldsymbol{q}$$

Then the Hamiltonian becomes

$$\begin{aligned}\hat{H} &= \sum_{\boldsymbol{k}\sigma} \frac{\hbar^2|\overline{\boldsymbol{k}}/r_0|^2}{2m} a^{\dagger}_{\overline{\boldsymbol{k}}\sigma} a_{\overline{\boldsymbol{k}}\sigma} + \frac{e^2}{2V} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_{\boldsymbol{q}}{}' \sum_{\sigma_1,\sigma_2} \frac{4\pi}{|\overline{\boldsymbol{q}}/r_0|^2} a^{\dagger}_{\overline{\boldsymbol{k}}_1\sigma_1} a^{\dagger}_{\overline{\boldsymbol{k}}_2\sigma_2} a_{\overline{\boldsymbol{k}}_2-\overline{\boldsymbol{q}},\sigma_2} a_{\overline{\boldsymbol{k}}_1+\overline{\boldsymbol{q}},\sigma_1} \\ &= \frac{\hbar^2}{m|r_0|^2} \left(\sum_{\boldsymbol{k}\sigma} \frac{|\overline{\boldsymbol{k}}|^2}{2} a^{\dagger}_{\overline{\boldsymbol{k}}\sigma} a_{\overline{\boldsymbol{k}}\sigma} + \frac{r_0 m e^2}{2\overline{V}\hbar^2} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_{\boldsymbol{q}}{}' \sum_{\sigma_1,\sigma_2} \frac{4\pi}{|\overline{\boldsymbol{q}}|^2} a^{\dagger}_{\overline{\boldsymbol{k}}_1\sigma_1} a^{\dagger}_{\overline{\boldsymbol{k}}_2\sigma_2} a_{\overline{\boldsymbol{k}}_2-\overline{\boldsymbol{q}},\sigma_2} a_{\overline{\boldsymbol{k}}_1+\overline{\boldsymbol{q}},\sigma_1} \right) \\ &= \frac{e^2}{a_0|r_s|^2} \left(\sum_{\boldsymbol{k}\sigma} \frac{|\overline{\boldsymbol{k}}|^2}{2} a^{\dagger}_{\overline{\boldsymbol{k}}\sigma} a_{\overline{\boldsymbol{k}}\sigma} + \frac{r_s}{2\overline{V}} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_{\boldsymbol{q}}{}' \sum_{\sigma_1,\sigma_2} \frac{4\pi}{|\overline{\boldsymbol{q}}|^2} a^{\dagger}_{\overline{\boldsymbol{k}}_1\sigma_1} a^{\dagger}_{\overline{\boldsymbol{k}}_2\sigma_2} a_{\overline{\boldsymbol{k}}_2-\overline{\boldsymbol{q}},\sigma_2} a_{\overline{\boldsymbol{k}}_1+\overline{\boldsymbol{q}},\sigma_1} \right)\end{aligned} \tag{1.11}$$

When $r_s \to 0$, i.e. $r_0 \to 0$, i.e. the high density limit, it is reasonable to consider the perturbation theory.
Let $\hat{H}_0, \hat{H}_1$ be

$$\hat{H}_0 = \sum_{\boldsymbol{k}\sigma} \frac{\hbar^2 k^2}{2m} a^{\dagger}_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma} \tag{1.12}$$

$$\hat{H}_1 = \frac{e^2}{2V} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} \sum_{\boldsymbol{q}}{}' \sum_{\sigma_1,\sigma_2} \frac{4\pi}{|\boldsymbol{q}|^2} a^{\dagger}_{\boldsymbol{k}_1\sigma_1} a^{\dagger}_{\boldsymbol{k}_2\sigma_2} a_{\boldsymbol{k}_2-\boldsymbol{q},\sigma_2} a_{\boldsymbol{k}_1+\boldsymbol{q},\sigma_1} \tag{1.13}$$

We want to treat $\hat{H}_0$ as the unperturbed system and $\hat{H}_1$ as the perturbation.
For the unperturbed system governed by $\hat{H}_0$ (also known as the free Fermi electron gas), the ground state, denoted by $|F\rangle$, is obtained by filling all the states with momentum smaller than a maximum value, called *Fermi momentum* $p_F = \hbar k_F$. The value of k_F is decided by:

$$N = \langle F|\hat{N}|F\rangle = \sum_{\boldsymbol{k}\sigma} \langle F\,|\hat{n}_{\boldsymbol{k}\lambda}|\,F\rangle = \sum_{\boldsymbol{k}\sigma} \theta\,(k_F - k) \tag{1.14}$$

where $\theta(x)$ is the step function

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

Note that when $L \to \infty$, the summation over $\boldsymbol{k}$ becomes an integral:

$$\sum_{\boldsymbol{k}} f(\boldsymbol{k}) = \sum_{n_x n_y n_z} f\left(\frac{2\pi\boldsymbol{n}}{L}\right) \underset{L\to\infty}{\to} \iiint \mathrm{d}n_x \mathrm{d}n_y \mathrm{d}n_z f\left(\frac{2\pi\boldsymbol{n}}{L}\right) = V(2\pi)^{-3} \int \mathrm{d}\boldsymbol{k} f(\boldsymbol{k})$$

Therefore

$$N = \langle F|\hat{N}|F\rangle = \sum_{\boldsymbol{k}\sigma} \theta\,(k_F - |\boldsymbol{k}|) = \frac{V}{(2\pi)^3} \sum_{\sigma} \int \mathrm{d}\boldsymbol{k}\theta\,(k_F - |\boldsymbol{k}|) = \frac{V k_F^3}{3\pi^2} \tag{1.15}$$

We finally obtain that

$$k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}} = \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} r_0^{-1} \approx 1.92 r_0^{-1} \tag{1.16}$$

and the ground state energy for this unperturbed system would be

$$
\begin{aligned}
E^{(0)} &= \left\langle F \left| \hat{H}_0 \right| F \right\rangle = \frac{\hbar^2}{2m} \sum_{\boldsymbol{k}\sigma} |\boldsymbol{k}|^2 \left\langle F \left| \hat{n}_{\boldsymbol{k}\sigma} \right| F \right\rangle = \frac{\hbar^2}{2m} \sum_{\boldsymbol{k}\sigma} |\boldsymbol{k}|^2 \theta\left(k_F - |\boldsymbol{k}|\right) \\
&= \frac{\hbar^2}{2m} \sum_{\sigma} V(2\pi)^{-3} \int \mathrm{d}\boldsymbol{k} |\boldsymbol{k}|^2 \theta\left(k_F - k\right) \\
&= \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} N = \frac{e^2}{2a_0} \frac{N}{r_s^2} \frac{3}{5} \left(\frac{9\pi}{4}\right)^{\frac{2}{3}} = \frac{e^2}{2a_0} N \frac{2.21}{r_s^2}.
\end{aligned} \tag{1.17}
$$

In other words, in the free Fermi gas, the energy per particle is 3/5 of the Fermi energy $\frac{\hbar^2 k_F^2}{2m}$. The Fermi energy is the maximum of single-particle energy in the system. Now let us compute the first order perturbation of the ground state energy:

$$
E^{(1)} = \left\langle F \left| \hat{H}_1 \right| F \right\rangle = \frac{e^2}{2V} \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2} \sum_{\boldsymbol{q}}{}' \sum_{\sigma_1, \sigma_2} \frac{4\pi}{|\boldsymbol{q}|^2} \left\langle F \left| a^\dagger_{\boldsymbol{k}_1 \sigma_1} a^\dagger_{\boldsymbol{k}_2 \sigma_2} a_{\boldsymbol{k}_2 - \boldsymbol{q}, \sigma_2} a_{\boldsymbol{k}_1 + \boldsymbol{q}, \sigma_1} \right| F \right\rangle \tag{1.18}
$$

After some calculation (left as an exercise), we have

$$
\begin{aligned}
E^{(1)} &= -\frac{e^2}{2V} \sum_{\boldsymbol{k}} \sum_{\boldsymbol{q}}{}' \sum_{\sigma_1} \frac{4\pi}{|\boldsymbol{q}|^2} \theta(k_F - |\boldsymbol{k} + \boldsymbol{q}|) \theta(k_F - |\boldsymbol{k}|) \\
&= -\frac{e^2}{2} \frac{4\pi V}{(2\pi)^6} 2 \int \mathrm{d}\boldsymbol{k} \mathrm{d}\boldsymbol{q} |\boldsymbol{q}|^{-2} \theta\left(k_F - |\boldsymbol{k} + \boldsymbol{q}|\right) \theta\left(k_F - |\boldsymbol{k}|\right)
\end{aligned} \tag{1.19}
$$

With a substitution of variable, the above integral becomes

$$
E^{(1)} = -\frac{e^2 V k_F^4}{4\pi^3} = -\frac{e^2}{2a_0} \frac{N}{r_s} \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{3}{2\pi} = -\frac{e^2}{2a_0} N \frac{0.916}{r_s} \tag{1.20}
$$

Therefore the ground state energy per particle is

$$
\frac{E}{N} \underset{r_s \to 0}{=} \frac{e^2}{2a_0} \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \cdots \right] \tag{1.21}
$$

where the first term is the kinetic energy, and the second term is called the exchange energy and is negative. It is called exchange energy since in the calculation of $E^{(1)}$, only the term that $\boldsymbol{k}_2 = \boldsymbol{k_1} - q$ and $\boldsymbol{k}_2 = \boldsymbol{k_1}$ could contribute, where the former one is formally an exchange of particles, and the latter one, often called the direct term, has been shown to cancel $H_b + H_{el-b}$. The remaining terms in this series (indicated by dots) are called the correlation energy.

1.2 Exercise

1. Derive the electronic Hamiltonian (eq 1.8) from eq 1.3.

2. Derive the first order perturbation (eq 1.19) of ground state energy of electron gas from the previous formulation (eq 1.18). Calculate the integral in eq 1.19.

3. Consider the electron gas in the high density limit. With $P = -\left(\frac{\partial E}{\partial V}\right)_N$, please derive the value of r_s when the system is at equilibrium (i.e. $P = 0$).

2 Statistical Mechanics

2.1 Quick review

Let us only consider systems with a single kind of particles. The internal energy E is regarded as a function of the entropy S, the volume V and the number of particles N . In other words, $E = E(S, V, N)$. We define the temperature T, pressure P and chemical potential μ as

$$T = \left(\frac{\partial E}{\partial S}\right)_{V,N}, \quad -P = \left(\frac{\partial E}{\partial V}\right)_{S,N}, \quad \mu = \left(\frac{\partial E}{\partial N}\right)_{S,V} \tag{2.1}$$

With this definition, we recover a fundamental law of thermodynamics:

$$\mathrm{d}E = T\mathrm{d}S - P\mathrm{d}V + \mu\mathrm{d}N \tag{2.2}$$

Here, we adopt the very confusing physicist's notation, for example in $\left(\frac{\partial E}{\partial S}\right)_{V,N}$, we write V, N in subscript. Many textbooks interpret it as emphasizing that we are taking derivative w.r.t S, we keep V, N unchanged. This sounds really stupid if you first hear it, since in the definition of partial derivatives, of course other variables are not changing.

But, what physicists actually mean is that: for a thermodynamic system , we have defined six quantities S, V, N, T, P, μ, and (more or less) any three of them are sufficient to describe the whole system. By writing $\left(\frac{\partial E}{\partial S}\right)_{V,N}$, we are reminding ourselves that we are considering E as a function of (S, V, N) instead of as functions of other quantities.

To further illustrate what I am talking about, let us define resulting functions the Helmholtz free energy F and the Gibbs free energy G through Legendre transformation

$$F = E - TS, \quad \mathrm{d}F = -S\mathrm{d}T - P\mathrm{d}V + \mu\mathrm{d}N \tag{2.3}$$

$$G = E - TS + PV, \quad \mathrm{d}G = -S\mathrm{d}T + V\mathrm{d}P + \mu\mathrm{d}N \tag{2.4}$$

$$\Omega = E - TS - \mu N, \quad \mathrm{d}\Omega = -S\mathrm{d}T - P\mathrm{d}V - N\mathrm{d}\mu \tag{2.5}$$

With this, we can see that $F = F(T, V, N)$, $G = G(T, P, N)$ and $\Omega = \Omega(T, V, \mu)$ and using the above notation:

$$\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V} = \left(\frac{\partial G}{\partial N}\right)_{T,P} \tag{2.6}$$

$$S = -\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu}, \quad P = -\left(\frac{\partial \Omega}{\partial V}\right)_{T,\mu}, \quad N = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} \tag{2.7}$$

Note that T, P, μ are intensive variables and E, S, V, N are extensive variables, therefore we have

$$\lambda E = E(\lambda S, \lambda V, \lambda N) \tag{2.8}$$

and differentiate it with respect to λ,

$$E = S\left(\frac{\partial E}{\partial S}\right)_{V,N} + V\left(\frac{\partial E}{\partial V}\right)_{S,N} + N\left(\frac{\partial E}{\partial N}\right)_{S,V} = TS - PV + \mu N \tag{2.9}$$

therefore

$$F = -PV + \mu N, \quad G = \mu N, \quad \Omega = -PV \tag{2.10}$$

Now let us turn to the microscopic aspect of the system. We introduce the concept of grand canonical ensemble with chemical potential μ and temperature $T = \frac{1}{k_B \beta}$. Here k_B is the Boltzmann constant. Let us define the grand partition function Z_G as

$$\begin{aligned} Z_G &= \sum_N \sum_j e^{-\beta(E_j - \mu N)} = \sum_N \sum_j \left\langle \psi_{N,j} \left| e^{-\beta(\hat{H} - \mu \hat{N})} \right| \psi_{N,j} \right\rangle \\ &= \mathrm{Tr}\left(e^{-\beta(\hat{H} - \mu\hat{N})}\right) \end{aligned} \tag{2.11}$$

where $|\psi_{N,j}\rangle$ is the j-th eigenfunction of $\hat{H}$ when the particle number is N. Statistical mechanics asserts that

$$\Omega(T, V, \mu) = -k_{\mathrm{B}} T \ln Z_{\mathrm{G}} \tag{2.12}$$

We also define the density operator $\hat{\rho}_G$ as

$$\hat{\rho}_G = Z_G^{-1} e^{-\beta(\hat{H} - \mu\hat{N})} = e^{\beta(\Omega - \hat{H} + \mu\hat{N})} \tag{2.13}$$

Then for any operator $\hat{O}$, the ensemble average $\langle \hat{O} \rangle$ is

$$\langle \hat{O} \rangle = \mathrm{Tr}\left(\hat{\rho}_G \hat{O}\right) = \frac{\mathrm{Tr}\left(e^{-\beta(\hat{H} - \mu\hat{N})}\hat{O}\right)}{\mathrm{Tr}\left(e^{-\beta(\hat{H} - \mu\hat{N})}\right)} \tag{2.14}$$

2.2 Ideal gas

Let us consider the noninteracting Boson and Fermi gas. Assume that ϵ_l is the eigenvalue of one-particle system. Using occupation number basis, we have

$$\begin{aligned} Z_G &= \mathrm{Tr}\left(e^{-\beta(\hat{H} - \mu\hat{N})}\right) \\ &= \sum_{n_1, n_2, \cdots} \left\langle n_1 \cdots n_\infty \left| e^{-\beta(\hat{H} - \mu\hat{N})} \right| n_1 \cdots n_\infty \right\rangle \\ &= \sum_{n_1, n_2, \cdots} \left\langle n_1 \cdots \cdot n_\infty \left| \exp\left[\beta\left(\mu \sum_i n_i - \sum_i \epsilon_i n_i\right)\right] \right| n_1 \cdots \cdot n_\infty \right\rangle \\ &= \prod_{i=1}^{\infty} \sum_{n_i} e^{\beta(\mu n_i - \epsilon_i n_i)} \end{aligned} \tag{2.15}$$

Let us discuss the two cases: bosons and fermions.

- For bosons, the summation on n_i is from 0 to ∞, and we have

$$Z_G = \prod_{i=1}^{\infty} \sum_{n_i=0}^{\infty} e^{\beta(\mu n_i - \epsilon_i n_i)} = \prod_{i=1}^{\infty} \left(1 - e^{\beta(\mu-\epsilon_i)}\right)^{-1} \tag{2.16}$$

  Therefore

$$\Omega_0(T,V,\mu) = -k_B T \ln Z_{\mathrm{G}} = k_B T \sum_{i=1}^{\infty} \ln\left(1 - e^{\beta(\mu-\epsilon_i)}\right), \quad \text{for Bosons} \tag{2.17}$$

  and

$$\langle \hat{N} \rangle = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} = \sum_{i=1}^{\infty} n_i^0 = \sum_{i=1}^{\infty} \frac{1}{e^{\beta(\epsilon_i-\mu)} - 1}, \quad \text{for Bosons} \tag{2.18}$$

  here n_i^0 is the mean occupation number in the i-th state.

- For fermions, n_i is either 0 or 1, and we have

$$Z_G = \prod_{i=1}^{\infty} \sum_{n_i=0}^{1} e^{\beta(\mu n_i - \epsilon_i n_i)} = \prod_{i=1}^{\infty} \left(1 - e^{\beta(\mu+\epsilon_i)}\right) \tag{2.19}$$

  Therefore

$$\Omega_0(T,V,\mu) = -k_B T \ln Z_{\mathrm{G}} = -k_B T \sum_{i=1}^{\infty} \ln\left(1 + e^{\beta(\mu-\epsilon_i)}\right), \quad \text{for fermions} \tag{2.20}$$

  and

$$\langle \hat{N} \rangle = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} = \sum_{i=1}^{\infty} n_i^0 = \sum_{i=1}^{\infty} \frac{1}{e^{\beta(\epsilon_i-\mu)} + 1}, \quad \text{for fermions} \tag{2.21}$$

  here n_i^0 is the mean occupation number in the i-th state.

2.3 A treatment on noninteracting bosons

Let us first focus on the noninteracting bosons. The energy spectrum is given by

$$\epsilon_p = \frac{|\boldsymbol{p}|^2}{2m} = \frac{\hbar^2 |\boldsymbol{k}|^2}{2m}$$

Since $\boldsymbol{p}$ is continuous, the sum over i becomes an integral:

$$\sum_i \to g \int \mathrm{d}n_1 \mathrm{d}n_2 \mathrm{d}n_3 = gV(2\pi)^{-3} \int \mathrm{d}\boldsymbol{k}$$

where g is the degeneracy of each single-particle momentum state. (For spinless particles, $g = 1$.) We actually want to write an integral about ϵ, therefore for any quantity f, we have

$$\frac{gV}{(2\pi)^3}\int f\mathrm{d}\boldsymbol{k} = \int \mathrm{d}k\frac{gV}{(2\pi)^3}4\pi k^2 f = \int \mathrm{d}\epsilon\frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\epsilon^{\frac{1}{2}}f \tag{2.22}$$

Apply this to Boson gas, we have

$$-\frac{\Omega_0}{k_BT} = \frac{PV}{k_BT} = -\frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty \mathrm{d}\epsilon\epsilon^{\frac{1}{2}}\ln\left(1-e^{\beta(\mu-\epsilon)}\right) \tag{2.23}$$

and

$$PV = \frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{2}{3}\int_0^\infty \mathrm{d}\epsilon\frac{\epsilon^{\frac{3}{2}}}{e^{\beta(\epsilon-\mu)}-1} \tag{2.24}$$

On the other hand, we have

$$E = \sum_i n_i^0\epsilon_i = \frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty d\epsilon\frac{\epsilon^{\frac{3}{2}}}{e^{\beta(\epsilon-\mu)}-1} \tag{2.25}$$

Therefore, we have a very crucial result:

$$PV = \frac{2}{3}E \tag{2.26}$$

Similarly, we have

$$\frac{N}{V} = \frac{g}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty d\epsilon\frac{\epsilon^{\frac{1}{2}}}{e^{\beta(\epsilon-\mu)}-1} \tag{2.27}$$

This integral is meaningful only if $\epsilon-\mu \geqslant 0$. Otherwise the mean occupation number n^0 would be less than zero for some values of ϵ. In particular, we should have $\mu \leq 0$.

We can also regard μ as a function of N/V and β in 2.27. For a fixed particle number N/V, when T gets smaller, i.e. β gets bigger, μ needs to get bigger to make N/V unchanged. As μ gets bigger, it will hit zero!

What I'm saying is, there exists a critical temperature T_0, for this N/V, the chemical potential hits 0. This T_0 could be found:

$$\frac{N}{V} = \frac{g}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty \mathrm{d}\epsilon\frac{\epsilon^{\frac{1}{2}}}{e^{\epsilon/k_BT_0}-1} = \frac{g}{4\pi^2}\left(\frac{2mk_BT_0}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty \mathrm{d}x\frac{x^{\frac{1}{2}}}{e^x-1} \tag{2.28}$$

which can be solved as

$$T_0 = \frac{\hbar^2}{2mk_B}\left(\frac{4\pi^2}{g\Gamma\left(\frac{3}{2}\right)\zeta\left(\frac{3}{2}\right)}\right)^{\frac{2}{3}}\left(\frac{N}{V}\right)^{\frac{2}{3}} = \frac{3.31}{g^{\frac{2}{3}}}\frac{\hbar^2}{mk_B}\left(\frac{N}{V}\right)^{\frac{2}{3}} \tag{2.29}$$

A physical interpretation is thermal energy k_BT_0 is comparable with the zero-point energy $\frac{\hbar^2}{m}\left(\frac{N}{V}\right)^{\frac{2}{3}}$, which is the ground state of putting a particle in volume V/N.

If we lower the temperature below T_0, mathematically speaking, since μ can not get bigger than 0, the integral on the right hand side in 2.27 will be smaller than N/V. If we go back to the summation picture, we can see that the term $\frac{\epsilon^{\frac{1}{2}}}{e^{\beta(\epsilon-\mu)}-1} = \frac{\epsilon^{\frac{1}{2}}}{e^{\beta\epsilon}-1}$ is $+\infty$ at $\epsilon = 0$. This term is not passed into the integral.

Therefore, the physical picture for $T < T_0$ is that: the particles with energy $\epsilon > 0$ is:

$$\frac{N_{\epsilon>0}}{V} = \frac{g}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty \mathrm{d}\epsilon \frac{\epsilon^{\frac{1}{2}}}{e^{\epsilon/k_B T}-1} = \frac{g}{4\pi^2}\left(\frac{2mk_B T}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty \mathrm{d}x \frac{x^{\frac{1}{2}}}{e^{x}-1} = \frac{N}{V}\left(\frac{T}{T_0}\right)^{\frac{3}{2}} \tag{2.30}$$

with density of states

$$\frac{\mathrm{d}N_\epsilon}{V} = \frac{g}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{\epsilon^{\frac{1}{2}}\mathrm{d}\epsilon}{e^{\beta\epsilon}-1} \tag{2.31}$$

and there is a portion of particles with energy $\epsilon = 0$:

$$\frac{N_{\epsilon=0}}{V} = \frac{N}{V}\left[1-\left(\frac{T}{T_0}\right)^{\frac{3}{2}}\right] \tag{2.32}$$

We say that these particles condensate at $\epsilon = 0$, and we often let chemical potential $\mu = 0^-$ in this case. T_0 is often identified as the point where phase transitions happens. For example, the constant-volume heat capacity C_V's derivative has a discontinuity at T_0.

2.4 A similar treatment on fermions

We have a similar treatment on fermions. Similarly we can get

$$PV = \frac{2}{3}E = \frac{2}{3}\frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty \mathrm{d}\epsilon \frac{\epsilon^{\frac{3}{2}}}{e^{\beta(\epsilon-\mu)}+1} \tag{2.33}$$

$$\frac{N}{V} = \frac{g}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty \mathrm{d}\epsilon \frac{\epsilon^{\frac{1}{2}}}{e^{\beta(\epsilon-\mu)}+1} \tag{2.34}$$

where g is the degeneracy factor ($g = 2$ for a spin- $\frac{1}{2}$ Fermi gas). The chemical potential could be positive now.

In the zero temperature limit, the Fermi distrubution becomes

$$\frac{1}{e^{(\epsilon-\mu)/k_B T}+1} \underset{T\to 0}{\to} \left\{\begin{array}{ll} 0 & \epsilon > \mu \\ 1 & \epsilon < \mu \end{array}\right\} = \theta(\mu-\epsilon) \tag{2.35}$$

Recall that the lowest energy state of the system is obtained by filling the energy levels up to.

$$\mu = \epsilon_F \quad \text{at } T = 0$$

Exercises

1. When $T < T_0$, the energy of the noninteracting Bose gas only comes from the particles that are not in the condensate. Prove that we have:

$$E = \frac{\zeta\left(\frac{5}{2}\right)\Gamma\left(\frac{5}{2}\right)}{\zeta\left(\frac{3}{2}\right)\Gamma\left(\frac{3}{2}\right)} N k_B T \left(\frac{T}{T_0}\right)^{\frac{3}{2}} \simeq 0.770 N k_B T \left(\frac{T}{T_0}\right)^{\frac{3}{2}}, \quad T \leqslant T_0 \tag{2.36}$$

2. Prove that for noninteracting Boson gas, we have

$$\left(\frac{\partial E}{\partial \mu}\right)_{TV} = \frac{3}{2} N \tag{2.37}$$

and therefore

$$E(T, V, \mu) = \begin{cases} E(T, V, 0) & T < T_0 \\ E(T, V, 0) + \frac{3}{2} N\mu & T > T_0 \end{cases} \tag{2.38}$$

3. Prove that for zero temperature Fermi gas, we have

$$\frac{E}{N} = \frac{3}{5}\mu = \frac{3}{5}\epsilon_F, \quad P = \frac{2}{5}\left(\frac{6\pi^2}{g}\right)^{\frac{2}{3}} \frac{\hbar^2}{2m}\left(\frac{N}{V}\right)^{\frac{5}{3}} \tag{2.39}$$

3 Zero Temperature Green's function

3.1 Pictures

Schrödinger picture

The Schrödinger picture is the first picture that we encounter in quantum mechanics. For a time-independent Hamiltonian $\hat{H}$, we regard the operator $\hat{H}$ as unchanged and the wavefunction changing according to Schrödinger's equation:

$$i\hbar\frac{\partial}{\partial t}\left|\Psi_s(t)\right\rangle = \hat{H}\left|\Psi_s(t)\right\rangle \tag{3.1}$$

Interacting picture

Assume that the Hamiltonian $\hat{H}$ could be split into two parts:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \tag{3.2}$$

We are secretly hoping that $\hat{H}_0$ itself is a problem solvable at least in some sense. Let us define

$$\left|\Psi_I(t)\right\rangle \equiv \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\left|\Psi_S(t)\right\rangle \tag{3.3}$$

We have

$$\begin{aligned}\mathrm{i}\hbar\frac{\partial}{\partial t}\left|\Psi_I(t)\right\rangle &= -\hat{H}_0\mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\left|\Psi_S(t)\right\rangle + \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\mathrm{i}\hbar\frac{\partial}{\partial t}\left|\Psi_S(t)\right\rangle \\ &= \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\left[-\hat{H}_0 + \hat{H}_0 + \hat{H}_1\right]\mathrm{e}^{-\mathrm{i}\hat{H}_0 t/\hbar}\left|\Psi_I(t)\right\rangle\end{aligned} \tag{3.4}$$

Therefore, let

$$\hat{H}_1(t) = \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\hat{H}_1\mathrm{e}^{-\mathrm{i}\hat{H}_0 t/\hbar}\left|\Psi_I(t)\right\rangle \tag{3.5}$$

we have

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\left|\Psi_I(t)\right\rangle = \hat{H}_1(t)\left|\Psi_I(t)\right\rangle \tag{3.6}$$

For an operator $\hat{O}$, assume that it is $\hat{O}_S$ in the Schrödinger picture, and we have

$$\left\langle\Psi_S(t)\left|\hat{O}_S\right|\Psi_S(t)\right\rangle = \left\langle\Psi_I(t)\left|\mathrm{e}^{\mathrm{i}H_0 t/\hbar}\hat{O}_S\mathrm{e}^{-\mathrm{i}H_0 t/\hbar}\right|\Psi_I(t)\right\rangle \tag{3.7}$$

Therefore it is only natural to define the operator in the interacting picture as

$$\hat{O}_I(t) \equiv \mathrm{e}^{\mathrm{i}H_0 t/\hbar}\hat{O}_S\mathrm{e}^{-\mathrm{i}H_0 t/\hbar} \tag{3.8}$$

The differentiation of above yields

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\hat{O}_I(t) = \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\left(\hat{O}_S\hat{H}_0 - \hat{H}_0\hat{O}_S\right)\mathrm{e}^{-\mathrm{i}\hat{H}_0 t/\hbar} = \left[\hat{O}_I(t), \hat{H}_0\right] \tag{3.9}$$

Now let us find out the equation of motion in the interaction picture, i.e. we want to find the propogator $\hat{U}(t,t_0)$ such that

$$|\Psi_I(t)\rangle = \hat{U}(t,t_0)\,|\Psi_I(t_0)\rangle \tag{3.10}$$

We have

$$\begin{aligned}|\Psi_I(t)\rangle &= \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\,|\Psi_S(t)\rangle = \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\mathrm{e}^{-\mathrm{i}\hat{H}(t-t_0)/\hbar}\,|\Psi_S(t_0)\rangle \\ &= \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\mathrm{e}^{-\mathrm{i}\hat{H}(t-t_0)/\hbar}\mathrm{e}^{-\mathrm{i}\hat{H}_0 t_0/\hbar}\,|\Psi_I(t_0)\rangle\end{aligned} \tag{3.11}$$

Therefore

$$\hat{U}(t,t_0) = \mathrm{e}^{\mathrm{i}\hat{H}_0 t/\hbar}\mathrm{e}^{-\mathrm{i}\hat{H}(t-t_0)/\hbar}\mathrm{e}^{-\mathrm{i}\hat{H}_0 t_0/\hbar} \tag{3.12}$$

It is not hard to verify (left as an exercise) that $\hat{U}(t,t_0)$ satisfy

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}_1(t)\hat{U}(t,t_0)\,, \quad \hat{U}(t_0,t_0) = \mathbf{1} \tag{3.13}$$

We can write this into an integral equation

$$\hat{U}(t,t_0) = \mathbf{1} - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\,\hat{H}_1(t')\,\hat{U}(t',t_0) \tag{3.14}$$

This equation could be substituted into itself iteratively:

$$\hat{U}(t,t_0) = \mathbf{1} + \left(\frac{-\mathrm{i}}{\hbar}\right)\int_{t_0}^{t} dt'\,\hat{H}_1(t') + \left(\frac{-\mathrm{i}}{\hbar}\right)^2\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\,\hat{H}_1(t')\,\hat{H}_1(t'') + \cdots \tag{3.15}$$

Note that we have

$$\begin{aligned}&\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\,\hat{H}_1(t')\,\hat{H}_1(t'') \\ =&\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t'}\mathrm{d}t''\,\hat{H}_1(t')\,\hat{H}_1(t'') + \frac{1}{2}\int_{t_0}^{t}\mathrm{d}t''\int_{t''}^{t}\mathrm{d}t'\,\hat{H}_1(t')\,\hat{H}_1(t'') \\ =&\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t}\mathrm{d}t''\left[\hat{H}_1(t')\,\hat{H}_1(t'')\,\theta(t'-t'') + \hat{H}_1(t'')\,\hat{H}_1(t')\,\theta(t''-t')\right]\end{aligned} \tag{3.16}$$

Here we see, for the first time, the kind of feature that the operators with the larger(later) time stays at the left. Therefore we introduce the time ordering operator T, so that

$$\begin{aligned}=&\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t}\mathrm{d}t''\left[\hat{H}_1(t')\,\hat{H}_1(t'')\,\theta(t'-t'') + \hat{H}_1(t'')\,\hat{H}_1(t')\,\theta(t''-t')\right] \\ =&\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t'\int_{t_0}^{t}\mathrm{d}t''\,T\left(\hat{H}_1(t')\,\hat{H}_1(t'')\right)\end{aligned} \tag{3.17}$$

where T is defined as

$$T\left(\hat{H}_1(t_1)\,\hat{H}_2(t_2)\right) = \hat{H}_1(t_1)\,\hat{H}_2(t_2)\,\theta(t_1-t_2) + \hat{H}_2(t_2)\,\hat{H}_1(t_1)\,\theta(t_2-t_1) \tag{3.18}$$

Carrying this on, one can verify that (left as an exercise)

$$\hat{U}\left(t, t_0\right)=\sum_{n=0}^{\infty}\left(\frac{-\mathrm{i}}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t \mathrm{d} t_1 \cdot \int_{t_0}^t \mathrm{d} t_n T\left[\hat{H}_1\left(t_1\right) \cdot \cdots \hat{H}_1\left(t_n\right)\right] \tag{3.19}$$

It is worth mentioning that under the time ordering operator, any two operators are commutable, while generally they don't.

Heisenberg picture

In Heisenberg picture, the wavefunction remains the same:

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\left|\Psi_H(t)\right\rangle=0, \quad\left|\Psi_H(t)\right\rangle=\left|\Psi_S(0)\right\rangle=e^{\mathrm{i} \hat{H} t / \hbar}\left|\Psi_S(t)\right\rangle \tag{3.20}$$

Similarly as above, we can deduce that an operator in Heisenberg picture should be

$$\hat{O}_H(t) \equiv \mathrm{e}^{\mathrm{i} H t / \hbar} \hat{O}_S \mathrm{e}^{-\mathrm{i} H t / \hbar} \tag{3.21}$$

and we have

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \hat{O}_H(t)=e^{\mathrm{i} \hat{H} t / \hbar}\left[\hat{O}_S, \hat{H}\right] e^{-\mathrm{i} H t / \hbar}=\left[\hat{O}_H(t), \hat{H}\right] \tag{3.22}$$

Adiabatic switching on

Consider the Hamiltonian

$$\hat{H}(t)=\hat{H}_0+e^{-\epsilon|t|} \hat{H}_1 \tag{3.23}$$

This could be understood as having the noninteracting Hamiltonian at $t=-\infty$ and gradually turning on the interacting part $\hat{H}_1$ till $t=0$. Let us consider the following interacting picture:

$$\left|\Psi_I(t)\right\rangle=\hat{U}_\epsilon\left(t, t_0\right)\left|\Psi_I\left(t_0\right)\right\rangle \tag{3.24}$$

where

$$\hat{U}_\epsilon\left(t, t_0\right)=\sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^t \mathrm{d} t_1 \cdots \int_{t_0}^t \mathrm{d} t_n \times \mathrm{e}^{-\epsilon\left(\left|t_1\right|+\cdots+\left|t_n\right|\right)} T\left[\hat{H}_1\left(t_1\right) \cdots \hat{H}_1\left(t_n\right)\right] \tag{3.25}$$

Note that we derive this result for time-independent $\hat{H}$. We need to verify that this equation holds for time-dependent Hamiltonian and for all t, t_0.

Starting from $t_0=-\infty$, and we start from $\left|\Phi_0\right\rangle$, which is the ground state of H_0, as t goes to 0, we can intuitively understand that we are slowly turning on $\hat{H}_1$, and at $t=0$ we get

$$\left|\Psi_H^\epsilon\right\rangle=\left|\Psi_I^\epsilon(0)\right\rangle=\hat{U}_\epsilon(0,-\infty)\left|\Phi_0\right\rangle \tag{3.26}$$

As ϵ goes to 0, i.e. we are turning on the H_1 more and more slowly, we are approaching the so called *adiabatic* switching regime, in which as $\hat{H}(t)$ changes very slowly, the quantum states changes and always stays at the ground state of $\hat{H}(t)$.

We are hoping that the adiabatic switching is reached as $\epsilon \to 0$. However, $\hat{U}_\epsilon(0,-\infty)\left|\Phi_0\right\rangle$ doesn't have a limit as $\epsilon \to 0$. In fact, if we let $\epsilon = 0$, the phase in $\hat{U}_{\epsilon=0}(0,t)\left|\Phi_0\right\rangle$ diverges as $t \to -\infty$.

A remedy for this is the following Gell-Mann and Low theorem, which considers the following quantity:

$$\lim_{\epsilon\to 0} \frac{\hat{U}_\epsilon(0,-\infty)\left|\Phi_0\right\rangle}{\left\langle\Phi_0\middle|\hat{U}_\epsilon(0,-\infty)\middle|\Phi_0\right\rangle} \tag{3.27}$$

Here the phases cancel out in the numerator and denominator. Gell-Mann and Low theorem states that if the above quantity exists to all orders in perturbation theory, then its limit is the ground state of $\hat{H}$:

$$\lim_{\epsilon\to 0} \frac{\hat{U}_\epsilon(0,-\infty)\left|\Phi_0\right\rangle}{\left\langle\Phi_0\middle|\hat{U}_\epsilon(0,-\infty)\middle|\Phi_0\right\rangle} \equiv \frac{\left|\Psi_0\right\rangle}{\left\langle\Phi_0 \mid \Psi_0\right\rangle} \tag{3.28}$$

Exercises

1. For $\hat{H}_0 = \sum_k \hbar\omega_k c_k^\dagger c_k$, prove that

   $$i\hbar\frac{\partial}{\partial t}c_{kI}(t) = \hbar\omega_k c_{kI}(t)$$

   and therefore $c_{kI}(t) = c_k \mathrm{e}^{-\mathrm{i}\omega_k t}$, $c_{kI}^\dagger(t) = c_k^\dagger \mathrm{e}^{\mathrm{i}\omega_k t}$.

2. Derive eq 3.13 from previous equations.

3. Derive eq 3.19. And verify that the following formulation reproduces eq 3.19 by term.

   $$U(t,t_0) = T\left\{\exp\left[-\mathrm{i}\hbar^{-1}\int_{t_0}^{t}\mathrm{d}t'\hat{H}_1(t')\right]\right\} \tag{3.29}$$

4. Prove that for Φ_0 and Ψ_0 in Gell-Mann and Low theorem, we have

   $$E - E_0 = \frac{\left\langle\Phi_0\middle|\hat{H}_1\middle|\Psi_0\right\rangle}{\left\langle\Phi_0 \mid \Psi_0\right\rangle} \tag{3.30}$$

5. Prove Gell-Mann and Low theorem in a physical manner. (See Fetter & Walecka Page 62-64)

3.2 Green's functions

Definition

Let $|\Psi_0\rangle$ be the ground state of the interacting system.

$$\hat{H}\,|\Psi_0\rangle = E\,|\Psi_0\rangle$$

Let us define the Heisenberg operator

$$\hat{\psi}_{\alpha,H}(\boldsymbol{x},t) = e^{\mathrm{i}\hat{H}t/\hbar}\hat{\psi}_\alpha(\boldsymbol{x})e^{-\mathrm{i}\hat{H}t/\hbar} \tag{3.31}$$

where α denotes spin and $\psi_\alpha(x)$ is the field operator. It can take two values for spin-$\frac{1}{2}$ fermions, whereas there are no indices for spin-zero bosons.
The single particle Green's function is defined as

$$G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) = -\mathrm{i}\left\langle \Psi_0 \left| T\left[\hat{\psi}_{\alpha,H}(\boldsymbol{x},t)\hat{\psi}^\dagger_{\beta,H}\left(\boldsymbol{x}',t'\right)\right]\right| \Psi_0\right\rangle \tag{3.32}$$

The time-ordering operator T is modified a little bit here;

$$T\left[\hat{\psi}_{\alpha,H}(\boldsymbol{x},t)\hat{\psi}^\dagger_{\beta,H}\left(\boldsymbol{x}',t'\right)\right] = \begin{cases} \hat{\psi}_{\alpha,H}(\boldsymbol{x},t)\hat{\psi}^\dagger_{\beta,H}\left(\boldsymbol{x}',t'\right) & t > t' \\ \pm\hat{\psi}^\dagger_{\beta,H}\left(\boldsymbol{x}',t'\right)\hat{\psi}_{\alpha,H}(\boldsymbol{x},t) & t' > t \end{cases} \tag{3.33}$$

where the upper (lower) sign refers to bosons (fermions). More generally, the T product of several operators orders them from right to left in ascending time order and adds a factor $(-1)^P$, where P is the number of interchanges of fermion operators from the original given order.

$$G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) = \begin{cases} -\mathrm{i}\left\langle \Psi_0 \left|\hat{\psi}_{\alpha,H}(\boldsymbol{x},t)\hat{\psi}^\dagger_{\beta,H}\left(\boldsymbol{x}',t'\right)\right| \Psi_0\right\rangle & t > t' \\ \mp\mathrm{i}\left\langle \Psi_0 \left|\hat{\psi}^\dagger_{\beta,H}\left(\boldsymbol{x}',t'\right)\hat{\psi}_{\alpha,H}(\boldsymbol{x},t)\right| \Psi_0\right\rangle & t' > t \end{cases} \tag{3.34}$$

If $\hat{H}$ is time-independent, we have

$$G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) = \begin{cases} -\mathrm{i}\mathrm{e}^{\mathrm{i}E(t-t')/\hbar}\left\langle \Psi_0 \left|\hat{\psi}_\alpha(\boldsymbol{x})\mathrm{e}^{-\mathrm{i}\hat{H}(t-t')/\hbar}\hat{\psi}^\dagger_\beta\left(\boldsymbol{x}'\right)\right| \Psi_0\right\rangle & t > t' \\ \mp\mathrm{i}\mathrm{e}^{-\mathrm{i}E(t-t')/\hbar}\left\langle \Psi_0 \left|\hat{\psi}^\dagger_\beta\left(\boldsymbol{x}'\right)\mathrm{e}^{\mathrm{i}\hat{H}(t-t')/\hbar}\hat{\psi}_\alpha(\boldsymbol{x})\right| \Psi_0\right\rangle & t' > t \end{cases} \tag{3.35}$$

We can see that $G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right)$ only depends on $(t-t')$.
Consider the single particle operator

$$\hat{J} = \int \mathrm{d}\boldsymbol{x}\hat{\mathcal{J}}(\boldsymbol{x}) = \int \mathrm{d}\boldsymbol{x}\hat{\psi}^\dagger_\beta(\boldsymbol{x})J^{\beta\alpha}(\boldsymbol{x})\hat{\psi}_\alpha(\boldsymbol{x}) \tag{3.36}$$

where $\hat{\mathcal{J}}(\boldsymbol{x})$ is the second quantized density. We have

$$\begin{aligned}\langle\hat{\mathcal{J}}(\boldsymbol{x})\rangle &= \langle\Psi_0|\,\hat{\mathcal{J}}(\boldsymbol{x})\,|\Psi_0\rangle = \lim_{\boldsymbol{x}'\to\boldsymbol{x}} J^{\beta\alpha}(\boldsymbol{x})\left\langle \Psi_0 \left|\hat{\psi}^\dagger_\beta\left(\boldsymbol{x}'\right)\hat{\psi}_\alpha(\boldsymbol{x})\right| \Psi_0\right\rangle \\ &= \pm\mathrm{i}\lim_{t'\to t^+}\lim_{\boldsymbol{x}'\to\boldsymbol{x}} J^{\beta\alpha}(\boldsymbol{x})G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) = \pm\mathrm{i}\lim_{t'\to t^+}\lim_{\boldsymbol{x}'\to\boldsymbol{x}}\mathrm{tr}(J(\boldsymbol{x})G\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right))\end{aligned} \tag{3.37}$$

$$\langle \hat{J} \rangle = \int \mathrm{d}\boldsymbol{x} \langle \hat{\mathcal{J}}(\boldsymbol{x}) \rangle = \pm \mathrm{i} \int \mathrm{d}\boldsymbol{x}\, \mathrm{tr}(J(\boldsymbol{x}) G\left(\boldsymbol{x}, t; \boldsymbol{x}, t_{+}\right)) \tag{3.38}$$

For example, we have particle density

$$\langle \hat{n}(\boldsymbol{x}) \rangle = \pm \mathrm{i}\, \mathrm{tr}\, G\left(\boldsymbol{x}, t; \boldsymbol{x}, t_{+}\right) \tag{3.39}$$

and we have the spin density

$$\langle \hat{\boldsymbol{\sigma}}(\boldsymbol{x}) \rangle = \pm \mathrm{i}\, \mathrm{tr}\left[\boldsymbol{\sigma} G\left(\boldsymbol{x}, t; \boldsymbol{x}, t_{+}\right)\right] \tag{3.40}$$

We have the kinetic energy as

$$\langle \hat{T} \rangle = \pm \mathrm{i} \int \mathrm{d}\boldsymbol{x} \lim_{\boldsymbol{x}' \to \boldsymbol{x}} \left[-\frac{\hbar^2 \nabla^2}{2m}\, \mathrm{tr}\, G\left(\boldsymbol{x}, t; \boldsymbol{x}', t_{+}\right) \right] \tag{3.41}$$

Now we want to give an expression for $\langle \hat{V} \rangle$, which is a two-particle quantity. Normally, the one-particle Green's function can not be used to express a two-particle operator, but $\langle \hat{V} \rangle$ is different since it is a part of $\hat{H}$:

$$\begin{aligned} \hat{H} = & \sum_{\alpha} \int \mathrm{d}\boldsymbol{x} \hat{\psi}_{\alpha}^{\dagger}(\boldsymbol{x}) T(\boldsymbol{x}) \hat{\psi}_{\alpha}(\boldsymbol{x}) \\ & + \frac{1}{2} \sum_{\substack{\alpha\alpha' \\ \beta\beta'}} \int \mathrm{d}\boldsymbol{x} \mathrm{d}\boldsymbol{x}' \hat{\psi}_{\alpha}^{\dagger}(\boldsymbol{x}) \hat{\psi}_{\beta}^{\dagger}\left(\boldsymbol{x}'\right) V\left(\boldsymbol{x}, \boldsymbol{x}'\right)_{\alpha\alpha', \beta\beta'} \hat{\psi}_{\beta'}\left(\boldsymbol{x}'\right) \hat{\psi}_{\alpha'}(\boldsymbol{x}) \end{aligned} \tag{3.42}$$

Then from

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \hat{\psi}_{\alpha, H}(\boldsymbol{x}t) = e^{\mathrm{i}\hat{H}t/\hbar} \left[\hat{\psi}_{\alpha}(\boldsymbol{x}), \hat{H}\right] e^{-\mathrm{i}\hat{H}t/\hbar} \tag{3.43}$$

we have (left as an exercise)

$$\left[\mathrm{i}\hbar \frac{\partial}{\partial t} - T(\boldsymbol{x})\right] \hat{\psi}_{\alpha, H}(\boldsymbol{x}, t) = \sum_{\beta'\gamma\gamma'} \int \mathrm{d}\boldsymbol{z}' \hat{\psi}_{\gamma, H}^{\dagger}\left(\boldsymbol{z}', t\right) V\left(\boldsymbol{x}, \boldsymbol{z}'\right)_{\alpha\beta', \gamma\gamma'} \hat{\psi}_{\gamma', H}\left(\boldsymbol{z}', t\right) \hat{\psi}_{\beta', H}(\boldsymbol{x}, t) \tag{3.44}$$

therefore we have (left as an exercise)

$$\langle \hat{V} \rangle = \pm \frac{1}{2} \mathrm{i} \int \mathrm{d}x \lim_{t' \to t^{+}} \lim_{\boldsymbol{x}' \to \boldsymbol{x}} \sum_{\alpha} \left[\mathrm{i}\hbar \frac{\partial}{\partial t} - T(\boldsymbol{x})\right] G_{\alpha\alpha}\left(\boldsymbol{x}, t; \boldsymbol{x}', t'\right) \tag{3.45}$$

Then

$$E = \langle \hat{T} + \hat{V} \rangle = \langle \hat{H} \rangle = \pm \frac{1}{2} \mathrm{i} \int \mathrm{d}\boldsymbol{x} \lim_{t' \to t^{+}} \lim_{\boldsymbol{x}' \to \boldsymbol{x}} \left[\mathrm{i}\hbar \frac{\partial}{\partial t} + T(\boldsymbol{x})\right] \mathrm{tr}\, G\left(\boldsymbol{x}, t; \boldsymbol{x}', t'\right) \tag{3.46}$$

If we express $\boldsymbol{x}$ in plane wave basis, and transform $(t - t')$ to its frequency domain, we have Green's funtion $G_{\alpha\beta}(\boldsymbol{k}, \omega)$:

$$G_{\alpha\beta}\left(\boldsymbol{x}, t; \boldsymbol{x}', t'\right) = (2\pi)^{-4} \int \mathrm{d}\boldsymbol{k} \int_{-\infty}^{\infty} \mathrm{d}\omega e^{\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{x} - \boldsymbol{x}')} e^{-\mathrm{i}\omega(t - t')} G_{\alpha\beta}(\boldsymbol{k}, \omega) \tag{3.47}$$

Exercises

1. Derive equation 3.45 and 3.46 from previous equations.

2. For $G(\boldsymbol{k}, \omega)$ (3.47), verify that we have

$$N = \int \mathrm{d}\boldsymbol{x} \langle \hat{n}(\boldsymbol{x}) \rangle = \pm \mathrm{i} \frac{V}{(2\pi)^4} \lim_{\eta \to 0^+} \int \mathrm{d}\boldsymbol{k} \int_{-\infty}^{\infty} \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \operatorname{tr} G(\boldsymbol{k}, \omega) \tag{3.48}$$

$$E = \pm \frac{1}{2} \mathrm{i} \frac{V}{(2\pi)^4} \lim_{\eta \to 0^+} \int \mathrm{d}\boldsymbol{k} \int_{-\infty}^{\infty} \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \left(\frac{\hbar^2 |\boldsymbol{k}|^2}{2m} + \hbar\omega \right) \operatorname{tr} G(\boldsymbol{k}, \omega) \tag{3.49}$$

   In the future we will use η to mean 0_+, and drop the $\lim_{\eta \to 0^+}$ for convenience.

3. Consider $\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}_1$ and $\hat{H}(\lambda) |\Psi_0(\lambda)\rangle = E(\lambda) |\Psi_0(\lambda)\rangle$. Let $E(\lambda) = \left\langle \Psi_0(\lambda) | \hat{H}(\lambda) | \Psi_0(\lambda) \right\rangle$.

   (a) Prove that

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} E(\lambda) = \left\langle \Psi_0(\lambda) \left| \hat{H}_1 \right| \Psi_0(\lambda) \right\rangle \tag{3.50}$$

   (b) Based on (a), prove that

$$E - E_0 = \pm \frac{\mathrm{i}}{2} \frac{V}{(2\pi)^4} \int_0^1 \frac{\mathrm{d}\lambda}{\lambda} \int \mathrm{d}\boldsymbol{k} \int_{-\infty}^{\infty} \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \left(\hbar\omega - \frac{\hbar^2 |\boldsymbol{k}|^2}{2m} \right) \operatorname{tr} G^{\lambda}(\boldsymbol{k}, \omega) \tag{3.51}$$

4. Let us investigate the Green's function of the noninteracting system of free fermions. Let

$$\hat{\psi}(\boldsymbol{x}) = \sum_{\boldsymbol{k}\lambda} \psi_{\boldsymbol{k}\lambda}(\boldsymbol{x}) c_{\boldsymbol{k}\lambda} \tag{3.52}$$

   where

$$c_{\boldsymbol{k}\lambda} = \begin{cases} a_{\boldsymbol{k}\lambda} & k > k_F \quad \text{particles} \\ b^{\dagger}_{-\boldsymbol{k}\lambda} & k < k_F \quad \text{holes} \end{cases} \tag{3.53}$$

   Here

$$\left\{ a_k, a^{\dagger}_{k'} \right\} = \left\{ b_k, b^{\dagger}_{k'} \right\} = \delta_{kk'} \tag{3.54}$$

   Consider the following Hamiltonian

$$\hat{H}_0 = \sum_{\boldsymbol{k}\lambda} \hbar\omega_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\lambda} c_{\boldsymbol{k}\lambda} \tag{3.55}$$

   (a) Prove that

$$\hat{H}_0 = \sum_{\boldsymbol{k}\lambda > k_F} \hbar\omega_{\boldsymbol{k}} a^{\dagger}_{\boldsymbol{k}\lambda} a_{\boldsymbol{k}\lambda} - \sum_{\boldsymbol{k}\lambda < k_F} \hbar\omega_{\boldsymbol{k}} b^{\dagger}_{\boldsymbol{k}\lambda} b_{\boldsymbol{k}\lambda} + \sum_{\boldsymbol{k}\lambda < k_F} \hbar\omega_{\boldsymbol{k}} \tag{3.56}$$

(b) Prove that

$$\mathrm{i}G^0_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right) = \delta_{\alpha\beta}(2\pi)^{-3}\int \mathrm{d}\boldsymbol{k}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')}e^{-\mathrm{i}\omega_{\boldsymbol{k}}(t-t')} \times\left[\theta\left(t-t'\right)\theta\left(|\boldsymbol{k}|-k_F\right)-\theta\left(t'-t\right)\theta\left(k_F-|\boldsymbol{k}|\right)\right] \tag{3.57}$$

(c) Prove that

$$G^0_{\alpha\beta}(\boldsymbol{k},\omega) = \delta_{\alpha\beta}\left[\frac{\theta\left(|\boldsymbol{k}|-k_F\right)}{\omega-\omega_{\boldsymbol{k}}+\mathrm{i}\eta}+\frac{\theta\left(k_F-|\boldsymbol{k}|\right)}{\omega-\omega_{\boldsymbol{k}}-\mathrm{i}\eta}\right] \tag{3.58}$$

Hint: use

$$\theta\left(t-t'\right) = -\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{\mathrm{e}^{-\mathrm{i}\omega(t-t')}}{\omega+\mathrm{i}\eta} \tag{3.59}$$

3.3 Lehmann representation

Before we started, I must confess that I am not satisfied with the following treatment on Lehmann representation. The downside of this note is that it is restricted to the case that G only relies on $\boldsymbol{x}-\boldsymbol{x}'$ (w.r.t rely on both of them). I recommend readers first take a look at the other note that I write on this. After that, go back to this note, and there are some new things mentioned here.

Below we focus on the fermionic case. Let us go back to the definition of Green's function:

$$\begin{aligned} G_{\alpha\beta}(\boldsymbol{x},t;\boldsymbol{x}',t') = &-\mathrm{i}\left\langle \Psi_0 \left| \hat{\psi}_{\alpha,H}(\boldsymbol{x},t)\hat{\psi}^\dagger_{\beta,H}(\boldsymbol{x}',t')\,\theta(t-t') \right| \Psi_0 \right\rangle \\ &+\mathrm{i}\left\langle \Psi_0 \left| \hat{\psi}^\dagger_{\beta,H}(\boldsymbol{x}',t')\,\hat{\psi}_{\alpha,H}(\boldsymbol{x},t)\theta(t'-t) \right| \Psi_0 \right\rangle \end{aligned} \tag{3.60}$$

We want to insert a complete basis $\sum_n |\Psi_n\rangle\langle\Psi_n|$, then we have:

$$\begin{aligned} G_{\alpha\beta}(\boldsymbol{x},t;\boldsymbol{x}',t') = &-\mathrm{i}\sum_n \theta(t-t')\left\langle \Psi_0 \left| \hat{\psi}_{\alpha,H}(\boldsymbol{x},t) \right| \Psi_n \right\rangle \left\langle \Psi_n \left| \hat{\psi}^\dagger_{\beta,H}(\boldsymbol{x}',t') \right| \Psi_0 \right\rangle \\ &+\mathrm{i}\sum_n \theta(t'-t)\left\langle \Psi_0 \left| \hat{\psi}^\dagger_{\beta,H}(\boldsymbol{x}',t') \right| \Psi_n \right\rangle \left\langle \Psi_n \left| \hat{\psi}_{\alpha,H}(\boldsymbol{x},t) \right| \Psi_0 \right\rangle \end{aligned} \tag{3.61}$$

Recall the definition of Heisenberg operators, we have

$$\begin{aligned} G_{\alpha\beta}(\boldsymbol{x},t;\boldsymbol{x}',t') = &-\mathrm{i}\sum_n \theta(t-t')\mathrm{e}^{-\mathrm{i}(E_n-E)(t-t')/\hbar}\left\langle \Psi_0 \left| \hat{\psi}_{\alpha}(\boldsymbol{x}) \right| \Psi_n \right\rangle \left\langle \Psi_n \left| \hat{\psi}^\dagger_{\beta}(\boldsymbol{x}') \right| \Psi_0 \right\rangle \\ &+\mathrm{i}\sum_n \theta(t'-t)\mathrm{e}^{\mathrm{i}(E_n-E)(t-t')}\left\langle \Psi_0 \left| \hat{\psi}^\dagger_{\beta}(\boldsymbol{x}') \right| \Psi_n \right\rangle \left\langle \Psi_n \left| \hat{\psi}_{\alpha}(\boldsymbol{x}) \right| \Psi_0 \right\rangle \end{aligned} \tag{3.62}$$

Since we have the property of number operator $\hat{N}$ (left as an exercise):

$$\left[\hat{N},\hat{\psi}_\beta(\boldsymbol{z})\right] = -\hat{\psi}_\beta(\boldsymbol{z}),\ \text{ where } \hat{N} = \sum_\alpha \int \mathrm{d}\boldsymbol{x}\hat{\psi}^\dagger_\alpha(\boldsymbol{x})\hat{\psi}_\alpha(\boldsymbol{x}) \tag{3.63}$$

then we have

$$\hat{N}\left[\hat{\psi}_\beta(\boldsymbol{z})\,|\Psi_0\rangle\right] = (N-1)\left[\hat{\psi}_\beta(\boldsymbol{z})\,|\Psi_0\rangle\right] \tag{3.64}$$

In other words $\hat{\psi}_\beta(\boldsymbol{z})\,|\Psi_0\rangle$ is a $(N-1)$-particle state. Similarly, $\hat{\psi}^\dagger_\beta(\boldsymbol{z})\,|\Psi_0\rangle$ is a $(N+1)$-particle state.

Now, let us assume $\hat{H}$ is translation invariant. In other words, $\hat{H}$ commutes with the momentum operator $\boldsymbol{P}$:

$$\hat{\boldsymbol{P}} = \sum_\alpha \int \mathrm{d}\boldsymbol{x}\hat{\psi}^\dagger_\alpha(\boldsymbol{x})(-\mathrm{i}\hbar\nabla)\hat{\psi}_\alpha(\boldsymbol{x}) = \sum_{\boldsymbol{k}\lambda}\hbar\boldsymbol{k}c^\dagger_{\boldsymbol{k}\lambda}c_{\boldsymbol{k}\lambda} \tag{3.65}$$

and therefore we have (left as an exercise):

$$\hat{\psi}_\alpha(\boldsymbol{x}) = e^{-\mathrm{i}\hat{\boldsymbol{P}}\cdot\boldsymbol{x}/\hbar}\hat{\psi}_\alpha(0)e^{\mathrm{i}\hat{\boldsymbol{P}}\cdot\boldsymbol{x}/\hbar} \tag{3.66}$$

Since $\hat{P}|\Psi_0\rangle = 0$ (left as an exercise), we have:

$$\begin{aligned}
&\mathrm{i}G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right)\\
=&\sum_n\Big[\theta\left(t-t'\right)e^{-\mathrm{i}(E_n-E)(t-t')/\hbar}e^{\mathrm{i}\boldsymbol{P}_n\cdot(\boldsymbol{x}-\boldsymbol{x}')/\hbar}\times\left\langle\Psi_0\left|\hat{\psi}_\alpha(0)\right|\Psi_n\right\rangle\left\langle\Psi_n\left|\hat{\psi}^\dagger_\beta(0)\right|\Psi_0\right\rangle\\
&-\theta\left(t'-t\right)e^{\mathrm{i}(E_n-E)(t-t')/\hbar}e^{-\mathrm{i}\boldsymbol{P}_n\cdot(\boldsymbol{x}-\boldsymbol{x}')/\hbar}\times\left\langle\Psi_0\left|\hat{\psi}^\dagger_\beta(0)\right|\Psi_n\right\rangle\left\langle\Psi_n\left|\hat{\psi}_\alpha(0)\right|\Psi_0\right\rangle\Big]
\end{aligned}\tag{3.67}$$

Therefore

$$\begin{aligned}
G_{\alpha\beta}(\boldsymbol{k},\omega)&=\int\mathrm{d}\left(\boldsymbol{x}-\boldsymbol{x}'\right)\int\mathrm{d}\left(t-t'\right)e^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\dot{\boldsymbol{x}}')}e^{i\omega(t-t')}G_{\alpha\beta}\left(\boldsymbol{x},t;\boldsymbol{x}',t'\right)\\
&=V\sum_n\delta_{\boldsymbol{k},\boldsymbol{P}_n/\hbar}\frac{\left\langle\Psi_0\left|\hat{\psi}_\alpha(0)\right|\Psi_n\right\rangle\left\langle\Psi_n\left|\hat{\psi}^\dagger_\beta(0)\right|\Psi_0\right\rangle}{\omega-\hbar^{-1}\left(E_n-E\right)+\mathrm{i}\eta}\\
&+V\sum_n\delta_{\boldsymbol{k},-\boldsymbol{P}_n/\hbar}\frac{\left\langle\Psi_0\left|\hat{\psi}^\dagger_\beta(0)\right|\Psi_n\right\rangle\left\langle\Psi_n\left|\hat{\psi}_\alpha(0)\right|\Psi_0\right\rangle}{\omega+\hbar^{-1}\left(E_n-E\right)-\mathrm{i}\eta}
\end{aligned}\tag{3.68}$$

Let us write $|\Psi_n\rangle = |N,\boldsymbol{P}/\hbar,m\rangle$, meaning that it is the m-th eigenfunction with particle number N and momentum $\boldsymbol{P}$, then we have

$$\begin{aligned}
G_{\alpha\beta}(\boldsymbol{k},\omega)=&V\sum_m\frac{\left\langle\Psi_0\left|\hat{\psi}_\alpha(0)\right|N+1,\boldsymbol{k},m\right\rangle\left\langle N+1,\boldsymbol{k},m\left|\hat{\psi}^\dagger_\beta(0)\right|\Psi_0\right\rangle}{\omega-\hbar^{-1}\left(E_{N+1,\boldsymbol{k},m}-E_{N,\boldsymbol{0},0}\right)+\mathrm{i}\eta}\\
&+V\sum_m\frac{\left\langle\Psi_0\left|\hat{\psi}^\dagger_\beta(0)\right|N-1,-\boldsymbol{k},m\right\rangle\left\langle N-1,-\boldsymbol{k},m\left|\hat{\psi}_\alpha(0)\right|\Psi_0\right\rangle}{\omega+\hbar^{-1}\left(E_{N-1,-\boldsymbol{k},m}-E_{N,\boldsymbol{0},0}\right)-\mathrm{i}\eta}\\
&=\hbar V\sum_m\frac{\left\langle\Psi_0\left|\hat{\psi}_\alpha(0)\right|N+1,\boldsymbol{k},m\right\rangle\left\langle N+1,\boldsymbol{k},m\left|\hat{\psi}^\dagger_\beta(0)\right|\Psi_0\right\rangle}{\hbar\omega-\mu-\epsilon_{N+1,\boldsymbol{k},m}+\mathrm{i}\eta}\\
&+\hbar V\sum_m\frac{\left\langle\Psi_0\left|\hat{\psi}^\dagger_\beta(0)\right|N-1,-\boldsymbol{k},m\right\rangle\left\langle N-1,-\boldsymbol{k},m\left|\hat{\psi}_\alpha(0)\right|\Psi_0\right\rangle}{\hbar\omega-\mu+\epsilon_{N-1,-\boldsymbol{k},m}-\mathrm{i}\eta}
\end{aligned}\tag{3.69}$$

where

$$E_{N+1,\boldsymbol{k},m}-E_{N,\boldsymbol{0},0}=\left(E_{N+1,\boldsymbol{k},m}-E_{N+1,\boldsymbol{0},0}\right)+\mu=\epsilon_{N+1,\boldsymbol{k},m}+\mu,\quad\epsilon_{N+1,\boldsymbol{k},m}>0$$

$$E_{N-1,\boldsymbol{k},m}-E_{N,\boldsymbol{0},0}=\left(E_{N-1,\boldsymbol{k},m}-E_{N-1,\boldsymbol{0},0}\right)-\mu=\epsilon_{N-1,\boldsymbol{k},m}-\mu,\quad\epsilon_{N-1,\boldsymbol{k},m}>0$$

Note that if the Hamiltonian is invariant under rotation, then we have

$$G_{\alpha\beta}(\boldsymbol{k},\omega)=\delta_{\alpha\beta}G(\boldsymbol{k},\omega)=\delta_{\alpha\beta}G(|\boldsymbol{k}|,\omega)\tag{3.70}$$

Let us give the following remark on the analytic property of Green's function:

- $G(\boldsymbol{k}, \omega)$ is a meromorphic function of $\hbar\omega$, with simple poles at the exact excitation energies of the interacting system corresponding to a momentum $\hbar\boldsymbol{k}$.

- For frequencies below $\mu/\hbar$, these singularities lie slightly above the real axis, and for frequencies above $\mu/\hbar$, these singularities lie slightly below the real axis. In this way, the singularities of the Green's function immediately yield the energies of those excited states for which the numerator does not vanish.

- For an interacting system, the field operator connects the ground state with very many excited states of the system containing $N \pm 1$ particles.

- For the non-interacting system, however, the field operator connects only one state to the ground state, so that $G^0(\boldsymbol{k}, \omega)$ has only a single pole, slightly below the real axis at $\hbar\omega = \hbar^2 k^2/2m$ if $k > k_F$ and slightly above the real axis at the same value of $\hbar\omega$ if $k < k_F$.

- It is clear from this discussion that the Green's function G is analytic in neither the upper nor the lower w plane.

We therefore define the retarded Green's function and advanced Green's function.

$$\begin{aligned} G^R_{\alpha\beta}(\boldsymbol{x}, t; \boldsymbol{x}', t') &= -\mathrm{i}\left\langle \Psi_0 \left| \left\{ \hat{\psi}_{\alpha,H}(\boldsymbol{x}, t), \hat{\psi}^\dagger_{\beta,H}(\boldsymbol{x}', t') \right\} \right| \Psi_0 \right\rangle \theta(t - t') \\ G^A_{\alpha\beta}(\boldsymbol{x}, t; \boldsymbol{x}', t') &= +\mathrm{i}\left\langle \Psi_0 \left| \left\{ \hat{\psi}_{\alpha,H}(\boldsymbol{x}, t), \hat{\psi}^\dagger_{\beta,H}(\boldsymbol{x}', t') \right\} \right| \Psi_0 \right\rangle \theta(t' - t) \end{aligned} \tag{3.71}$$

and we have

$$\begin{aligned} G^{\mathrm{R},A}_{\alpha\beta}(\boldsymbol{k}, \omega) = {} & \hbar V \sum_m \frac{\left\langle \Psi_0 \left| \hat{\psi}_\alpha(0) \right| N+1, \boldsymbol{k}, m \right\rangle \left\langle N+1, \boldsymbol{k}, m \left| \hat{\psi}^\dagger_\beta(0) \right| \Psi_0 \right\rangle}{\hbar\omega - \mu - \epsilon_{N+1,\boldsymbol{k},m} \pm \mathrm{i}\eta} \\ & + \hbar V \sum_m \frac{\left\langle \Psi_0 \left| \hat{\psi}^\dagger_\beta(0) \right| N-1, -\boldsymbol{k}, m \right\rangle \left\langle N-1, -\boldsymbol{k}, m \left| \hat{\psi}_\alpha(0) \right| \Psi_0 \right\rangle}{\hbar\omega - \mu + \epsilon_{N-1,-\boldsymbol{k},m} \pm \mathrm{i}\eta} \end{aligned} \tag{3.72}$$

- $G^R(\boldsymbol{k}, \omega)$ and $G^A(\boldsymbol{k}, \omega)$ are again meromorphic functions of ω.

- All the poles of $G^R(\boldsymbol{k}, \omega)$ lie in the lower half plane, so that $G^R(\boldsymbol{k}, \omega)$ is analytic for $\mathrm{Im}\,\omega > 0$; in contrast, all the poles of $G^A(\boldsymbol{k}, \omega)$ lie in the upper half plane, so that $G^A(\mathrm{k}, \omega)$ is analytic for $\mathrm{Im}\,\omega < 0$.

- For real ω, we have
$$\left[G^R_{\alpha\beta}(\boldsymbol{k}, \omega)\right]^* = G^A_{\beta\alpha}(\boldsymbol{k}, \omega) \tag{3.73}$$

Now, let us consider the infinite volume limit, where the summation should be replaced by an integral. Let us introduce $A(\boldsymbol{k},\omega')$ by

$$\begin{aligned}
&V\int \mathrm{d}m \frac{\left|\left\langle \Psi_0 \left| \hat{\psi}_\alpha(0) \right| N+1,\boldsymbol{k},m\right\rangle\right|^2}{\omega-\mu/\hbar-\epsilon_{N+1,\boldsymbol{k},m}/\hbar\pm\mathrm{i}\eta} \\
=&V\int_0^\infty \mathrm{d}\omega' \frac{\left|\left\langle \Psi_0 \left| \hat{\psi}_\alpha(0) \right| N+1,\boldsymbol{k},m(\omega')\right\rangle\right|^2}{\omega-\mu/\hbar-\omega'\pm\mathrm{i}\eta}\frac{\mathrm{d}m}{\mathrm{d}\omega'} \\
=&\int_0^\infty \mathrm{d}\omega' \frac{A(\boldsymbol{k},\omega')}{\omega-\mu/\hbar-\omega'\pm\mathrm{i}\eta}
\end{aligned} \tag{3.74}$$

and similarly introduce $B(\boldsymbol{k},\omega')$ by

$$\begin{aligned}
&V\int \mathrm{d}m \frac{\left|\left\langle \Psi_0 \left| \hat{\psi}_\alpha(0) \right| N-1,-\boldsymbol{k},m\right\rangle\right|^2}{\omega-\mu/\hbar+\epsilon_{N-1,-\boldsymbol{k},m}/\hbar\pm\mathrm{i}\eta} \\
=&V\int_0^\infty \mathrm{d}\omega' \frac{\left|\left\langle \Psi_0 \left| \hat{\psi}_\alpha(0) \right| N-1,-\boldsymbol{k},m(\omega')\right\rangle\right|^2}{\omega-\mu/\hbar+\omega'\pm\mathrm{i}\eta}\frac{\mathrm{d}m}{\mathrm{d}\omega'} \\
=&\int_0^\infty \mathrm{d}\omega' \frac{B(\boldsymbol{k},\omega')}{\omega-\mu/\hbar+\omega'\pm\mathrm{i}\eta}
\end{aligned} \tag{3.75}$$

We then have

$$G(\boldsymbol{k},\omega)=\int_0^\infty \mathrm{d}\omega' \left[\frac{A(\boldsymbol{k},\omega')}{\omega-\hbar^{-1}\mu-\omega'+i\eta}+\frac{B(\boldsymbol{k},\omega')}{\omega-\hbar^{-1}\mu+\omega'-i\eta}\right] \tag{3.76}$$

As a result, in the infinite volume limit, $G(\boldsymbol{k},\omega)$ now has a branch cut in the complex ω plane along the whole real axis instead of having a bunch of poles in the finite system case. Similarly, we have

$$G^{R,A}(\boldsymbol{k},\omega)=\int_0^\infty \mathrm{d}\omega' \left[\frac{A(\boldsymbol{k},\omega')}{\omega-\hbar^{-1}\mu-\omega'\pm i\eta}+\frac{B(\boldsymbol{k},\omega')}{\omega-\hbar^{-1}\mu+\omega'\pm i\eta}\right] \tag{3.77}$$

Since we have

$$\frac{1}{\omega\pm\mathrm{i}\eta}=\mathcal{P}\frac{1}{\omega}\mp\mathrm{i}\pi\delta(\omega) \tag{3.78}$$

where $\mathcal{P}$ denotes a Cauchy principal value, therefore we have

$$\operatorname{Re}G^{R,A}(\boldsymbol{k},\omega)=\mp\mathcal{P}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{\pi}\frac{\operatorname{Im}G^{R,A}(\boldsymbol{k},\omega')}{\omega-\omega'} \tag{3.79}$$

This equation also holds for finite systems, where $\operatorname{Im}G$ is a sum of delta functions.

Now consider

$$\left\langle \Psi_0 \left| \left\{ \hat{\psi}_\alpha(\boldsymbol{x}),\hat{\psi}^\dagger_\beta(\boldsymbol{x}')\right\} \right| \Psi_0 \right\rangle=\delta_{\alpha\beta}\delta(\boldsymbol{x}-\boldsymbol{x}') \tag{3.80}$$

Using a similar analysis as before, we have

$$\delta\left(\boldsymbol{x}-\boldsymbol{x}'\right)=\sum_n\left[\mathrm{e}^{\mathrm{i}\boldsymbol{P}_n\cdot(\boldsymbol{x}-\boldsymbol{x}')/\hbar}\left|\left\langle\Psi_n\left|\hat{\psi}_\alpha^\dagger(0)\right|\Psi_0\right\rangle\right|^2+\mathrm{e}^{-\mathrm{i}\boldsymbol{P}_n\cdot(\boldsymbol{x}-\boldsymbol{x}')/\hbar}\left|\left\langle\Psi_n\left|\hat{\psi}_\alpha(0)\right|\Psi_0\right\rangle\right|^2\right] \tag{3.81}$$

With a Fourier transform, we have

$$1=\int_0^\infty \mathrm{d}\omega[A(\boldsymbol{k},\omega)+B(\boldsymbol{k},\omega)] \tag{3.82}$$

As a result, we have, for $|\omega|\to\infty$,

$$\begin{aligned}G(\boldsymbol{k},\omega)=G^R(\boldsymbol{k},\omega)=G^A(\boldsymbol{k},\omega)&\sim\frac{1}{\omega}\int_0^\infty d\omega'\left[A\left(\boldsymbol{k},\omega'\right)+B\left(\boldsymbol{k},\omega'\right)\right]\\&\sim\frac{1}{\omega}\quad|\omega|\to\infty\end{aligned} \tag{3.83}$$

Exercise

1. Prove equation 3.63.
2. Prove equation 3.66.
3. Prove that if $\hat{P}$ commutes with $\hat{H}$, (with reasonable assumptions) $\hat{P}|\Psi_0\rangle=0$.
4. Please derive 3.58 again using the Lehmann representation.

3.4 Physical interpretation

The first straightforward physical interpretation of Green's function comes from the following identity: for $t > t'$, we have

$$\left\langle \Psi_I(t) \left| \hat{\psi}_{\alpha,I}(\boldsymbol{x},t)\hat{U}\left(t,t'\right)\hat{\psi}^{\dagger}_{\beta,I}\left(\boldsymbol{x}',t'\right) \right| \Psi_I\left(t\right) \right\rangle = \left\langle \Psi_0 \left| \hat{\psi}_{\alpha,H}(\boldsymbol{x},t)\hat{\psi}^{\dagger}_{\beta,H}\left(\boldsymbol{x}',t'\right) \right| \Psi_0 \right\rangle \tag{3.84}$$

where I represents interaction picture. A similar relation could be derived between Schrödinger picture and Heisenberg picture.

The physical interpretation of this is that for $|\Psi_I\left(t'\right)\rangle$, add a particle at the point $(\boldsymbol{x}',t')$, it becomes $\hat{\psi}^{\dagger}_{I\beta}\left(\boldsymbol{x}',t'\right)|\Psi_I'\left(t'\right)\rangle$. Then it propogates through time t' to time t and becomes $\hat{U}\left(t,t'\right)\hat{\psi}^{\dagger}_{I\beta}\left(\boldsymbol{x}',t'\right)|\Psi_I\left(t'\right)\rangle$, and then calculate its overlap with $\hat{\psi}^{\dagger}_{\alpha,I}(\boldsymbol{x},t)\,|\Psi_I(t)\rangle$.

In other words, the Green's function for $t > t'$, characterizes the propagation of a state containing an additional particle. In a similar way, if $t < t'$, the field operator first creates a hole at time t, and the system then propagates according to the full hamiltonian. The Green's function is the probability amplitude at a later time t' for finding a single hole in the ground state of the interacting system.

Now, let us consider

$$G(\boldsymbol{k},t) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}e^{-\mathrm{i}\omega t}G(\boldsymbol{k},\omega) = \int_{-\infty}^{\mu/\hbar}\frac{\mathrm{d}\omega}{2\pi}e^{-\mathrm{i}\omega t}G(\boldsymbol{k},\omega) + \int_{\mu/\hbar}^{\infty}\frac{\mathrm{d}\omega}{2\pi}e^{-\mathrm{i}\omega t}G(\boldsymbol{k},\omega) \tag{3.85}$$

For the first term, i.e. the integral on $[-\infty,\mu/\hbar]$, we have $G(\boldsymbol{k},\omega) = G^A(\boldsymbol{k},\omega)$

$$\int_{-\infty}^{\mu/\hbar}\frac{\mathrm{d}\omega}{2\pi}e^{-\mathrm{i}\omega t}G(\boldsymbol{k},\omega) = \int_{-\infty}^{\mu/\hbar}\frac{\mathrm{d}\omega}{2\pi}e^{-\mathrm{i}\omega t}G^A(\boldsymbol{k},\omega) \tag{3.86}$$

and $G(\boldsymbol{k},\omega)$ is analytic on the lower half plane. We can then use the widely applied complex analysis trick (in 1):

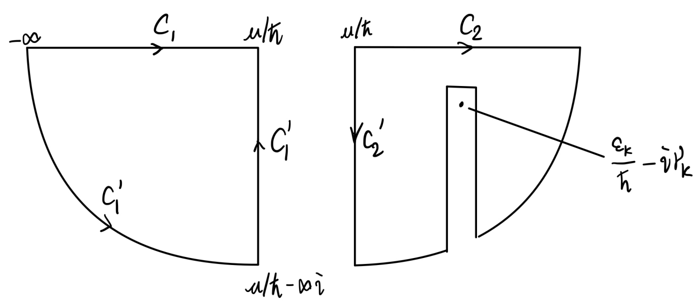

Figure 1: contour for $G(k,t)$

The contribution from the arc vanishes at $\omega \to \infty$ (since we have proved that $G(\omega) \sim 1/\omega$ as $\omega \to \infty$), therefore we have

$$\int_{-\infty}^{\mu/\hbar}\frac{\mathrm{d}\omega}{2\pi}e^{-\mathrm{i}\omega t}G(\boldsymbol{k},\omega) = \int_{\mu/\hbar-\mathrm{i}\infty}^{\mu/\hbar}\frac{\mathrm{d}\omega}{2\pi}e^{-\mathrm{i}\omega t}G^A(\boldsymbol{k},\omega) \tag{3.87}$$

For the second term, i.e. the integral on $[\mu/\hbar, \infty]$, we would like to use the same trick since $G = G^R$, However, G^R is not analytic on the lower half plane. We don't have any particular knowledge about the poles of G^R on the lower half plane at all. But, in order to demonstrate what $G(\boldsymbol{k}, t)$ looks like (and the physics within), let us assume for now that G^R has a single pole close to the real axis on the lower half plane at $\omega = \hbar^{-1}\epsilon_k - \mathrm{i}\gamma_k$ with residue a. Then we have

$$\int_{\mu/\hbar}^{\infty} \frac{\mathrm{d}\omega}{2\pi} e^{-\mathrm{i}\omega t} G(\boldsymbol{k}, \omega) = \int_{\mu/\hbar}^{\mu/\hbar - \mathrm{i}\infty} \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} G^R(\boldsymbol{k}, \omega) - \mathrm{i}a e^{-\mathrm{i}\epsilon_k t/\hbar} e^{-\gamma_k t} \tag{3.88}$$

Therefore we have

$$G(\boldsymbol{k}, t) = \int_{\mu/\hbar - \mathrm{i}\infty}^{\mu/\hbar} \frac{\mathrm{d}\omega}{2\pi} e^{-\mathrm{i}\omega t} \left[G^A(\boldsymbol{k}, \omega) - G^R(\boldsymbol{k}, \omega)\right] - \mathrm{i}a e^{-\mathrm{i}\epsilon_k t/\hbar} e^{-\gamma_k t} \tag{3.89}$$

where

$$\begin{aligned} G^R(\boldsymbol{k}, \omega) &\approx \frac{a}{\omega - \epsilon_k/\hbar + i\gamma_k} \\ G^A(\boldsymbol{k}, \omega) = \left[G^R(\boldsymbol{k}, \omega)\right]^* &\approx \frac{a}{\omega - \epsilon_k/\hbar - i\gamma_k} \end{aligned} \tag{3.90}$$

Let us consider the following regime, i.e. $|t|$ is not too large and not too small:

$$|t|\gamma_k \lesssim 1, \quad |t|\left(\epsilon_k - \mu\right) \gg \hbar, \quad \epsilon_k - \mu \geq \hbar\gamma_k \tag{3.91}$$

Then we have

$$\begin{aligned} &\int_{\mu/\hbar - \mathrm{i}\infty}^{\mu/\hbar} \frac{\mathrm{d}\omega}{2\pi} e^{-\mathrm{i}\omega t} \left[G^A(\boldsymbol{k}, \omega) - G^R(\boldsymbol{k}, \omega)\right] \\ &\approx 2\mathrm{i}\gamma_k a \int_{\mu/\hbar - \mathrm{i}\infty}^{\mu/\hbar} \frac{\mathrm{d}\omega}{2\pi} \frac{e^{-\mathrm{i}\omega t}}{\left(\omega - \hbar^{-1}\epsilon_k\right)^2 + \gamma_k^2} \\ &= -\frac{\gamma_k a e^{-\mathrm{i}\mu t/\hbar}}{\pi} \int_0^{\infty} \mathrm{d}u \frac{e^{-ut}}{\gamma_k^2 + \left[\hbar^{-1}\left(\mu - \epsilon_k\right) - \mathrm{i}u\right]^2} \\ &\approx -(\pi t)^{-1} \gamma_k a \hbar^2 \left(\mu - \epsilon_k\right)^{-2} e^{-\mathrm{i}\mu t/\hbar} \ll -\mathrm{i}a e^{-\mathrm{i}\epsilon_k t/\hbar} e^{-\gamma_k t} \end{aligned} \tag{3.92}$$

In other words, we have

$$G(\boldsymbol{k}, t) \approx -\mathrm{i}a \mathrm{e}^{-\mathrm{i}\epsilon_k t/\hbar} \mathrm{e}^{-\gamma_k t} \tag{3.93}$$

This shows that the real and imaginary parts of the poles of the analytic continuation of $G^R(\boldsymbol{k}, \omega)$ into the lower half plane determine the *frequency and lifetime* of the excited states obtained by adding a particle to an interacting ground state.

Similarly, the poles of the analytic continuation of $G^A(\boldsymbol{k}, \omega)$ into the upper half ω plane determine the frequency and lifetime of the state obtained by creating a hole (destroying a particle) in the interacting ground state.