Green's function in many body physics, using contour formalism

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This is largely based on the excellent textbook: *Nonequilibrium Many-body Theory of Quantum Systems: A Modern Introduction*, by Gianluca Stefanucci and Robert van Leeuwen.

Contents

1   Time-dependent Schrödinger equation and evolution operators

We aim to find a solution for the time-dependent Schrödinger equation.

$$\mathrm{i}\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}(t)\,|\Psi(t)\rangle$$

For time-independent Hamitonian $\hat{H}(t) = \hat{H}(t_0)$ (for all t), we have

$$|\Psi(t)\rangle = e^{-\mathrm{i}\hat{H}(t_0)(t-t_0)}|\Psi(t_0)\rangle$$

What we are actually looking for, is the evolution operator.

- The evolution operator $\hat{U}(t, t_0)$ is defined as:

$$|\Psi(t)\rangle = \hat{U}(t, t_0)\,|\Psi(t_0)\rangle$$

  where $\hat{U}(t, t_0)$ is unitary.

- If $t > t_0$, $\hat{H}$ is piecewise constant, i.e. for $t_0 < t_1 < \cdots < t_n < t_{n+1} = t$

$$\hat{H}(\tau) = \hat{H}(t_p) \text{ for } t_p < \tau < t_{p+1},$$

  Then we have

$$|\Psi(t)\rangle = e^{-\mathrm{i}\hat{H}(t_n)(t-t_n)}\,|\Psi(t_n)\rangle = e^{-\mathrm{i}\hat{H}(t_n)(t-t_n)}e^{-\mathrm{i}\hat{H}(t_{n-1})(t_n-t_{n-1})}\,|\Psi(t_{n-1})\rangle$$
$$= e^{-\mathrm{i}\hat{H}(t_n)(t-t_n)}e^{-\mathrm{i}\hat{H}(t_{n-1})(t_n-t_{n-1})}\cdots e^{-\mathrm{i}\hat{H}(t_0)(t_1-t_0)}\,|\Psi(t_0)\rangle$$

  For simplicity, let's assume for now all $t_{p+1} - t_p = \Delta t$.

- Now we are ready to introduce time-ordering operator $\hat{T}$. $\hat{T}$ acts on the product of m Hamitonians of different time in the following way:

$$\hat{T}\left(\hat{H}\,(t_1)\cdots\hat{H}\,(t_m)\right) = \hat{H}\left(t_{P(1)}\right)\cdots\hat{H}\left(t_{P(m)}\right)$$

  where $t_1, \cdots, t_m$ are rearranged in the increasing order: $t_{P(1)} \geq \cdots \geq t_{P(m)}$.

- Why do we introduce the time-ordering operator? It is because we want to write

$$e^{-\mathrm{i}\hat{H}(t_n)\Delta t}e^{-\mathrm{i}\hat{H}(t_{n-1})\Delta t)}\cdots e^{-\mathrm{i}\hat{H}(t_0)\Delta t}$$

in a more compact way. However, $\hat{H}(t_i)$ and $\hat{H}(t_j)$ probably doesn't commute, therefore

$$\mathrm{e}^{-\mathrm{i}\hat{H}(t_n)\Delta t}\mathrm{e}^{-\mathrm{i}\hat{H}(t_{n-1})\Delta t)}\cdots\mathrm{e}^{-\mathrm{i}\hat{H}(t_0)\Delta t} \neq \mathrm{e}^{-\mathrm{i}\Delta t\left(\hat{H}(t_n)+\hat{H}(t_{n-1})+\cdots+\hat{H}(t_0)\right)}$$

But with time ordering operators, we actually have:

$$\mathrm{e}^{-\mathrm{i}\hat{H}(t_n)\Delta t}\mathrm{e}^{-\mathrm{i}\hat{H}(t_{n-1})\Delta t)}\cdots\mathrm{e}^{-\mathrm{i}\hat{H}(t_0)\Delta t} = \hat{T}\left(\mathrm{e}^{-\mathrm{i}\Delta t\left(\hat{H}(t_n)+\hat{H}(t_{n-1})+\cdots+\hat{H}(t_0)\right)}\right)$$

You can verify this through Taylor expansion, but another straightforward way to see this is that under $\hat{T}$, $\hat{H}(t_i)$ and $\hat{H}(t_j)$ does commute.

- In one word, for pieceswise constant Hamiltonian, we have

$$|\Psi(t)\rangle = \hat{T}\left(\mathrm{e}^{-\mathrm{i}\Delta t\left(\sum_p \hat{H}(t_p)\right)}\right)|\Psi(t_0)\rangle$$

- In the spirit of Riemann integral, for general time-dependent Hamiltonian, we should have

$$|\Psi(t)\rangle = \lim_{\Delta t \to 0} \hat{T}\left(\mathrm{e}^{-\mathrm{i}\Delta t\left(\sum_p \hat{H}(t_p)\right)}\right)|\Psi(t_0)\rangle$$
$$= \hat{T}\left(\mathrm{e}^{-\mathrm{i}\int_{t_0}^t \mathrm{d}\tau \hat{H}(\tau)}\right)|\Psi(t_0)\rangle$$

The time evolution operator is, for $t > t_0$

$$\hat{U}(t,t_0) = \hat{T}\left(\mathrm{e}^{-\mathrm{i}\int_{t_0}^t \mathrm{d}\tau \hat{H}(\tau)}\right)$$

- The time evolution operator satisfies the time-dependent Schrödinger equation itself:

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

From this we can also derive the formalism for time evolution opeartor above. We have

$$\hat{U}(t,t_0) = \mathbf{1} - \mathrm{i}\int_{t_0}^t \mathrm{d}t_1 \hat{H}(t_1)\hat{U}(t_1,t_0)$$

We can substitute $\hat{U}$ back into itself again and again, and get:

$$\hat{U}(t,t_0) = \mathbf{1} - \mathrm{i}\int_{t_0}^t \mathrm{d}t_1 \hat{H}(t_1) + (-\mathrm{i})^2 \int_{t_0}^t \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \hat{H}(t_1)\hat{H}(t_2)\hat{U}(t_2,t_0)$$
$$= \sum_{k=0}^{\infty}(-\mathrm{i})^k \int_{t_0}^t \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \cdots \int_{t_0}^{t_{k-1}} \mathrm{d}t_k \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_k)$$

Note that

$$\int_{t_0}^t \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \cdots \int_{t_0}^{t_{k-1}} \mathrm{d}t_k \hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_k) = \frac{1}{k!}\int_{t_0}^t \mathrm{d}t_1 \int_{t_0}^t \mathrm{d}t_2 \cdots \int_{t_0}^t \mathrm{d}t_k \hat{T}\left(\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_k)\right)$$

Therefore

$$\hat{U}(t,t_0) = \sum_{k=0}^{\infty}\frac{(-\mathrm{i})^k}{k!}\int_{t_0}^t \mathrm{d}t_1 \int_{t_0}^t \mathrm{d}t_2 \cdots \int_{t_0}^t \mathrm{d}t_k \hat{T}\left(\hat{H}(t_1)\hat{H}(t_2)\cdots\hat{H}(t_k)\right)$$
$$= \hat{T}\left(\mathrm{e}^{-\mathrm{i}\int_{t_0}^t \mathrm{d}\tau \hat{H}(\tau)}\right)$$

- Similarly, we can prove, for $t < t_0$, we have

$$\hat{U}(t, t_0) = \bar{T}\left(e^{i \int_t^{t_0} d\tau \hat{H}(\tau)}\right)$$

where $\bar{T}$ is the anti-chronological time ordering operator, which reorders the operators with time increasing from the left to the right.

2 Operators in the Heisenberg picture

- With the evolution operator $\hat{U}(t, t_0)$,

$$|\Psi(t)\rangle = \hat{U}(t, t_0)|\Psi_0\rangle$$

- For operator $\hat{O}(t)$, the observation expection is

$$\left\langle \Psi(t)\left|\hat{O}(t)\right|\Psi(t)\right\rangle = \left\langle \Psi_0\left|\hat{U}(t_0, t)\hat{O}(t)\hat{U}(t, t_0)\right|\Psi_0\right\rangle$$

Therefore we define the following operator $\hat{O}_H$, which is called operator in the Heisenberg representation:

$$\hat{O}_H(t) = \hat{U}(t_0, t)\hat{O}(t)\hat{U}(t, t_0)$$

- For example, for density operator $\hat{n}(\boldsymbol{x}) = \hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}(\boldsymbol{x})$, we have $\hat{n}_H(\boldsymbol{x}, t)$ as followed:

$$\hat{n}_H(\boldsymbol{x}, t) = \hat{U}(t_0, t)\hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}(\boldsymbol{x})\hat{U}(t, t_0) = \hat{U}(t_0, t)\hat{\psi}^\dagger(\boldsymbol{x})\hat{U}(t, t_0)\hat{U}(t_0, t)\hat{\psi}(\boldsymbol{x})\hat{U}(t, t_0)$$
$$= \hat{\psi}_H^\dagger(\boldsymbol{x})\hat{\psi}_H(\boldsymbol{x})$$

- Basic property: if $C = AB$, then $C_H = A_H B_H$; $[A_H, B_H] = ([A, B])_H$.

- (Anti-)commutation relation:

$$\left[\hat{\psi}(\boldsymbol{x}, t), \hat{\psi}^\dagger(\boldsymbol{x}', t)\right] = \delta(\boldsymbol{x} - \boldsymbol{x}')$$

- With some calculation, we have the equation of motion:

$$i\frac{\partial}{\partial t}\hat{O}_H(t) = [\hat{O}_H(t), \hat{H}_H(t)]_- + i\left(\frac{\partial \hat{O}}{\partial t}\right)_H(t)$$

- We consider the following Hamiltonian $\hat{H}(t)$

$$\hat{H}(t) = \int d\boldsymbol{x}\hat{\psi}^\dagger(\boldsymbol{x})\hat{h}(\boldsymbol{x}, t)\hat{\psi}(\boldsymbol{x}) + \frac{1}{2}\int d\boldsymbol{x}d\boldsymbol{x}'\hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}^\dagger(\boldsymbol{x}')v(\boldsymbol{x}, \boldsymbol{x}')\hat{\psi}^\dagger(\boldsymbol{x}')\hat{\psi}^\dagger(\boldsymbol{x})$$
$$= H_0 + H_{\text{int}}$$

- With this Hamiltonian, we can figure out the equation of motion for field oprator. We need to calculate:

$$\left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}')\right] = \hat{\psi}(\boldsymbol{x})\hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}') - \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x})$$

$$= \hat{\psi}(\boldsymbol{x})\hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}') \mp \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x})\hat{\psi}(\boldsymbol{x}') = \hat{\psi}(\boldsymbol{x}')\delta(\boldsymbol{x} - \boldsymbol{x}')$$

$$\left[\hat{\psi}^{\dagger}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}')\right] = \hat{\psi}^{\dagger}(\boldsymbol{x})\hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}') - \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x})$$

$$= \pm\hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x})\hat{\psi}(\boldsymbol{x}') - \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x}) = -\hat{\psi}^{\dagger}(\boldsymbol{x}')\delta(\boldsymbol{x}' - \boldsymbol{x})$$

$$\left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}')\right] = \hat{\psi}(\boldsymbol{x})\hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}') - \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x})$$

$$= \hat{\psi}(\boldsymbol{x})\hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}') - \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x})\hat{\psi}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}')$$

$$= \left(\hat{\psi}(\boldsymbol{x})\hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x}'') - \hat{\psi}^{\dagger}(\boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x})\right)\hat{\psi}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}')$$

$$= \left([\hat{\psi}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{x}')]_{\mp}\hat{\psi}^{\dagger}(\boldsymbol{x}'') \pm \hat{\psi}^{\dagger}(\boldsymbol{x}')[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{x}'')]_{\mp}\right)\hat{\psi}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}')$$

$$= \left(\delta(\boldsymbol{x} - \boldsymbol{x}')\hat{\psi}^{\dagger}(\boldsymbol{x}'') \pm \hat{\psi}^{\dagger}(\boldsymbol{x}')\delta(\boldsymbol{x} - \boldsymbol{x}'')]\right)\hat{\psi}(\boldsymbol{x}'')\hat{\psi}(\boldsymbol{x}')$$

Then we have:

$$\mathrm{i}\frac{\partial}{\partial t}\hat{\psi}_H(\boldsymbol{x}, t) = \hat{h}(\boldsymbol{x}, t)\hat{\psi}_H(\boldsymbol{x}, t) + \int \mathrm{d}\boldsymbol{x}' v(\boldsymbol{x}, \boldsymbol{x}')\hat{\psi}^{\dagger}_H(\boldsymbol{x}', t)\hat{\psi}_H(\boldsymbol{x}', t)\hat{\psi}_H(\boldsymbol{x}, t)$$

$$\mathrm{i}\frac{\partial}{\partial t}\hat{\psi}^{\dagger}_H(\boldsymbol{x}, t) = -\hat{h}(\boldsymbol{x}, t)\hat{\psi}^{\dagger}_H(\boldsymbol{x}, t) - \int \mathrm{d}\boldsymbol{x}' v(\boldsymbol{x}, \boldsymbol{x}')\hat{\psi}^{\dagger}_H(\boldsymbol{x}, t)\hat{\psi}^{\dagger}_H(\boldsymbol{x}', t)\hat{\psi}_H(\boldsymbol{x}', t)$$

3 Schwinger-Keldysh contour

We start by considering how to calculate the time-dependent quantum average of an operator $\hat{O}(t)$. Let $|\Psi(t_0)\rangle = |\Psi_0\rangle$, for $t > t_0$, we have:

$$\langle\hat{O}\rangle(t) = \langle\Psi(t)|\hat{O}(t)|\Psi(t)\rangle = \langle\Psi_0|\hat{U}(t_0, t)|\hat{O}(t)|\hat{U}(t, t_0)|\Psi_0\rangle$$

With the formula derived in the previous section, we have:

$$\langle\hat{O}\rangle(t) = \left\langle\Psi_0\left|\bar{T}\left(\mathrm{e}^{-\mathrm{i}\int_t^{t_0} \mathrm{d}\tau\hat{H}(\tau)}\right)\right|\hat{O}(t)\left|T\left(\mathrm{e}^{-\mathrm{i}\int_{t_0}^t \mathrm{d}\tau\hat{H}(\tau)}\right)\right|\Psi_0\right\rangle$$

If we do Taylor expansions, our job will be reduced to evaluate the integrals of the following forms:

$$\bar{T}\left(\hat{H}(t_1)\cdots\hat{H}(t_n)\right)\hat{O}(t)\hat{T}\left(\hat{H}(t'_1)\cdots\hat{H}(t'_m)\right)$$

in which t_i, t'_i is between t_0 and t.

There are two separate time-ordering operators in this formula. We want to use a general time-ordering operator $\mathcal{T}$ to simplify this formulation.

- We start by defining an oriented contour:

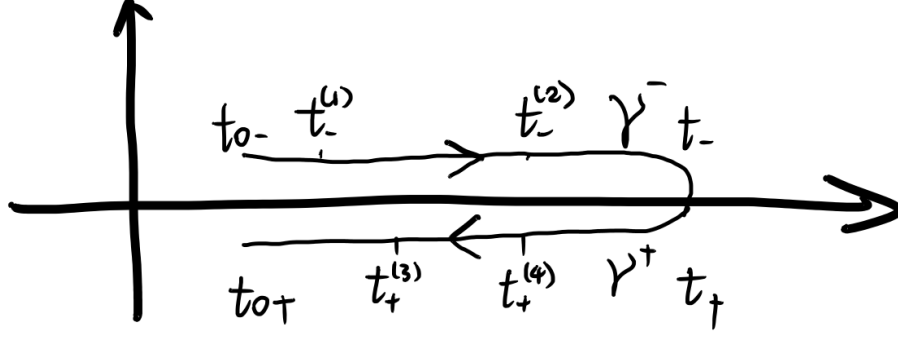$$\gamma := (t_0, t) \oplus (t, t_0) = \gamma_- \oplus \gamma_+$$

Figure 1: The oriented contour $\gamma = \gamma_- \oplus \gamma_+$

- γ_- is the forward branch. γ_+ is the backward branch.

- For a time $z \in \gamma$, if it's time t and it's on forward branch γ_-, we call it $z = t_-$, meaning that it's time t and it's used on the forward branch.

- For a time $z \in \gamma$, if it's time t and it's on backward branch γ_+, we call it $z = t_+$, meaning that it's time t and it's used on the backward branch.

- We have
$$\hat{H}(t_+) = \hat{H}(t_-) = \hat{H}(t), \quad \hat{O}(t_+) = \hat{O}(t_-) = \hat{O}(t)$$

- The oriented contour defines an ordering of time. For $t_-^{(1)}, t_-^{(2)}, t_+^{(3)}, t_+^{(4)}$, we have:
$$t_{0+} > t_+^{(3)} > t_+^{(4)} > t_+ = t_- > t_-^{(2)} > t_-^{(1)} > t_{0-}$$

- With this well-defined ordering, we can define a generic time-ordering operator $\mathcal{T}$, called the contour ordering operator, which operates as followed: for $z_1, \cdots, z_m \in \gamma$
$$\mathcal{T}\left(\hat{A}_1(z_1) \cdots \hat{A}_m(z_m) \right) = \hat{A}_{P(1)}(z_{P(1)}) \cdots \hat{A}_{P(m)}(z_{P(m)})$$

where $z_{P(1)} > \cdots > z_{P(m)}$, which is the ordering defined by the contour.

- Therefore, we have
$$\bar{T}\left(\hat{H}(t_1) \cdots \hat{H}(t_n) \right) \hat{O}(t) \hat{T}\left(\hat{H}(t_1') \cdots \hat{H}(t_m') \right)$$
$$= \mathcal{T}\left(\hat{H}(t_{1+}) \cdots \hat{H}(t_{n+}) \hat{O}(t_\pm) \hat{H}(t_{1-}') \cdots \hat{H}(t_{m-}') \right)$$

- Now we are ready to rewrite the quantum average in contour integral. We have
$$\int_t^{t_0} dt_1 \cdots \int_t^{t_0} dt_n \int_{t_0}^t dt_1' \cdots \int_{t_0}^t dt_m' \bar{T}\left(\hat{H}(t_1) \cdots \hat{H}(t_n) \right) \hat{O}(t) \hat{T}\left(\hat{H}(t_1') \cdots \hat{H}(t_m') \right)$$
$$= \int_{\gamma_+} dz_1 \cdots \int_{\gamma_+} dz_n \int_{\gamma_-} dz_1' \cdots \int_{\gamma_-} dz_m' \mathcal{T}\left(\hat{H}(z_1) \cdots \hat{H}(z_n) \hat{O}(t_\pm) \hat{H}(z_1') \cdots \hat{H}(z_m') \right)$$

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- Then, the original quantum average could be written in the form of

$$\langle O \rangle (t) = \left\langle \Psi_0 \left| \mathcal{T} \left(e^{-i \int_{\gamma_+} dz \hat{H}(z)} \hat{O}(t_\pm) e^{-i \int_{\gamma_-} dz \hat{H}(z)} \right) \right| \Psi_0 \right\rangle$$

Note that all these operators in $\mathcal{T}$ commutes, therefore we have

$$\langle O \rangle (t) = \left\langle \Psi_0 \left| \mathcal{T} \left(e^{-i \int_{\gamma} dz \hat{H}(z)} \hat{O}(t_\pm) \right) \right| \Psi_0 \right\rangle$$

In fact, there is more that we can do. As γ here actually rely on t, we can replace γ with a new contour that doesn't rely on t. Let our new $\tilde{\gamma}$ be

$$\tilde{\gamma} = (t_0, +\infty) \oplus (+\infty, t_0)$$

Then, with this γ, we have

$$\mathcal{T} \left(e^{-i \int_{\tilde{\gamma}} dz \hat{H}(z)} O(t_-) \right) = \hat{U}(t_0, \infty) \hat{U}(\infty, t) \hat{O}(t) \hat{U}(t, t_0) = \hat{U}(t_0, t) \hat{O}(t) \hat{U}(t, t_0)$$

$$\mathcal{T} \left(e^{-i \int_{\tilde{\gamma}} dz \hat{H}(z)} O(t_+) \right) = \hat{U}(t_0, t) \hat{O}(t) \hat{U}(t, \infty) \hat{U}(\infty, t_0) = \hat{U}(t_0, t) \hat{O}(t) \hat{U}(t, t_0)$$

Then, we have the final result, which is very elegant:

$$\langle O \rangle (t) = \left\langle \Psi_0 \left| \mathcal{T} \left(e^{-i \int_{\tilde{\gamma}} dz \hat{H}(z)} \hat{O}(t_\pm) \right) \right| \Psi_0 \right\rangle$$

This $\tilde{\gamma}$ is refered to as Schwinger-Keldysh contour.

4   Konstantinov-Perel contour for ensemble averages

Now we turn to the ensemble averages, which is probably a mixed state, rather than a pure state in the previous section.

The setup of the problem is as followed:

- For Hamiltonian $\hat{H}^M$, (M is credited to Matsubra), let's assume its eigenpairs being $(E_k^M, |\Psi_k\rangle)$. The Hamiltonian could be reconstructed as

$$\hat{H} = \sum_k E_k^M |\Psi_k\rangle \langle \Psi_k|$$

- The density matrix, $\hat{\rho}$, is defined as

$$\hat{\rho} = \frac{1}{Z} e^{-\beta H} = \frac{1}{Z} \sum_k e^{-\beta E_k^M} |\Psi_k\rangle \langle \Psi_k|$$

where Z is set to be $\text{Tr}(e^{-\beta H}) = \sum_k e^{-\beta E_k^M}$ to make sure $\text{Tr}(\hat{\rho}) = 1$. Here β is

$$\beta = \frac{1}{k_B T}$$

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- With density matrix $\hat{\rho}$, the ensemble average of an operator $\hat{O}$ is

$$\langle \hat{O} \rangle = \text{Tr}(\hat{\rho}\hat{O})$$

- For an ensemble in thermodynamic equilibrium, described by temperature T and chemical potential μ, the Hamlitonian $\hat{H}^M$ is

$$\hat{H}^M = \hat{H} - \mu\hat{N}$$

- In the previous section, we have the result

$$\hat{U}(t_0, t)\hat{O}(t)\hat{U}(t, t_0) = \mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz\hat{H}(z)}\hat{O}(t_\pm)\right)$$

Then the ensemble average is

$$\langle \hat{O} \rangle(t) = \left\langle \text{Tr}(\hat{U}(t_0, t)\hat{O}(t)\hat{U}(t, t_0))\right\rangle = \text{Tr}\left(\hat{\rho}\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz\hat{H}(z)}\hat{O}(t_\pm)\right)\right)$$

$$= \frac{\text{Tr}\left(e^{-\beta H^M}\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz\hat{H}(z)}\hat{O}(t_\pm)\right)\right)}{\text{Tr}\left(e^{-\beta H^M}\right)}$$

This is partly written using the contour formalism.

- In fact, we can try to express the above formula only using contour integrals. Let z_a, z_b be the points in complex plane, such that

$$z_b - z_a = -i\beta$$

- Let γ^M be (any of) the contour starting from z_a ending in z_b, then we have

$$e^{-\beta\hat{H}^M} = e^{-i\int_{\gamma^M} dz\hat{H}^M}$$

For $z \in \gamma^M$, we can also define the value of Hamiltonian $H^M(z)$ on γ^M. We just choose $H^M(z) = H(t_0)$.

- We also have

$$\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz\hat{H}(z)}\right) = \hat{U}(t_0, \infty)\hat{U}(\infty, t_0) = \mathbf{1}$$

- Then, combined those two equations, we have:

$$\langle \hat{O} \rangle(t) = \frac{\text{Tr}\left(e^{-i\int_{\gamma^M} dz\hat{H}^M}\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz\hat{H}(z)}\hat{O}(t_\pm)\right)\right)}{\text{Tr}\left(e^{-i\int_{\gamma^M} dz\hat{H}^M}\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz\hat{H}(z)}\right)\right)}$$

- In this case, $\hat{H}(z) = \hat{H}^M$ for all z.

- We haven't decided what is z_a, z_b and γ^M yet, just saying that $z_b - z_a = -i\beta$. As shown in figure 2, we do have different choices.

Using γ^M and the original γ_-, γ_+, we can construct new oriented contour γ:

$$\gamma = \gamma_- \oplus \gamma_+ \oplus \gamma^M = \tilde{\gamma} \oplus \gamma^M$$
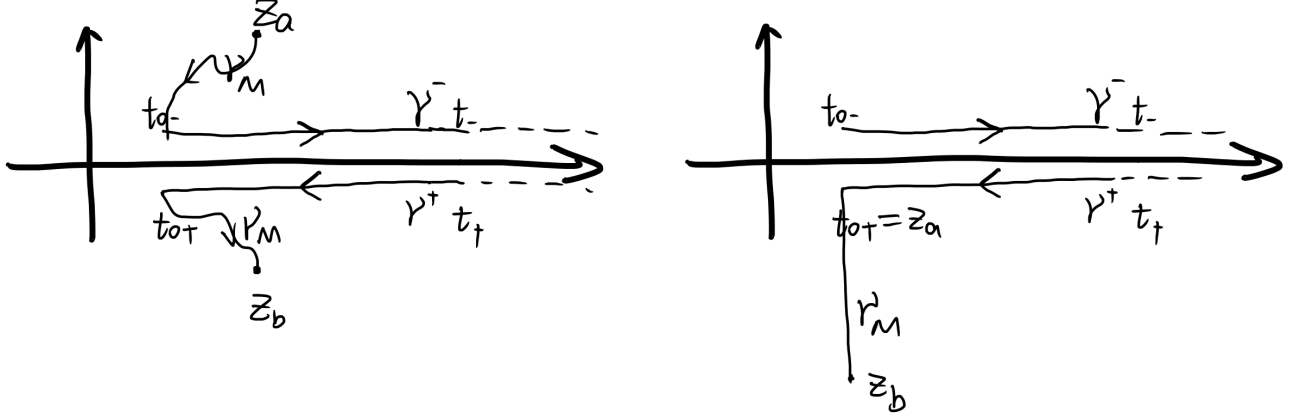
and define the ordering using this oriented contour γ.

Figure 2: Different choices of z_a, z_b

- Now, for example, for the left choice of figure 2, we have:

$$\mathrm{Tr}\left(e^{-i\int_{\gamma^M} dz \hat{H}^M} \mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz \hat{H}(z)} \hat{O}(t_\pm)\right)\right) = \mathrm{Tr}\left(e^{-i\int_{z_a}^{t_{0-}} dz \hat{H}^M} \mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz \hat{H}(z)} \hat{O}(t_\pm)\right) e^{-i\int_{t_{0+}}^{z_b} dz \hat{H}^M}\right)$$

$$= \mathrm{Tr}\left(\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}\oplus\gamma^M} dz \hat{H}(z)} \hat{O}(t_\pm)\right)\right)$$

- In general, we have

$$\langle \hat{O} \rangle(t) = \frac{\mathrm{Tr}\left(\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}\oplus\gamma^M} dz \hat{H}(z)} \hat{O}(t_\pm)\right)\right)}{\mathrm{Tr}\left(\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}\oplus\gamma^M} dz \hat{H}(z)}\right)\right)}$$

In fact, this value could also be generalized to any $z \in \gamma$, not only real-time t, but also imaginary time z on γ^M:

$$\langle \hat{O} \rangle(z) = \frac{\mathrm{Tr}\left(\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}\oplus\gamma^M} dz \hat{H}(z)} \hat{O}(z)\right)\right)}{\mathrm{Tr}\left(\mathcal{T}\left(e^{-i\int_{\tilde{\gamma}\oplus\gamma^M} dz \hat{H}(z)}\right)\right)}$$

5 Equation of motion on the contour

- As an analogy to the evolution operator for quantum system, we define the following evolution operator on the contour:

$$\hat{U}(z_2, z_1) = \begin{cases} \mathcal{T}\left(e^{-i\int_{z_1}^{z_2} dz \hat{H}(z)}\right), & z_2 \text{ later than } z_1 \\ \bar{\mathcal{T}}\left(e^{+i\int_{z_2}^{z_1} dz \hat{H}(z)}\right), & z_1 \text{ later than } z_2 \end{cases}$$

The integral is taken along the contour.

- This evolution operator has the following property:

$$\hat{U}(z, z) = \mathbf{1}, \quad \hat{U}(z_3, z_2)\hat{U}(z_2, z_1) = \hat{U}(z_3, z_1)$$

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- Now let's calculate the derivative. If z is later than z_0, we have

$$\mathrm{i}\frac{\partial}{\partial z}\hat{U}(z,z_0) = \mathcal{T}\left(\mathrm{i}\frac{\partial}{\partial z}e^{-\mathrm{i}\int_{z_0}^{z}\mathrm{d}\bar{z}\hat{H}(\bar{z})}\right) = \mathcal{T}\left(\hat{H}(z)e^{-\mathrm{i}\int_{z_0}^{z}\mathrm{d}\bar{z}\hat{H}(\bar{z})}\right) = \hat{H}(z)\hat{U}(z,z_0)$$

$$\mathrm{i}\frac{\partial}{\partial z}\hat{U}(z_0,z) = \bar{\mathcal{T}}\left(\mathrm{i}\frac{\partial}{\partial z}e^{\mathrm{i}\int_{z_0}^{z}\mathrm{d}\bar{z}\hat{H}(\bar{z})}\right) = -\bar{\mathcal{T}}\left(\hat{H}(z)e^{\mathrm{i}\int_{z_0}^{z}\mathrm{d}\bar{z}\hat{H}(\bar{z})}\right) = -\hat{U}(z_0,z)\hat{H}(z)$$

- We have the following relation between evolution operator on contour $\hat{U}(z_2,z_1)$ and the ordinary evolution operator $\hat{U}(t_2,t_1)$:

$$\hat{U}(t_2,t_1) = \hat{U}(t_{2-},t_{1-}) = \hat{U}(t_{2+},t_{1+})$$

- Let's denote by z_i the initial point of the contour, by z_f the final point of the contour. Then:

$$O(z) = \frac{\mathrm{Tr}\left(\hat{U}(z_f,z_i)\hat{U}(z_i,z)\hat{O}(z)\hat{U}(z,z_i)\right)}{\mathrm{Tr}\left(\hat{U}(z_f,z_i)\right)}$$

- It seems natural to define the contour Heisenberg picture:

$$\hat{O}_H(z) = \hat{U}(z_i,z)\hat{O}(z)\hat{U}(z,z_i)$$

- If z lies on the horizontal branches, the contour Heisenberg picture and the standard Heisenberg picture is:

$$\hat{O}_H(t_1) = \hat{O}_H(t_2) = \hat{O}_H(t)$$

- Equation of motion:

$$\mathrm{i}\frac{\partial}{\partial z}\hat{O}_H(z) = \hat{U}(z_i,z)[\hat{O}(z),\hat{H}(z)]\hat{U}(z,z_i) + \mathrm{i}\left(\frac{\partial\hat{O}}{\partial z}\right)_H(z)$$

$$= [\hat{O}_H(z),\hat{H}_H(z)] + \mathrm{i}\left(\frac{\partial\hat{O}}{\partial z}\right)_H(z)$$

- For example, field operators $\hat{\psi}_H(\boldsymbol{x},t), \hat{\psi}_H^\dagger(\boldsymbol{x},t)$ also have the contour analog $\hat{\psi}_H(\boldsymbol{x},z), \hat{\psi}_H^\dagger(\boldsymbol{x},z)$.

- For $\hat{\psi}(\boldsymbol{x},z), \hat{\psi}^\dagger(\boldsymbol{x},z)$, we only need to specify the definition on the γ^M:

$$\hat{\psi}(\boldsymbol{x}, z \in \gamma^M) = \hat{\psi}(\boldsymbol{x}), \quad \hat{\psi}^\dagger(\boldsymbol{x}, z \in \gamma^M) = \hat{\psi}^\dagger(\boldsymbol{x})$$

In other words, the field operators are constant over the entire contour. Generally, we only consider $\hat{H}^M$ of the form:

$$\hat{H}^M = \int \mathrm{d}\boldsymbol{x}\hat{\psi}^\dagger(\boldsymbol{x})\hat{h}(\boldsymbol{x},z)\hat{\psi}(\boldsymbol{x}) + \frac{1}{2}\int \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{x}'\hat{\psi}^\dagger(\boldsymbol{x})\hat{\psi}^\dagger(\boldsymbol{x}')v(\boldsymbol{x},\boldsymbol{x}')\hat{\psi}(\boldsymbol{x}')\hat{\psi}(\boldsymbol{x})$$

$$= \hat{H}_0^M + \hat{H}_{\mathrm{int}}^M$$

- Neglecting spins, we have the following equation of motion:

$$\mathrm{i}\frac{\partial}{\partial z}\hat{\psi}_H(\boldsymbol{x},z) = \hat{h}(\boldsymbol{x},z)\hat{\psi}_H(\boldsymbol{x},z) + \int \mathrm{d}\boldsymbol{x}'v(\boldsymbol{x},\boldsymbol{x}',z)\hat{\psi}_H^\dagger(\boldsymbol{x}',z)\hat{\psi}_H(\boldsymbol{x}',z)\hat{\psi}_H(\boldsymbol{x},z)$$

$$\mathrm{i}\frac{\partial}{\partial z}\hat{\psi}_H^\dagger(\boldsymbol{x},z) = -\hat{h}(\boldsymbol{x},z)\hat{\psi}_H^\dagger(\boldsymbol{x},z) - \int \mathrm{d}\boldsymbol{x}'v(\boldsymbol{x},\boldsymbol{x}',z)\hat{\psi}_H^\dagger(\boldsymbol{x},z)\hat{\psi}_H^\dagger(\boldsymbol{x}',z)\hat{\psi}_H(\boldsymbol{x}',z)$$

6 Operators correlators on the contour

- It has been shown that, in order to calculate $\langle O \rangle(t)$, after taylor expansion, the quantity that we are concerned about are traces of the following forms:

$$\hat{k}(z_1, \cdots, z_n) = \mathcal{T}\left(\hat{O}_1(z_1) \cdots \hat{O}_n(z_n)\right)$$

These are what we call operator correlators.

- Define $\theta(z_1, z_2)$:

$$\theta(z_1, z_2) = \begin{cases} 1 & z_1 > z_2 \\ 0 & z_1 \leq z_2 \end{cases}$$

its derivative is the delta function:

$$\frac{\mathrm{d}}{\mathrm{d}z_1}\theta(z_1, z_2) = \delta(z_1, z_2), \quad \frac{\mathrm{d}}{\mathrm{d}z_2}\theta(z_1, z_2) = -\delta(z_1, z_2)$$

- For two operator case $\mathcal{T}\left(\hat{O}_1(z_1)\hat{O}_2(z_2)\right)$, we have:

$$\mathcal{T}\left(\hat{O}_1(z_1)\hat{O}_2(z_2)\right) = \theta(z_1, z_2)\hat{O}_1(z_1)\hat{O}_2(z_2) + \theta(z_2, z_1)\hat{O}_2(z_2)\hat{O}_1(z_1)$$

Then the derivative is:

$$\frac{\mathrm{d}}{\mathrm{d}z_1}\mathcal{T}\left(\hat{O}_1(z_1)\hat{O}_2(z_2)\right) = \delta(z_1, z_2)\left[\hat{O}_1(z_1), \hat{O}_2(z_2)\right] + \mathcal{T}\left(\left(\frac{\mathrm{d}}{\mathrm{d}z_1}\hat{O}_1(z_1)\right)\hat{O}_2(z_2)\right)$$

- The commutator is actual for bosons. For fermions, we prefer anti-commutators. Therefore, if $\hat{O}_1, \hat{O}_2$ are fermionic operators, we modify our definition of time-ordering operator:

$$\mathcal{T}\left(\hat{O}_1(z_1)\hat{O}_2(z_2)\right) = \theta(z_1, z_2)\hat{O}_1(z_1)\hat{O}_2(z_2) - \theta(z_2, z_1)\hat{O}_2(z_2)\hat{O}_1(z_1)$$

Then, the derivative is:

$$\frac{\mathrm{d}}{\mathrm{d}z_1}\mathcal{T}\left(\hat{O}_1(z_1)\hat{O}_2(z_2)\right) = \delta(z_1, z_2)\left\{\hat{O}_1(z_1), \hat{O}_2(z_2)\right\} + \mathcal{T}\left(\left(\frac{\mathrm{d}}{\mathrm{d}z_1}\hat{O}_1(z_1)\right)\hat{O}_2(z_2)\right)$$

- Generally, for n operators, we define

$$\mathcal{T}\left(\hat{O}_1(z_1) \cdots \hat{O}_n(z_n)\right) = \sum_P (\pm)^P \theta(z_{P(1)}, \cdots, z_{P(n)})\hat{O}_{P(1)}(z_{P(1)}) \cdots \hat{O}_{P(n)}(z_{P(n)})$$

where $\theta(z_1, \cdots, z_n)$ is defined as

$$\theta(z_1, \cdots, z_n) = \begin{cases} 1 & z_1 > z_2 > \cdots > z_n \\ 0 & \text{otherwise} \end{cases}$$

we have

$$\mathcal{T}\left(\hat{O}_1(z_1) \cdots \hat{O}_n(z_n)\right) = (\pm)^P \mathcal{T}\left(\hat{O}_{P(1)}(z_{P(1)}) \cdots \hat{O}_{P(n)}(z_{P(n)})\right)$$

The plus sign is for Bosonic operator, and the minus sign is for Fermionic operator. Hamiltonian is treated as Bosonic operator.

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- In other words, we have:

$$\frac{\mathrm{d}}{\mathrm{d}z_1}\mathcal{T}\left(\hat{O}_1(z_1)\hat{O}_2(z_2)\right) = \delta(z_1,z_2)\left[\hat{O}_1(z_1),\hat{O}_2(z_2)\right]_{\mp} + \mathcal{T}\left(\left(\frac{\mathrm{d}}{\mathrm{d}z_1}\hat{O}_1(z_1)\right)\hat{O}_2(z_2)\right)$$

- For M equal time operators, it acts like a bosonic/fermionic operator under $\mathcal{T}$, for M being even/odd.

- For n operators, we have:

$$\frac{\mathrm{d}}{\mathrm{d}z_k}\mathcal{T}\left(\hat{O}_1(z_1)\cdots\hat{O}_n(z_n)\right) = \mathcal{T}\left(\hat{O}_1(z_1)\cdots\hat{O}_{k-1}(z_{k-1})\left(\frac{\mathrm{d}}{\mathrm{d}z_k}\hat{O}_k(z_k)\right)\hat{O}_{k+1}(z_{k+1})\cdots\hat{O}_n(z_n)\right)$$

$$+ \sum_P (\pm)^P\left(\frac{\mathrm{d}}{\mathrm{d}z_k}\theta(z_{P(1)},\cdots,z_{P(n)})\right)\hat{O}_{P(1)}(z_{P(1)})\cdots\hat{O}_{P(n)}(z_{P(n)})$$

- Now we dedicate to calculate the second term. When moving z_k along the contour, only of when it passes along another z_l, will create a term like $\delta(z_k - z_l)$ in the derivative. Consider z_l is the term closest to z_k, there is nothing between them. We have:

  - if $l > k$,

  $$\mathcal{T}\left(\hat{O}_1\cdots\hat{O}_n\right) = (\pm)^{l-k-1}\mathcal{T}\left(\hat{O}_1\cdots\hat{O}_k\hat{O}_l\hat{O}_{k+1}\cdots\hat{O}_{l-1}\hat{O}_{l+1}\cdots\hat{O}_n\right)$$

  $$= (\pm)^{l-k-1}(\pm)^Q\left(\theta(z_k-z_l)\hat{O}_{Q(1)}\cdots\hat{O}_k\hat{O}_l\hat{O}_{Q(n)} \pm \theta(z_l-z_k)\hat{O}_{Q(1)}\cdots\hat{O}_l\hat{O}_k\hat{O}_{Q(n)}\right)$$

  We see the above second term of the derivative in this case becomes:

  $$(\pm)^{l-k-1}(\pm)^Q\left(\delta(z_k-z_l)\hat{O}_{Q(1)}\cdots\left[\hat{O}_k,\hat{O}_l\right]_{\mp}\hat{O}_{Q(n)}\right)$$

  $$= (\pm)^{l-k-1}\delta(z_k,z_l)\mathcal{T}\left(\hat{O}_1\cdots\left[\hat{O}_k,\hat{O}_l\right]_{\mp}\hat{O}_{k+1}\cdots\hat{O}_{l-1}\hat{O}_{l+1}\cdots\hat{O}_n\right)$$

  - if $k > l$, similarly we have the derivative as

  $$(\pm)^{k-l}\delta(z_k,z_l)\mathcal{T}\left(\hat{O}_1\cdots\hat{O}_{l-1}\hat{O}_{l+1}\cdots\left[\hat{O}_k,\hat{O}_l\right]_{\mp}\hat{O}_{k+1}\cdots\hat{O}_n\right)$$

- Put them together, we have

$$\sum_{l=k+1}^{n}(\pm)^{l-k-1}\delta(z_k,z_l)\mathcal{T}\left(\hat{O}_1\cdots\left[\hat{O}_k,\hat{O}_l\right]_{\mp}\hat{O}_{k+1}\cdots\hat{O}_{l-1}\hat{O}_{l+1}\cdots\hat{O}_n\right)$$

$$+ \sum_{l=1}^{k-1}(\pm)^{k-l}\delta(z_k,z_l)\mathcal{T}\left(\hat{O}_1\cdots\hat{O}_{l-1}\hat{O}_{l+1}\cdots\left[\hat{O}_k,\hat{O}_l\right]_{\mp}\hat{O}_{k+1}\cdots\hat{O}_n\right)$$

- We will be working with field operators, which has a nice property that the (anti)commutator is a scalar function. Therefore the above formalism could be simplified further:

$$\sum_{l=k+1}^{n}(\pm)^{l-k-1}\delta(z_k,z_l)\left[\hat{O}_k,\hat{O}_l\right]_{\mp}\mathcal{T}\left(\hat{O}_1\cdots\tilde{\hat{O}}_k\cdots\tilde{\hat{O}}_l\cdots\hat{O}_n\right)$$

$$+ \sum_{l=1}^{k-1}(\pm)^{k-l}\delta(z_k,z_l)\left[\hat{O}_k,\hat{O}_l\right]_{\mp}\mathcal{T}\left(\hat{O}_1\cdots\tilde{\hat{O}}_l\cdots\tilde{\hat{O}}_k\cdots\hat{O}_n\right)$$

  where $\tilde{\hat{O}}_k$ means exclude this term from the multiplication.

- In order to deal with the field operators, we introduce the following notation:

$$i = \boldsymbol{x}_i, z_i, \quad j = \boldsymbol{x}_j, z_j, \cdots$$

$$\delta(j; k) = \delta(z_j, z_k)\delta(\boldsymbol{x}_j - \boldsymbol{x}_k)$$

- As an example, we have

$$\frac{\mathrm{d}}{\mathrm{d}z_2}\mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}_H^\dagger(3)\hat{\psi}_H^\dagger(4)\right\} = \mathcal{T}\left\{\hat{\psi}_H(1)\left(\frac{\mathrm{d}}{\mathrm{d}z_2}\hat{\psi}_H(2)\right)\hat{\psi}_H^\dagger(3)\hat{\psi}_H^\dagger(4)\right\}$$

$$+ \delta(2;3)\mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H^\dagger(4)\right\} \pm \delta(2;4)\mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H^\dagger(3)\right\}$$

- We are specifically interested in the following correlators:

$$\hat{G}_n(1,\cdots,n;1',\cdots,n') = \frac{1}{\mathrm{i}^n}\mathcal{T}\left(\hat{\psi}_H(1)\cdots\hat{\psi}_H(n)\psi_H^\dagger(n')\cdots\psi_H^\dagger(1')\right)$$

For $n = 0$, $\hat{G}_0 = \mathbf{1}$

- Therefore we have:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z_k}\hat{G}_n(1,\cdots,n;1',\cdots,n') = \frac{1}{\mathrm{i}^n}\mathcal{T}\left(\hat{\psi}_H(1)\cdots\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z_k}\hat{\psi}_H(k)\right)\cdots\hat{\psi}_H(n)\psi_H^\dagger(n')\cdots\psi_H^\dagger(1')\right)$$

$$+ \sum_{j=1}^n (\pm)^{k+j}\delta(k;j')\hat{G}_{n-1}(1,\cdots,\tilde{k},\cdots,n;1',\cdots,\tilde{j}',\cdots,n')$$

Similarly:

$$-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z_k'}\hat{G}_n(1,\cdots,n;1',\cdots,n') = \frac{1}{\mathrm{i}^n}\mathcal{T}\left(\hat{\psi}_H(1)\cdots\left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z_k'}\hat{\psi}_H(k)\right)\cdots\hat{\psi}_H(n)\psi_H^\dagger(n')\cdots\psi_H^\dagger(1')\right)$$

$$+ \sum_{j=1}^n (\pm)^{k+j}\delta(j;k')\hat{G}_{n-1}(1,\cdots,\tilde{j},\cdots,n;1',\cdots,\tilde{k}',\cdots,n')$$

- Recall the equation of motion for field operators:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z_k}\hat{\psi}_H(k) = \hat{h}(k)\hat{\psi}_H(k) + \int \mathrm{d}\bar{1}v(k,\bar{1})\hat{\psi}_H^\dagger(\bar{1})\hat{\psi}_H(\bar{1})\hat{\psi}_H(k)$$

$$-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z_k}\hat{\psi}_H^\dagger(k') = \hat{\psi}_H^\dagger(k')\hat{h}(k') + \int \mathrm{d}\bar{1}v(k',\bar{1})\hat{\psi}_H^\dagger(k')\hat{\psi}_H^\dagger(\bar{1})\hat{\psi}_H(\bar{1})$$

- If we insert the derivative of field operator back into the derivative of $\hat{G}_n$, we have something like $\hat{G}_{n+1}$. Note that: In order to ensure $\hat{\psi}_H^\dagger(1)$ is in front of $\hat{\psi}_H(1)$, we can introduce 1+:

$$\mathcal{T}\left(\cdots\hat{n}_H(\bar{1})\hat{\psi}_H(k)\cdots\right) = \mathcal{T}\left(\cdots\hat{\psi}_H^\dagger(\bar{1}^+)\hat{\psi}_H(\bar{1})\hat{\psi}_H(k)\cdots\right) = \pm\mathcal{T}\left(\cdots\hat{\psi}_H(k)\hat{\psi}_H(\bar{1})\hat{\psi}_H^\dagger(\bar{1}^+)\cdots\right)$$

Then we have:

$$\frac{1}{\mathrm{i}^n}\mathcal{T}\left\{\hat{\psi}_H(1)\ldots\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z_k}\hat{\psi}_H(k)\right)\ldots\hat{\psi}_H(n)\hat{\psi}_H^\dagger(n')\ldots\hat{\psi}_H^\dagger(1')\right\}$$

$$= h(k)\hat{G}_n(1,\ldots,n;1',\ldots,n') \pm \frac{1}{\mathrm{i}^n}\int \mathrm{d}\bar{1}v(k;\bar{1})\mathcal{T}\left\{\hat{\psi}_H(1)\ldots\hat{\psi}_H(n)\hat{\psi}_H(\bar{1})\hat{\psi}_H^\dagger\left(\bar{1}^+\right)\hat{\psi}_H^\dagger(n')\ldots\hat{\psi}_H^\dagger(1')\right\}$$

$$= h(k)\hat{G}_n(1,\ldots,n;1',\ldots,n') \pm \mathrm{i}\int \mathrm{d}\bar{1}v(k;\bar{1})\hat{G}_{n+1}\left(1,\ldots,n,\bar{1};1,\ldots,n',\bar{1}^+\right)$$

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Therefore we have:

$$\left[\mathrm{i}\frac{d}{dz_k} - h(k) \right] \hat{G}_n \left(1, \ldots, n; 1', \ldots, n'\right)$$

$$= \pm \mathrm{i} \int d\bar{1} v(k; \bar{1}) \hat{G}_{n+1} \left(1, \ldots, n, \bar{1}; 1', \ldots, n', \bar{1}^+\right) + \sum_{j=1}^{n} (\pm)^{k+j} \delta\left(k; j'\right) \hat{G}_{n-1} \left(1, \ldots \tilde{k} \ldots, n; 1', \ldots \tilde{j}' \ldots, n'\right)$$

Similarly, we have:

$$\hat{G}_n \left(1, \ldots, n; 1', \ldots, n'\right) \left[-\mathrm{i}\frac{\overleftarrow{d}}{dz'_k} - h\left(k'\right) \right]$$

$$= \pm \mathrm{i} \int d\bar{1} v\left(k'; \bar{1}\right) \hat{G}_{n+1} \left(1, \ldots, n, \bar{1}^-; 1', \ldots, n', \bar{1}\right) + \sum_{j=1}^{n} (\pm)^{k+j} \delta\left(j; k'\right) \hat{G}_{n-1} \left(1, \ldots \tilde{j} \ldots, n; 1', \ldots \tilde{k}' \ldots, n'\right)$$

7 Martin-Schwinger hierarchy

- The $n-$particle Green's function G_n, is defined using $\hat{G}_n$:

$$G_n(1, \cdots, n; 1, \cdots, n') = \frac{\mathrm{Tr}\left(e^{-\beta H^M} \hat{G}_n(1, \cdots, n; 1, \cdots, n'))\right)}{\mathrm{Tr}\left(e^{-\beta H^M}\right)}$$

$$= \frac{1}{\mathrm{i}^n} \frac{\mathrm{Tr}\left(\mathcal{T}\left(e^{-\mathrm{i}\int_\gamma d\bar{z}\hat{H}(\bar{z})} \hat{\psi}(1) \cdots \hat{\psi}(n)\psi^\dagger(n') \cdots \psi^\dagger(1')\right)\right)}{\mathrm{Tr}\left(\mathcal{T}\left(e^{-\mathrm{i}\int_\gamma d\bar{z}\hat{H}(\bar{z})}\right)\right)}$$

This requires derivation!

- For G_1, by choosing $z_1 = z$, $z'_1 = z^+$, we have the time dependent ensemble average for $\hat{\psi}^\dagger(\boldsymbol{x}'_1)\hat{\psi}(\boldsymbol{x}_1)$, which could be used to calculate the ensemble average of any one-body operator. For example, the density operator:

$$n(\boldsymbol{x}, z) = \frac{\mathrm{Tr}\left(e^{-\beta H^M} \hat{\psi}_H^\dagger(\boldsymbol{x}, z)\hat{\psi}_H(\boldsymbol{x}, z)\right)}{\mathrm{Tr}\left(e^{-\beta H^M}\right)} = \pm i G_1(\boldsymbol{x}, z; \boldsymbol{x}, z^+)$$

and the current density operator:

$$\boldsymbol{j}(\boldsymbol{x}, z) = \frac{1}{2m\mathrm{i}} \frac{\mathrm{Tr}\left(e^{-\beta H^M} \left(\hat{\psi}_H^\dagger(\boldsymbol{x}, z)\left(\nabla\hat{\psi}_H(\boldsymbol{x}, z)\right) - \left(\nabla\hat{\psi}_H^\dagger(\boldsymbol{x}, z)\right)\hat{\psi}_H(\boldsymbol{x}, z)\right)\right)}{\mathrm{Tr}\left(e^{-\beta H^M}\right)}$$

$$= \pm\frac{\nabla - \nabla'}{2m} G_1(\boldsymbol{x}, z; \boldsymbol{x}', z^+)|_{\boldsymbol{x}=\boldsymbol{x}'}$$

For G_n it's similar. For example, the interaction energy is:

$$E_{\mathrm{int}}(z) = -\frac{1}{2} \int d\boldsymbol{x} d\boldsymbol{x}' v(\boldsymbol{x}, \boldsymbol{x}', z) G_2(\boldsymbol{x}', z, \boldsymbol{x}, z; \boldsymbol{x}', z^+, \boldsymbol{x}, z^+)$$

- We have the differential equation for G_n:

$$\left[i\frac{d}{dz_k} - h(k)\right] G_n\left(1,\ldots,n;1',\ldots,n'\right)$$

$$= \pm i \int d\bar{1}v(k;\bar{1})G_{n+1}\left(1,\ldots,n,\bar{1};1',\ldots,n',\bar{1}^+\right) + \sum_{j=1}^{n}(\pm)^{k+j}\delta\left(k;j'\right)G_{n-1}\left(1,\ldots\tilde{k}\ldots,n;1',\ldots\tilde{j}'\ldots,n'\right)$$

and

$$G_n\left(1,\ldots,n;1',\ldots,n'\right)\left[-i\frac{\overleftarrow{d}}{dz_k'} - h\left(k'\right)\right]$$

$$= \pm i \int d\bar{1}v\left(k';\bar{1}\right)G_{n+1}\left(1,\ldots,n,\bar{1}^-;1',\ldots,n',\bar{1}\right) + \sum_{j=1}^{n}(\pm)^{k+j}\delta\left(j;k'\right)G_{n-1}\left(1,\ldots\tilde{j}\ldots,n;1',\ldots\tilde{k}'\ldots,n'\right)$$

This is called the Martin-Schwinger hierarchy.

- We also have the following boundary condition for Green's function:

$$G_n(1,\cdots,\boldsymbol{x}_k,z_i,\cdots,n;1',\cdots,n') = \pm G_n(1,\cdots,\boldsymbol{x}_k,z_f,\cdots,n;1',\cdots,n')$$

$$G_n(1,\cdots,n;1'\cdots,\boldsymbol{x}_k',z_i,\cdots,n') = \pm G_n(1,\cdots,n;1'\cdots,\boldsymbol{x}_k',z_f,\cdots,n')$$

This is called the Kubo-Martin-Schwinger(KMS) relations.

We'll now discuss an example of the truncation of hierarchy, i.e. the approximation of Green's function.

- For $G(1,1')$, we have:

$$\left(i\frac{d}{dz_1} - h(1)\right)G(1;1') = \delta(1;1') \pm i\int d2v(1,2)G_2(1,2;1',2^+)$$

$$G(1;1')\left(-i\frac{\overleftarrow{d}}{dz_1} - h(1')\right) = \delta(1;1') \pm i\int d2v(1',2)G_2(1,2^-;1',2)$$

- For $G_2(1,2;1',2')$, we have:

$$\left(i\frac{d}{dz_1} - h(1)\right)G_2(1,2;1',2') = \delta(1;1')G(2,2')\pm\delta(1;2')G(2;1')\pm i\int d3v(1,3)G_3(1,2,3;1',2',3^+)$$

$$\left(i\frac{d}{dz_2} - h(2)\right)G_2(1,2;1',2') = \pm\delta(2;1')G(1,2')+\delta(2;2')G(1;1')\pm i\int d3v(2,3)G_3(1,2,3;1',2',3^+)$$

$$G_2(1,2;1',2')\left(-i\frac{\overleftarrow{d}}{dz_1} - h(1')\right) = \delta(1;1')G(2,2')\pm\delta(2;1')G(1;2')\pm i\int d3v(1',3)G_3(1,2,3^-;1',2',3)$$

$$G_2(1,2;1',2')\left(-i\frac{\overleftarrow{d}}{dz_2} - h(2')\right) = \pm\delta(1;2')G(2,1')+\delta(2;2')G(1;1')\pm i\int d3v(2',3)G_3(1,2,3^-;1',2',3)$$

- This inspires us to write $G_2(1, 2; 1', 2')$ into the following formulation:

$$G_2(1, 2; 1', 2') = G(1; 1')G(2; 2') \pm G(1; 2')G(2; 1') + \Upsilon(1, 2; 1', 2')$$

$\Upsilon(1, 2; 1', 2')$ is called the correlation function. For $v = 0$, we can verify that $G_2(1, 2; 1', 2') = G(1; 1')G(2; 2') \pm G(1; 2')G(2; 1')$ satisfy the exact differential equation for G_2.

- The formulation

$$G_2(1, 2; 1', 2') = G(1; 1')G(2; 2') \pm G(1; 2')G(2; 1')$$

is called the Hartree-Fock approximation. If we insert it back to the differential equation for $G(1; 1')$, we have:

$$\left(i\frac{\mathrm{d}}{\mathrm{d}z_1} - h(1) \right) G(1; 1') = \delta(1; 1') \pm i \int \mathrm{d}2 v(1, 2) \left(G(1; 1')G(2; 2^+) \pm G(1; 2^+)G(2; 1') \right)$$

$$G(1; 1') \left(-i\frac{\overleftarrow{\mathrm{d}}}{\mathrm{d}z_1} - h(1') \right) = \delta(1; 1') \pm i \int \mathrm{d}2 v(1', 2) \left(G(1; 1')G(2^-; 2) \pm G(1; 2')G(2^-; 1') \right)$$

- If we define Σ as:

$$\Sigma(1, 2) = \delta(1; 2)V_H(1) + iv(1; 2)G(1; 2^+)$$

where

$$V_H(1) = \pm i \int \mathrm{d}3 v(1; 3)G(3, 3^+) = \int \mathrm{d}\boldsymbol{x}_3 v(\boldsymbol{x}_1, \boldsymbol{x}_3, z_1)n(\boldsymbol{x}_3, z_1)$$

is the well-known Hartree potential. Then we have

$$\left(i\frac{\mathrm{d}}{\mathrm{d}z_1} - h(1) \right) G(1; 1') = \delta(1; 1') + i \int \mathrm{d}2 \Sigma(1, 2)G(2; 1')$$

$$G(1; 1') \left(-i\frac{\overleftarrow{\mathrm{d}}}{\mathrm{d}z_1} - h(1') \right) = \delta(1; 1') + i \int \mathrm{d}2 G(1; 2)\Sigma(2; 1')$$

This is the self-consistent equation.

- Now we discuss the derivation of Dyson's equation. Using integral by part and KMS boundary condition, we have:

$$\int \mathrm{d}1 G_0(2; 1) \left[i\frac{\mathrm{d}}{\mathrm{d}z_1} - h(1) \right] G(1; 1')$$

$$= \int \mathrm{d}1 G_0(2; 1) \left[-i\frac{\overleftarrow{\mathrm{d}}}{\mathrm{d}z_1} - h(1) \right] G(1; 1') + i \int \mathrm{d}\boldsymbol{x}_1 G_0(2; \boldsymbol{x}_1, z_1) G(\boldsymbol{x}_1, z_1; 1') \Big|_{z_1=z_1}^{z_1=z_t}$$

$$= \int \mathrm{d}1 \delta(2; 1)G(1; 1') = G(2, 1')$$

With this we can do integral on the self-consistent equation for $G(1; 1')$, and we have:

$$G(1; 2) = G_0(1; 2) + \int \mathrm{d}3\mathrm{d}4 G_0(1; 3)\Sigma(3; 4)G(4; 2)$$

Similarly, we can also get:

$$G(1; 2) = G_0(1; 2) + \int \mathrm{d}3\mathrm{d}4 G_{(}1; 3)\Sigma(3; 4)G_0(4; 2)$$

Dyson's equation is also correct for the general case, not only for the Hartree-Fock approximation here.

We also can discuss the approximation beyond Hartree-Fock.

- For
$$G_2(1, 2; 1', 2') = G(1; 1')G(2; 2') \pm G(1; 2')G(2; 1') + \Upsilon(1, 2; 1', 2')$$

  with
$$\left(i\frac{d}{dz_1} - h(1)\right) G(1; 1') = \delta(1; 1') \pm i \int d2v(1, 2)G_2(1, 2; 1', 2^+)$$
$$\left(i\frac{d}{dz_1} - h(1)\right) G(1; 2') = \delta(1; 2') \pm i \int d2v(1, 2)G_2(1, 2; 2', 2^+)$$
$$\left(i\frac{d}{dz_1} - h(1)\right) G_2(1, 2; 1', 2') = \delta(1; 1')G(2, 2') \pm \delta(1; 2')G(2; 1') \pm i \int d3v(1, 3)G_3(1, 2, 3; 1', 2', 3^+)$$

- Therefore we have
$$\left(i\frac{d}{dz_1} - h(1)\right) \Upsilon(1, 2; 1', 2')$$
$$= \pm i \int d3v(1, 3) \left(G_3(1, 2, 3; 1', 2', 3^+) - G_2(1, 3; 1', 3^+)G(2; 2') \mp G_2(1, 3; 2', 3^+)G(2; 1')\right)$$

- Because
$$\left[i\frac{d}{dz_2} - h(2)\right] G_3\left(1, 2, 3; 1', 2', 3'\right) = \pm\delta\left(2; 1'\right) G_2\left(1, 3; 2, 3'\right) + \delta\left(2; 2'\right) G_2\left(1, 3; 1', 3'\right)$$
$$\pm\delta\left(2; 3'\right) G_2\left(1, 3; 1', 2'\right) \pm i \int d4v(2; 4)G_4\left(1, 2, 3, 4; 1', 2', 3', 4^+\right)$$

- Therefore
$$\left[i\frac{d}{dz_1} - h(1)\right] \left[i\frac{d}{dz_2} - h(2)\right] \Upsilon\left(1, 2; 1', 2'\right) = iv(1; 2)G_2\left(1, 2; 1', 2'\right)$$
$$- \int d4v(1; 3)v(2; 4) \left[G_4\left(1, 2, 3, 4; 1', 2', 3^+, 4^+\right) - G_2\left(1, 3; 1', 3^+\right) G_2\left(2, 4; 2', 4^+\right)\right.$$
$$\left.\mp G_2\left(1, 3; 2', 3^+\right) G_2\left(2, 4; 1', 4^+\right)\right].$$

- If we neglect the higher order term, we have:
$$\left[i\frac{d}{dz_1} - h(1)\right] \left[i\frac{d}{dz_2} - h(2)\right] \Upsilon\left(1, 2; 1', 2'\right) = iv(1; 2)G_2\left(1, 2; 1', 2'\right)$$

  Therefore
$$\Upsilon\left(1, 2; 1', 2'\right) = i \int d3d4G_0(1; 3)G_0(2; 4)v(3; 4)G_2\left(3, 4; 1', 2'\right)$$

8   Exact solution of Martin-Schwinger's Hierarchy from Wick's theorem

- We'll first deal with the non-interacting case $G_{0,n}$, where $v = 0$. We have the following result:

$$G_{0,n}\left(1,\ldots,n;1',\ldots,n'\right) = \begin{vmatrix} G_0\left(1;1'\right) & \ldots & G_0\left(1;n'\right) \\ \vdots & & \vdots \\ G_0\left(n;1'\right) & \ldots & G_0\left(n;n'\right) \end{vmatrix}_{\pm}$$

This follows from Martin-Schwinger hierarchy if $v = 0$. This is the so-called Wick's theorem.

- This inspires us to calculate G_n in a brute-force way. From the definition, we have:

$$G_n = \frac{1}{i^n} \frac{\text{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}_0(\bar{z})} e^{-i\int_\gamma d\bar{z}\hat{H}_{\text{int}}(\bar{z})} \hat{\psi}(1)\ldots\hat{\psi}^\dagger(1')\right\}\right]}{\text{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}_0(\bar{z})} e^{-i\int_\gamma d\bar{z}\hat{H}_{\text{int}}(\bar{z})}\right\}\right]}$$

where $\hat{H}_0$ and $\hat{H}_{\text{int}}$ are respectively one-body and two-body terms for the Hamiltonian.

- If we introduce the notation:

$$\text{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}_0(\bar{z})}\ldots\right\}\right] = \langle\mathcal{T}\{\ldots\}\rangle_0$$

which could be physically interpreted as taking average over the non-interacting system. Then our interacting Green's function G_n, using Taylor's expansion, is

$$G_n = \frac{1}{i^n} \frac{\sum_{k=0}^\infty \frac{(-i)^k}{k!}\int_\gamma d\bar{z}_1\ldots d\bar{z}_k \left\langle\mathcal{T}\left\{\hat{H}_{\text{int}}\left(\bar{z}_1\right)\ldots\hat{H}_{\text{int}}\left(\bar{z}_k\right)\hat{\psi}(1)\ldots\hat{\psi}^\dagger(1')\right\}\right\rangle_0}{\sum_{k=0}^\infty \frac{(-i)^k}{k!}\int_\gamma d\bar{z}_1\ldots d\bar{z}_k \left\langle\mathcal{T}\left\{\hat{H}_{\text{int}}\left(\bar{z}_1\right)\ldots\hat{H}_{\text{int}}\left(\bar{z}_k\right)\right\}\right\rangle_0}$$

where $\hat{H}_{\text{int}}$ is

$$\hat{H}_{\text{int}}(z) = \frac{1}{2}\int dz'\int d\boldsymbol{x}d\boldsymbol{x}' v\left(\boldsymbol{x},z;\boldsymbol{x}',z'\right)\hat{\psi}^\dagger\left(\boldsymbol{x},z^+\right)\hat{\psi}^\dagger\left(\boldsymbol{x}',z^+\right)\hat{\psi}\left(\boldsymbol{x}',z'\right)\hat{\psi}(\boldsymbol{x},z)$$

where

$$v\left(\boldsymbol{x},z;\boldsymbol{x}',z'\right) = \delta\left(z,z'\right)\begin{cases} v\left(\boldsymbol{x},\boldsymbol{x}',t\right) & \text{if } z = t_\pm \text{is on the horizontal branches of } \gamma \\ v^{\text{M}}\left(\boldsymbol{x},\boldsymbol{x}'\right) & \text{if } z \text{ is on the vertical track of } \gamma \end{cases}$$

- Now we look at the case of one-particle Green's function. Let $a = (\boldsymbol{x}_a, z_a), b = (\boldsymbol{x}_b, z_b)$, we have

$$G(a;b) = \frac{1}{i} \frac{\sum_{k=0}^\infty \frac{(-i)^k}{k!}\int_\gamma dz_1\ldots dz_k \left\langle\mathcal{T}\left\{\hat{H}_{\text{int}}\left(z_1\right)\ldots\hat{H}_{\text{int}}\left(z_k\right)\hat{\psi}(a)\hat{\psi}^\dagger(b)\right\}\right\rangle_0}{\sum_{k=0}^\infty \frac{(-i)^k}{k!}\int_\gamma dz_1\ldots dz_k \left\langle\mathcal{T}\left\{\hat{H}_{\text{int}}\left(z_1\right)\ldots\hat{H}_{\text{int}}\left(z_k\right)\right\}\right\rangle_0}$$

The numerator could be rewritten as

$$\sum_{k=0}^\infty \frac{1}{k!}\left(-\frac{i}{2}\right)^k \int d1\ldots dk d1'\ldots dk' v\left(1;1'\right)\ldots v\left(k;k'\right)$$
$$\times\left\langle\mathcal{T}\left\{\hat{\psi}^\dagger\left(1^+\right)\hat{\psi}^\dagger\left(1'^+\right)\hat{\psi}\left(1'\right)\hat{\psi}(1)\ldots\hat{\psi}^\dagger\left(k^+\right)\hat{\psi}^\dagger\left(k'^+\right)\hat{\psi}\left(k'\right)\hat{\psi}(k)\hat{\psi}(a)\hat{\psi}^\dagger(b)\right\}\right\rangle_0$$

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The quantity inside time-ordering operator could be rewritten as

$$\left\langle \mathcal{T}\left\{ \hat{\psi}(a)\hat{\psi}(1)\hat{\psi}\left(1'\right)\ldots\hat{\psi}(k)\hat{\psi}\left(k'\right)\hat{\psi}^{\dagger}\left(k^{+}\right)\hat{\psi}^{\dagger}\left(k^{+}\right)\ldots\hat{\psi}^{\dagger}\left(1'^{+}\right)\hat{\psi}^{\dagger}\left(1^{+}\right)\hat{\psi}^{\dagger}(b)\right\}\right\rangle_{0}$$

which is exactly

$$i^{2k+1}Z_{0}G_{0,2k+1}\left(a,1,1',\ldots,k,k';b,1^{+},1'^{+},\ldots k^{+},k'^{+}\right)$$

Similarly, the k-th order term of the denominator is

$$i^{2k}Z_{0}G_{0,2k}\left(1,1',\ldots,k,k';1^{+},1'^{+},\ldots k^{+},k'^{+}\right)$$

Therefore we have

$$G(a;b)=\frac{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^{k}\int v\left(1;1'\right)\ldots v\left(k;k'\right)G_{0,2k+1}\left(a,1,1',\ldots;b,1^{+},1'^{+},\ldots\right)}{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^{k}\int v\left(1;1'\right)\ldots v\left(k;k'\right)G_{0,2k}\left(1,1',\ldots;1^{+},1'^{+},\ldots\right)}$$

which could be further written using Wick's theorem

$$G(a,b)=\frac{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^{k}\int v\left(1;1'\right)..v\left(k;k'\right)\begin{vmatrix}G_{0}(a;b)&G_{0}\left(a;1^{+}\right)&\ldots&G_{0}\left(a;k'^{+}\right)\\G_{0}(1;b)&G_{0}\left(1;1^{+}\right)&\ldots&G_{0}\left(1;k'^{+}\right)\\\vdots&\vdots&\ddots&\vdots\\G_{0}\left(k';b\right)&G_{0}\left(k';1^{+}\right)&\ldots&G_{0}\left(k';k'^{+}\right)\end{vmatrix}_{\pm}}{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^{k}\int v\left(1;1'\right)..v\left(k;k'\right)\begin{vmatrix}G_{0}\left(1;1^{+}\right)&G_{0}\left(1;1'^{+}\right)&\ldots&G_{0}\left(1;k'^{+}\right)\\G_{0}\left(1';1^{+}\right)&G_{0}\left(1';1'^{+}\right)&\ldots&G_{0}\left(1';k'^{+}\right)\\\vdots&\vdots&\ddots&\vdots\\G_{0}\left(k';1^{+}\right)&G_{0}\left(k';1'^{+}\right)&\ldots&G_{0}\left(k';k'^{+}\right)\end{vmatrix}_{\pm}}$$

where the integrals are over $1,1',\cdots k,k'$.

- Similarly, we have

$$G_{2}(a,b;c,d)=\frac{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^{k}\int v\left(1;1'\right)\ldots v\left(k;k'\right)\begin{vmatrix}G_{0}(a;c)&G_{0}(a;d)&\ldots&G_{0}\left(a;k'^{+}\right)\\G_{0}(b;c)&G_{0}(b;d)&\ldots&G_{0}\left(b;k'^{+}\right)\\\vdots&\vdots&\ddots&\vdots\\G_{0}\left(k';c\right)&G_{0}\left(k';d\right)&\ldots&G_{0}\left(k';k'^{+}\right)\end{vmatrix}_{\pm}}{\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^{k}\int v\left(1;1'\right)\ldots v\left(k;k'\right)\begin{vmatrix}G_{0}\left(1;1^{+}\right)&G_{0}\left(1;1'^{+}\right)&\ldots&G_{0}\left(1;k'^{+}\right)\\G_{0}\left(1';1^{+}\right)&G_{0}\left(1';1'^{+}\right)&\ldots&G_{0}\left(1';k'^{+}\right)\\\vdots&\vdots&\ddots&\vdots\\G_{0}\left(k';1^{+}\right)&G_{0}\left(k';1'^{+}\right)&\ldots&G_{0}\left(k';k'^{+}\right)\end{vmatrix}_{\pm}}$$

We also have Z/Z_{0}, which is just the denominator above

$$\frac{Z}{Z_{0}}=\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i}{2}\right)^{k}\int v\left(1;1'\right)\ldots v\left(k;k'\right)\begin{vmatrix}G_{0}\left(1;1^{+}\right)&G_{0}\left(1;1'^{+}\right)&\ldots&G_{0}\left(1;k'^{+}\right)\\G_{0}\left(1';1^{+}\right)&G_{0}\left(1';1'^{+}\right)&\ldots&G_{0}\left(1';k'^{+}\right)\\\vdots&\vdots&\ddots&\vdots\\G_{0}\left(k';1^{+}\right)&G_{0}\left(k';1'^{+}\right)&\ldots&G_{0}\left(k';k'^{+}\right)\end{vmatrix}_{\pm}$$

This is the full mathematical description of many body perturbation theory.

9 Analytic continuity rules

Here we consider the analytic property of two-point correlators $k(z, z')$, such as one-particle Green's function.

$$k\left(z, z'\right) = \mathrm{Tr}\left[\hat{\rho}\hat{k}\left(z, z'\right)\right] = \mathrm{Tr}\left[\hat{\rho}\mathcal{T}\left\{\hat{O}_1(z)\hat{O}_2\left(z'\right)\right\}\right]$$

and the discussion here based on $\hat{O}(t_+) = \hat{O}(t_-)$. We only consider the contour as being the right side of figure 2.

- We have

$$k\left(z, z'\right) = \theta\left(z, z'\right)k^>\left(z, z'\right) + \theta\left(z', z\right)k^<\left(z, z'\right)$$

  where $k^>$ and $k^<$ are:

$$k^>\left(z, z'\right) = \mathrm{Tr}\left[\hat{\rho}\hat{O}_1(z)\hat{O}_2\left(z'\right)\right], \quad k^<\left(z, z'\right) = \pm\,\mathrm{Tr}\left[\hat{\rho}\hat{O}_2\left(z'\right)\hat{O}_1(z)\right]$$

- $k(z, z')$ is the same value for z, z' being on forward/backward branch:

$$k^{\lessgtr}\left(t_+, z'\right) = k^{\lessgtr}\left(t_-, z'\right), \quad k^{\lessgtr}\left(z, t'_+\right) = k^{\lessgtr}\left(z, t'_-\right)$$

- A function is said to belong to Keldysh space, if

$$k\left(z, z'\right) = k^{\delta}(z)\delta\left(z, z'\right) + \theta\left(z, z'\right)k^>\left(z, z'\right) + \theta\left(z', z\right)k^<\left(z, z'\right)$$

  Here $k^{\delta}(t) = k^{\delta}(t_-) = k^{\delta}(t_+)$.

- On the real time axis, we can define the greater and lesser Keldysh components as followed:

$$k^>\left(t, t'\right) \equiv k\left(t_+, t'_-\right)$$
$$k^<\left(t, t'\right) \equiv k\left(t_-, t'_+\right)$$

- We also define the left and right Keldysh components from $k(z, z')$ with one real time t and one imaginary time $t_0 - i\tau$:

$$k^{\lceil}(\tau, t) \equiv k\left(t_0 - i\tau, t_{\pm}\right)$$
$$k^{\rceil}(t, \tau) \equiv k\left(t_{\pm}, t_0 - i\tau\right)$$

- We can also define the Matsubara component $k^M(\tau, \tau')$ with both contour arguments on the vertical track:

$$k^{\mathrm{M}}\left(\tau, \tau'\right) \equiv k\left(t_0 - i\tau, t_0 - i\tau'\right)$$
$$= \delta\left(t_0 - i\tau, t_0 - i\tau'\right)k^{\delta}\left(t_0 - i\tau\right) + k_r^{\mathrm{M}}\left(\tau, \tau'\right)$$

  where

$$k_r^{\mathrm{M}}\left(\tau, \tau'\right) = \theta\left(\tau - \tau'\right)k^>\left(t_0 - i\tau, t_0 - i\tau'\right) + \theta\left(\tau' - \tau\right)k^<\left(t_0 - i\tau, t_0 - i\tau'\right)$$

  Because $\delta\left(t_0 - i\tau, t_0 - i\tau'\right) = i\delta\left(\tau - \tau'\right)$, therefore

$$k^{\mathrm{M}}\left(\tau, \tau'\right) = i\delta\left(\tau - \tau'\right)k^{\delta}(\tau) + k_r^{\mathrm{M}}\left(\tau, \tau'\right)$$

- We also define the retarded and advanced component:

$$k^{\mathrm{R}}\left(t, t'\right) \equiv k^{\delta}(t)\delta\left(t - t'\right) + \theta\left(t - t'\right)\left[k^{>}\left(t, t'\right) - k^{<}\left(t, t'\right)\right]$$

$$k^{\mathrm{A}}\left(t, t'\right) \equiv k^{\delta}(t)\delta\left(t - t'\right) - \theta\left(t' - t\right)\left[k^{>}\left(t, t'\right) - k^{<}\left(t, t'\right)\right]$$

and the time-ordered and anti time-ordered component:

$$k^{\mathrm{T}}\left(t, t'\right) \equiv k\left(t_{-}, t'_{-}\right) = k^{\delta}(t)\delta\left(t - t'\right) + \theta\left(t - t'\right)k^{>}\left(t, t'\right) + \theta\left(t' - t\right)k^{<}\left(t, t'\right)$$

$$k^{\overline{\mathrm{T}}}\left(t, t'\right) \equiv k\left(t_{+}, t'_{+}\right) = -k^{\delta}(t)\delta\left(t - t'\right) + \theta\left(t' - t\right)k^{>}\left(t, t'\right) + \theta\left(t - t'\right)k^{<}\left(t, t'\right)$$

There are a lot to be filled in this section.....

10   Physics of one-particle Green's function

We begin by discussing some other formalism of Green's function.

- The Green's function could be regarded as a first quantization operator:

$$\hat{\mathcal{G}}\left(z_1, z_2\right) = \int d\boldsymbol{x}_1 d\boldsymbol{x}_2 \left|\boldsymbol{x}_1\right\rangle G(1; 2)\left\langle\boldsymbol{x}_2\right|$$

whose matrix element is

$$\left\langle\boldsymbol{x}_1 \left|\hat{\mathcal{G}}\left(z_1, z_2\right)\right| \boldsymbol{x}_2\right\rangle = G(1; 2)$$

- On the other hand, recall that

$$\hat{\psi}(\boldsymbol{x}) = \sum_i \varphi_i(\boldsymbol{x})\hat{d}_i, \quad \hat{\psi}^{\dagger}(\boldsymbol{x}) = \sum_i \varphi_i^{*}(\boldsymbol{x})\hat{d}_i^{\dagger}$$

we can also define the following matrix Green's function:

$$G_{ji}\left(z_1, z_2\right) = \frac{1}{\mathrm{i}} \frac{\mathrm{Tr}\left[e^{-\beta\hat{H}^{\mathrm{M}}}\mathcal{T}\left\{\hat{d}_{j,H}\left(z_1\right)\hat{d}_{i,H}^{\dagger}\left(z_2\right)\right\}\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^{\mathrm{M}}}\right]}$$

- Their relations are:

$$G(1; 2) = \sum_{ji} \varphi_j\left(\boldsymbol{x}_1\right) G_{ji}\left(z_1, z_2\right) \varphi_i^{*}\left(\boldsymbol{x}_2\right) = \sum_{ji} \left\langle\boldsymbol{x}_1 \mid j\right\rangle G_{ji}\left(z_1, z_2\right)\left\langle i \mid \boldsymbol{x}_2\right\rangle$$

$$\hat{\mathcal{G}}\left(z_1, z_2\right) = \sum_{ji} |j\rangle G_{ji}\left(z_1, z_2\right)\langle i|$$

- For non-interacting Green's function, we have:

$$\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z_1} - \hat{h}\left(z_1\right)\right)\hat{\mathcal{G}}_0\left(z_1, z_2\right) = \delta\left(z_1, z_2\right)$$

For interactimg case, we have

$$\left[\mathrm{i}\frac{d}{dz_1} - \hat{h}\left(z_1\right)\right]\hat{\mathcal{G}}\left(z_1, z_2\right) - \int_{\gamma} d\bar{z}\hat{\Sigma}\left(z_1, \bar{z}\right)\hat{\mathcal{G}}\left(\bar{z}, z_2\right) = \delta\left(z_1, z_2\right)$$

Now we talk about Matsubara Green's function.

- Let $z_1 = t_0 - \mathrm{i}\tau_1$ and $z_2 = t_0 - \mathrm{i}\tau_2$. The definition of Matsubara Green's function is

$$G_{ji}^{\mathrm{M}}(\tau_1, \tau_2) = \frac{1}{\mathrm{i}} \left\{ \theta(\tau_1 - \tau_2) \frac{\mathrm{Tr}\left[e^{(\tau_1 - \tau_2 - \beta)\hat{H}^{\mathrm{M}}} \hat{d}_j e^{(\tau_2 - \tau_1)\hat{H}^{\mathrm{M}}} \hat{d}_i^\dagger\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^{\mathrm{M}}}\right]} \pm \theta(\tau_2 - \tau_1) \frac{\mathrm{Tr}\left[e^{(\tau_2 - \tau_1 - \beta)\hat{H}^{\mathrm{M}}} \hat{d}_i^\dagger e^{(\tau_1 - \tau_2)\hat{H}^{\mathrm{M}}} \hat{d}_j\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^{\mathrm{M}}}\right]} \right\}$$

  Here $\hat{H}^M = \hat{H}(t_0) - \mu\hat{N}$.

- For any one-body operator $\hat{O}$

$$\hat{O} = \sum_{ij} O_{ij} \hat{d}_i^\dagger \hat{d}_j$$

  we have

$$\langle O \rangle = \frac{\mathrm{Tr}\left[e^{-\beta\hat{H}^M}\hat{O}\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^M}\right]} = \sum_{ij} O_{ij} \frac{\mathrm{Tr}\left[e^{-\beta\hat{H}^M}\hat{d}_i^\dagger \hat{d}_j\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^M}\right]} = \pm\mathrm{i}\sum_{ij} O_{ij} G_{ji}^{\mathrm{M}}(\tau, \tau^+)$$

- $G_{ji}^{M}(\tau_1, \tau_2)$ only depends on $\tau_1 - \tau_2$.

- KMS relation:
$$\hat{\mathcal{G}}^{\mathrm{M}}(0, \tau) = \pm\hat{\mathcal{G}}^{\mathrm{M}}(\beta, \tau), \quad \hat{\mathcal{G}}^{\mathrm{M}}(\tau, 0) = \pm\hat{\mathcal{G}}^{\mathrm{M}}(\tau, \beta)$$

- Therefore the Matsubara Green's function could be expended using Fourier series:

$$\hat{\mathcal{G}}^{\mathrm{M}}(\tau_1, \tau_2) = \frac{1}{-\mathrm{i}\beta} \sum_{m=-\infty}^{\infty} e^{-\omega_m(\tau_1 - \tau_2)} \hat{\mathcal{G}}^{\mathrm{M}}(\omega_m)$$

  where the Matsubara frequencies are

$$\omega_m = \begin{cases} \frac{\mathrm{i}2m\pi}{\beta} & \text{for bosons} \\ \frac{\mathrm{i}(2m+1)\pi}{\beta} & \text{for fermions} \end{cases}$$

- Let's look at example. For
$$\hat{H}^{\mathrm{M}} = \sum_{ij} h_{ij}^{\mathrm{M}} \hat{d}_i^\dagger \hat{d}_j$$

  with the equation of motion, we have

$$\left[-\frac{d}{d\tau_1} - \hat{h}^{\mathrm{M}}\right] \hat{\mathcal{G}}^{\mathrm{M}}(\tau_1, \tau_2) = \delta(-\mathrm{i}\tau_1 + \mathrm{i}\tau_2) = \mathrm{i}\delta(\tau_1 - \tau_2)$$

  with the help of

$$\delta(\tau) = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} \begin{cases} e^{-\mathrm{i}\frac{2m\pi}{\beta}\tau} \\ e^{-\mathrm{i}\frac{(2m+1)\pi}{\beta}\tau} \end{cases}_\tau = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} e^{-\omega_m\tau}$$

  we get

$$\hat{\mathcal{G}}^{\mathrm{M}}(\omega_m) = \frac{1}{\omega_m - \hat{h}^{\mathrm{M}}}$$

Now we discuss lesser/greater Green's function.

- The definition is

$$G_{ji}^{<}\left(t,t'\right) = \mp\mathrm{i}\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}^{M}}\hat{d}_{i,H}^{\dagger}\left(t'\right)\hat{d}_{j,H}(t)\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^{M}}\right]} = \mp\mathrm{i}\sum_{k}\rho_{k}\left\langle\Psi_{k}\left|\hat{d}_{i,H}^{\dagger}\left(t'\right)\hat{d}_{j,H}(t)\right|\Psi_{k}\right\rangle$$

$$G_{ji}^{>}\left(t,t'\right) = -\mathrm{i}\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}^{M}}\hat{d}_{j,H}(t)\hat{d}_{i,H}^{\dagger}\left(t'\right)\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^{M}}\right]} = -\mathrm{i}\sum_{k}\rho_{k}\left\langle\Psi_{k}\left|\hat{d}_{j,H}(t)\hat{d}_{i,H}^{\dagger}\left(t'\right)\right|\Psi_{k}\right\rangle$$

- We have:
$$\left[G_{ji}^{>}\left(t,t'\right)\right]^{*} = -G_{ij}^{>}\left(t',t\right),\quad \left[G_{ji}^{<}\left(t,t'\right)\right]^{*} = -G_{ij}^{<}\left(t',t\right)$$
and consequently
$$\hat{\mathcal{G}}^{\mathrm{R}}\left(t,t'\right) = \theta\left(t-t'\right)\left[\hat{\mathcal{G}}^{>}\left(t,t'\right) - \hat{\mathcal{G}}^{<}\left(t,t'\right)\right] = \left[\hat{\mathcal{G}}^{\mathrm{A}}\left(t',t\right)\right]^{\dagger}$$

- The lesser Green's function could be used to calculate one-body operator. For example:
$$n_{i}(t) = \pm\mathrm{i}\sum_{ij}O_{ij}G_{ji}^{<}(t,t)$$

- For $t = t_{0}$, we have for all τ:
$$\hat{\mathcal{G}}(t_{0},t_{0}) = \hat{\mathcal{G}}^{\mathrm{M}}(\tau,\tau^{+})$$

- If $\hat{H}(t) = \hat{H}$ for $t > t_{0}$, we have
$$G_{ji}^{<}\left(t,t'\right) = \mp\mathrm{i}\sum_{k}\rho_{k}\left\langle\Psi_{k}\left|e^{\mathrm{i}\hat{H}(t'-t_{0})}\hat{d}_{i}^{\dagger}e^{-\mathrm{i}\hat{H}(t'-t)}\hat{d}_{j}e^{-\mathrm{i}\hat{H}(t-t_{0})}\right|\Psi_{k}\right\rangle$$

- In general, $G_{ij}^{<}$ is not a function of $t' - t$, because Ψ_{k} is not necessarily the eigenstates of driving Hamiltonian $\hat{H}$.

11 Non-interacting Green's function

We are talking about non-interacting case, where the Hamiltonian is
$$\hat{H}(z) = \sum_{ij}h_{ij}(z)\hat{d}_{i}^{\dagger}\hat{d}_{j} = \sum_{ij}\langle i|\hat{h}(z)|j\rangle\hat{d}_{i}^{\dagger}\hat{d}_{j}$$

- We write $\hat{\mathcal{G}}$ as:
$$\hat{\mathcal{G}}(z_{1},z_{2}) = \hat{\mathcal{U}}_{L}(z_{1})\hat{\mathcal{F}}(z_{1},z_{2})\hat{\mathcal{U}}_{R}(z_{2})$$
Here $\hat{\mathcal{U}}_{L/R}(z)$ fulfill:
$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z}\hat{\mathcal{U}}_{L}(z) = \hat{h}(z)\hat{\mathcal{U}}_{L}(z),\quad \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z}\hat{\mathcal{U}}_{R}(z) = -\hat{\mathcal{U}}_{R}(z)\hat{h}(z)$$
with $\hat{\mathcal{U}}_{L}(t_{0-}) = \hat{\mathcal{U}}_{R}(t_{0-}) = \mathbf{1}$.

- The solution of $\hat{\mathcal{U}}_L$ and $\hat{\mathcal{U}}_R$ is

$$\hat{\mathcal{U}}_L(z) = \mathcal{T}\left\{e^{-i\int_{t_0}^z d\bar{z}\hat{h}(\bar{z})}\right\}, \quad \hat{\mathcal{U}}_R(z) = \overline{\mathcal{T}}\left\{e^{+i\int_{t_0}^z d\bar{z}\hat{h}(\bar{z})}\right\}$$

- Therefore we have the differential equation for $\hat{\mathcal{F}}$:

$$i\frac{d}{dz_1}\hat{\mathcal{F}}(z_1, z_2) = \delta(z_1, z_2), \quad -i\frac{d}{dz_2}\hat{\mathcal{F}}(z_1, z_2) = \delta(z_1, z_2)$$

- We have

$$\hat{\mathcal{F}}(z_1, z_2) = \theta(z_1, z_2)\hat{\mathcal{F}}^> + \theta(z_2, z_1)\hat{\mathcal{F}}^<$$

where

$$\hat{\mathcal{F}}^> - \hat{\mathcal{F}}^< = -i\hat{\mathbf{1}}$$

- With KMS relations:

$$\hat{\mathcal{G}}(t_{0-}, z') = \pm\hat{\mathcal{G}}(t_0 - i\beta, z') \quad \begin{cases} + \text{ for bosons} \\ - \text{ for fermions} \end{cases}$$

we have

$$\hat{\mathcal{F}}^< = \pm\hat{\mathcal{U}}_L(t_0 - i\beta)\hat{\mathcal{F}}^> = \pm e^{-\beta\hat{h}^M}\hat{\mathcal{F}}^> \quad \begin{cases} + \text{ for bosons} \\ - \text{ for fermions} \end{cases}$$

Then

$$\hat{\mathcal{F}}^< = \mp i\frac{1}{e^{\beta\hat{h}^M} \mp \hat{\mathbf{1}}} = \mp if\left(\hat{h}^M\right)$$

and

$$\hat{\mathcal{F}}^> = \pm i\frac{1}{e^{-\beta\hat{h}^M} \mp \hat{\mathbf{1}}} = -i\bar{f}\left(\hat{h}^M\right)$$

where

$$f(\omega) = 1/\left[e^{\beta\omega} \mp 1\right], \quad \bar{f}(\omega) = 1 \pm f(\omega) = e^{\beta\omega}f(\omega)$$

Now we are talking about the Matsubara component:

- Let $z_1 = t_0 - i\tau_1$, $z_2 = t_0 - i\tau_2$, we have

$$\hat{\mathcal{U}}_L(t_0 - i\tau) = e^{-\tau\hat{h}^M}, \quad \hat{\mathcal{U}}_R(t_0 - i\tau) = e^{\tau\hat{h}^M}$$

Then we have

$$\hat{\mathcal{G}}^M(\tau_1, \tau_2) = -i\left[\theta(\tau_1 - \tau_2)\bar{f}\left(\hat{h}^M\right) \pm \theta(\tau_2 - \tau_1)f\left(\hat{h}^M\right)\right]e^{-(\tau_1 - \tau_2)\hat{h}^M}$$

- Another way to write this, using result from previous section, is that

$$\hat{\mathcal{G}}^M(\tau_1, \tau_2) = \frac{1}{-i\beta}\sum_{m=-\infty}^{\infty}\frac{e^{-\omega_m(\tau_1 - \tau_2)}}{\omega_m - \hat{h}^M}$$

- We can prove they are equivalent.

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Now let's talk about lesser and greater component. Inspired by

$$\hat{\mathcal{G}}(z_1, z_2) = -i\hat{\mathcal{U}}_L(z_1)\left(\theta(z_1 - z_2)\bar{f}(\hat{h}^M) \pm \theta(z_2 - z_1)f(\hat{h}^M)\right)\hat{\mathcal{U}}_R(z_2)$$

and with

$$\hat{U}_L(t_\pm) = T\left(e^{-i\int_{t_0}^t d\bar{t}\hat{h}(\bar{t})}\right) = \hat{\mathcal{U}}(t), \quad \hat{\mathcal{U}}_R(t_\pm) = \hat{\mathcal{U}}^\dagger(t)$$

we have:

- The lesser component:
$$\hat{\mathcal{G}}^<(t_1, t_2) = \mp i\hat{\mathcal{U}}(t_1)f(\hat{h}^M)\hat{\mathcal{U}}^\dagger(t_2)$$

- The greater component:
$$\hat{\mathcal{G}}^>(t_1, t_2) = -i\hat{\mathcal{U}}(t_1)\bar{f}(\hat{h}^M)\hat{\mathcal{U}}^\dagger(t_2)$$

- Furthermore, we have:
$$\hat{\mathcal{G}}^<(t_1, t_2) = \mp i\sum_\lambda f(\epsilon_\lambda^M)\hat{\mathcal{U}}(t_1)|\lambda^M\rangle\langle\lambda^M|\hat{\mathcal{U}}^\dagger(t_2)$$
$$= \mp i\sum_\lambda f(\epsilon_\lambda^M)|\lambda^M(t_1)\rangle\langle\lambda^M(t_2)|$$

- The density is
$$n(\boldsymbol{x}, t) = \pm iG^<(\boldsymbol{x}, t; \boldsymbol{x}, t)$$

- If the Hamiltonian is constant, we have
$$\hat{\mathcal{G}}^<(t_1, t_2) = \mp if(\hat{h}^M)e^{-i\hat{h}(t_1 - t_2)}$$
$$\hat{\mathcal{G}}^>(t_1, t_2) = -i\bar{f}(\hat{h}^M)e^{-i\hat{h}(t_1 - t_2)}$$

There is no dependence on t_0! Only dependence on $t_1 - t_2$.

- We can define the Fourier transform:
$$\hat{\mathcal{G}}^<(t_1, t_2) = \int \frac{d\omega}{2\pi}e^{-i\omega(t_1 - t_2)}\hat{\mathcal{G}}^<(\omega)$$
$$\hat{\mathcal{G}}^>(t_1, t_2) = \int \frac{d\omega}{2\pi}e^{-i\omega(t_1 - t_2)}\hat{\mathcal{G}}^>(\omega)$$

We can directly see that
$$\hat{\mathcal{G}}^<(\omega) = \mp 2\pi if(\hat{h}^M)\delta(\omega - \hat{h})$$
$$\hat{\mathcal{G}}^>(\omega) = -2\pi i\bar{f}(\hat{h}^M)\delta(\omega - \hat{h}) = \pm e^{\beta\hat{h}^M}\hat{\mathcal{G}}^<(\omega)$$

Now let's discuss other components.

- The retarded Green's function is
$$\hat{\mathcal{G}}^R(t_1, t_2) = \theta(t_1 - t_2)\left(\hat{\mathcal{G}}^>(t_1, t_2) - \hat{\mathcal{G}}^<(t_1, t_2)\right)$$
$$= -i\theta(t_1 - t_2)\hat{\mathcal{U}}(t_1)\hat{\mathcal{U}}^\dagger(t_2) = -i\theta(t_1 - t_2)T\left(e^{-i\int_{t_2}^{t_1} d\bar{t}\hat{h}(\bar{t})}\right)$$

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- The advanced Green's function is

$$\hat{\mathcal{G}}^A(t_1, t_2) = \mathrm{i}\theta(t_2 - t_1)\bar{T}\left(e^{\mathrm{i}\int_{t_2}^{t_1} \mathrm{d}\bar{t}\hat{h}(\bar{t})}\right) = \left(\hat{\mathcal{G}}^R(t_2, t_1)\right)^\dagger$$

This doesn't depend on the original density matrix, only depends on the Hamiltonian.

- For constant Hamiltonian $\hat{h}(t) = \hat{h}$, we have

$$\hat{\mathcal{G}}^R(t_1, t_2) = -\mathrm{i}\theta(t_1 - t_2)e^{-\mathrm{i}\hat{h}(t_1 - t_2)}$$

$$\hat{\mathcal{G}}^A(t_1, t_2) = \mathrm{i}\theta(t_2 - t_1)e^{\mathrm{i}\hat{h}(t_2 - t_1)}$$

- The Fourier transform is defined as

$$\hat{\mathcal{G}}^{R,A}(t_1, t_2) = \int \frac{\mathrm{d}\omega}{2\pi} e^{-\mathrm{i}\omega(t_1 - t_2)}\hat{\mathcal{G}}^{R,A}(\omega)$$

- We have the integration form of step function:

$$\theta(t_1 - t_2) = \mathrm{i}\int \frac{d\omega}{2\pi} \frac{e^{-\mathrm{i}\omega(t_1 - t_2)}}{\omega + \mathrm{i}\eta}$$

- Therefore

$$\hat{\mathcal{G}}^{\mathrm{R}}(t_1, t_2) = \int \frac{d\omega}{2\pi} \frac{e^{-\mathrm{i}(\omega + \hat{h})(t_1 - t_2)}}{\omega + \mathrm{i}\eta}$$

Changing variables from $\omega \to \omega - \hat{h}$, we have

$$\hat{\mathcal{G}}^{\mathrm{R}}(\omega) = \frac{1}{\omega - \hat{h} + \mathrm{i}\eta} = \sum_\lambda \frac{|\lambda\rangle\langle\lambda|}{\omega - \epsilon_\lambda + \mathrm{i}\eta}$$

And because

$$\hat{\mathcal{G}}^{\mathrm{A}}(\omega) = \left[\hat{\mathcal{G}}^{\mathrm{R}}(\omega)\right]^\dagger$$

we have

$$\hat{\mathcal{G}}^{\mathrm{A}}(\omega) = \frac{1}{\omega - \hat{h} - \mathrm{i}\eta} = \sum_\lambda \frac{|\lambda\rangle\langle\lambda|}{\omega - \epsilon_\lambda - \mathrm{i}\eta}$$

- Given that

$$\hat{\mathcal{G}}^{\mathrm{R}} - \hat{\mathcal{G}}^{\mathrm{A}} = \hat{\mathcal{G}}^> - \hat{\mathcal{G}}^<$$

we have

$$\hat{\mathcal{G}}^<(\omega) = \pm f\left(\hat{h}^{\mathrm{M}}\right)\left[\hat{\mathcal{G}}^{\mathrm{R}}(\omega) - \hat{\mathcal{G}}^{\mathrm{A}}(\omega)\right]$$

and

$$\hat{\mathcal{G}}^>(\omega) = \bar{f}\left(\hat{h}^{\mathrm{M}}\right)\left[\hat{\mathcal{G}}^{\mathrm{R}}(\omega) - \hat{\mathcal{G}}^{\mathrm{A}}(\omega)\right]$$

- In the case $\hat{h}^{\mathrm{M}} = \hat{h} - \mu$, we have

$$\hat{\mathcal{G}}^<(\omega) = \pm f(\omega - \mu)\left[\hat{\mathcal{G}}^{\mathrm{R}}(\omega) - \hat{\mathcal{G}}^{\mathrm{A}}(\omega)\right], \quad \hat{\mathcal{G}}^>(\omega) = \bar{f}(\omega - \mu)\left[\hat{\mathcal{G}}^{\mathrm{R}}(\omega) - \hat{\mathcal{G}}^{\mathrm{A}}(\omega)\right]$$

- Left and right component:

$$\hat{\mathcal{G}}^{\rceil}(t, \tau) = \mp i \hat{\mathcal{U}}(t) f\left(\hat{h}^{\mathrm{M}}\right) e^{\tau \hat{h}^{\mathrm{M}}} = i \hat{\mathcal{G}}^{\mathrm{R}}(t, t_0) \hat{\mathcal{G}}^{\mathrm{M}}(0, \tau)$$

$$\hat{\mathcal{G}}^{\lceil}(\tau, t) = -i e^{-\tau \hat{h}^{\mathrm{M}}} \bar{f}\left(\hat{h}^{\mathrm{M}}\right) \hat{\mathcal{U}}^{\dagger}(t) = -i \hat{\mathcal{G}}^{\mathrm{M}}(\tau, 0) \hat{\mathcal{G}}^{\mathrm{A}}(t_0, t)$$

- We have time-ordered Green's function

$$\hat{\mathcal{G}}^{\mathrm{T}}(t_1, t_2) = -i \hat{\mathcal{U}}(t_1) \left[\theta(t_1 - t_2) \bar{f}\left(\hat{h}^{\mathrm{M}}\right) \pm \theta(t_2 - t_1) f\left(\hat{h}^{\mathrm{M}}\right)\right] \hat{\mathcal{U}}^{\dagger}(t_2)$$

and we have

$$\hat{\mathcal{G}}^{\mathrm{T}}(t_1, t_2) = \int \frac{d\omega}{2\pi} e^{-i\omega(t_1 - t_2)} \underbrace{\left[\frac{\bar{f}\left(\hat{h}^{\mathrm{M}}\right)}{\omega - \hat{h} + i\eta} \mp \frac{f\left(\hat{h}^{\mathrm{M}}\right)}{\omega - \hat{h} - i\eta}\right]}_{\hat{\mathcal{G}}^{\mathrm{T}}(\omega)}$$

- For fermions in zero temperature, $\hat{h}^{\mathrm{M}} = \hat{h} - \epsilon_{\mathrm{F}}$, ϵ_{F} is the Fermi energy, and we have $f(\epsilon_\lambda - \mu) = \theta(\epsilon_{\mathrm{F}} - \epsilon_\lambda)$. Then we have

$$\hat{\mathcal{G}}^{\mathrm{T}}(\omega) = \sum_{\epsilon_\lambda > \epsilon_{\mathrm{F}}} \frac{|\lambda\rangle\langle\lambda|}{\omega - \epsilon_\lambda + i\eta} + \sum_{\epsilon_\lambda < \epsilon_{\mathrm{F}}} \frac{|\lambda\rangle\langle\lambda|}{\omega - \epsilon_\lambda - i\eta}$$

12 Interacting Green's function

Consider Hamiltonian $\hat{H}$ and corresponding $\hat{H}^M = \hat{H} - \mu\hat{N}$. Consider the eigenstates of $|\Psi_k\rangle$ of $\hat{H}^M$.

- We have

$$G_{ji}^{<}(t, t') = \mp i \sum_k \rho_k \left\langle \Psi_k \left| \hat{d}_i^{\dagger} e^{-i(\hat{H} - E_k)(t' - t)} \hat{d}_j \right| \Psi_k \right\rangle$$

$$G_{ji}^{>}(t, t') = -i \sum_k \rho_k \left\langle \Psi_k \left| \hat{d}_j e^{-i(\hat{H} - E_k)(t - t')} \hat{d}_i^{\dagger} \right| \Psi_k \right\rangle$$

- Lehmann representation:

$$G_{ji}^{<}(t, t') = \mp i \sum_{pk} \rho_k \Phi_{pk}^{*}(i) \Phi_{pk}(j) e^{-i(E_p - E_k)(t' - t)}$$

$$G_{ji}^{>}(t, t') = -i \sum_{pk} \rho_k \Phi_{kp}(j) \Phi_{kp}^{*}(i) e^{-i(E_p - E_k)(t - t')}$$

where

$$\Phi_{kp}(i) = \left\langle \Psi_k \left| \hat{d}_i \right| \Psi_p \right\rangle$$

For this term to be nonzero, $|\Psi_p\rangle$ must contain one more particle than $|\Psi_k\rangle$.

- Then we get the Fourier transform:

$$G_{ji}^<(\omega) = \mp 2\pi i \sum_{pk} \rho_k \Phi_{pk}^*(i) \Phi_{pk}(j) \delta(\omega - E_k + E_p)$$

and

$$G_{ji}^>(\omega) = -2\pi i \sum_{pk} \rho_k \Phi_{kp}(j) \Phi_{kp}^*(i) \delta(\omega - E_p + E_k)$$

and we have the property

$$i G_{jj}^>(\omega) \geq 0$$

$$i G_{jj}^<(\omega) \geq 0 \quad \text{for bosons ;} \quad i G_{jj}^<(\omega) \leq 0 \quad \text{for fermions}$$

- For retarded and advanced function, we have

$$\hat{\mathcal{G}}^R(t, t') = i \int \frac{d\omega}{2\pi} \frac{e^{-i\omega(t-t')}}{\omega + i\eta} \int \frac{d\omega'}{2\pi} e^{-i\omega'(t-t')} \left[\hat{\mathcal{G}}^>(\omega') - \hat{\mathcal{G}}^<(\omega') \right]$$

therefore

$$\hat{\mathcal{G}}^R(\omega) = i \int \frac{d\omega'}{2\pi} \frac{\hat{\mathcal{G}}^>(\omega') - \hat{\mathcal{G}}^<(\omega')}{\omega - \omega' + i\eta}$$

with

$$\hat{\mathcal{G}}^A(\omega) = \left[\hat{\mathcal{G}}^R(\omega) \right]^\dagger$$

then

$$\hat{\mathcal{G}}^A(\omega) = i \int \frac{d\omega'}{2\pi} \frac{\hat{\mathcal{G}}^>(\omega') - \hat{\mathcal{G}}^<(\omega')}{\omega - \omega' - i\eta}$$

therefore

$$G_{ji}^{R/A}(\omega) = \sum_{pk} \frac{\Phi_{kp}(j) \Phi_{kp}^*(i)}{\omega - E_p + E_k \pm i\eta} [\rho_k \mp \rho_p]$$

- For thermodynamic equilibrium,

$$\hat{H}^M = \hat{H} - \mu \hat{N}$$

we have

$$\rho_k = \frac{e^{-\beta(E_k - \mu N_k)}}{\text{Tr}\left[e^{-\beta(\hat{H} - \mu \hat{N})} \right]} = e^{-\beta(E_k - E_p) + \beta\mu(N_k - N_p)} \rho_p$$

- We can prove that

$$\hat{\mathcal{G}}^>(\omega) = \pm e^{\beta(\omega - \mu)} \hat{\mathcal{G}}^<(\omega)$$

- We have

$$\hat{\mathcal{G}}^>(\omega) - \hat{\mathcal{G}}^<(\omega) = \hat{\mathcal{G}}^R(\omega) - \hat{\mathcal{G}}^A(\omega)$$

Then

$$\hat{\mathcal{G}}^<(\omega) = \pm f(\omega - \mu) \left[\hat{\mathcal{G}}^R(\omega) - \hat{\mathcal{G}}^A(\omega) \right]$$

$$\hat{\mathcal{G}}^>(\omega) = \bar{f}(\omega - \mu) \left[\hat{\mathcal{G}}^R(\omega) - \hat{\mathcal{G}}^A(\omega) \right]$$

- For left component, we have

$$G_{ji}^{\Gamma}\left(\tau, t'\right) = -\mathrm{i}\sum_k \rho_k \left\langle \Psi_k \right| \underbrace{e^{\mathrm{i}(\hat{H}-\mu\hat{N})(-\mathrm{i}\tau)}\hat{d}_j e^{-\mathrm{i}(\hat{H}-\mu\hat{N})(-\mathrm{i}\tau)}}_{\hat{d}_{j,H}(t_0-\mathrm{i}\tau)} \underbrace{e^{\mathrm{i}\hat{H}(t'-t_0)}\hat{d}_i^{\dagger}e^{-\mathrm{i}\hat{H}(t'-t_0)}}_{d_{i,H}^{\dagger}(t')} \left|\Psi_k\right\rangle$$

$$= -\mathrm{i}e^{\mu\tau}\sum_k \rho_k \left\langle \Psi_k \left| \hat{d}_j e^{-\mathrm{i}\left(\hat{H}-E_k\right)(t_0-\mathrm{i}\tau-t')}\hat{d}_i^{\dagger} \right| \Psi_k \right\rangle$$

then

$$\hat{\mathcal{G}}^{\lceil}\left(\tau, t'\right) = e^{\mu\tau}\hat{\mathcal{G}}^{>}\left(t_0 - \mathrm{i}\tau, t'\right)$$

Similarly

$$\hat{\mathcal{G}}^{\rceil}(t, \tau) = e^{-\mu\tau}\hat{\mathcal{G}}^{<}\left(t, t_0 - \mathrm{i}\tau\right)$$

- For system in thermodynamic equilibrium, we have

$$G_{ji}^{\mathrm{M}}\left(\tau_1, \tau_2\right) = \frac{1}{\mathrm{i}}\sum_{kn}\rho_p\left[\theta\left(\tau_1-\tau_2\right)e^{\beta\left(E_p^{\mathrm{M}}-E_k^{\mathrm{M}}\right)} \pm \theta\left(\tau_2-\tau_1\right)\right]e^{-(\tau_1-\tau_2)\left(E_p^{\mathrm{M}}-E_k^{\mathrm{M}}\right)}\Phi_{kp}(j)\Phi_{kp}^*(i)$$

where

$$E_p^{\mathrm{M}} = E_p - \mu N_p$$

Recall that we proved

$$\frac{1}{-\mathrm{i}\beta}\sum_{m=-\infty}^{\infty}\frac{e^{-\omega_m\tau}}{\omega_m - E} = \frac{1}{\mathrm{i}}\left[\theta(\tau)e^{\beta E} \pm \theta(-\tau)\right]f(E)e^{-\tau E}$$

Then we have

$$G_{ji}^{\mathrm{M}}\left(\tau_1, \tau_2\right) = \frac{1}{-\mathrm{i}\beta}\sum_{m=-\infty}^{\infty}e^{-\omega_m(\tau_1-\tau_2)}\underbrace{\sum_{kp}\frac{\rho_p}{f\left(E_p^{\mathrm{M}}-E_k^{\mathrm{M}}\right)}\frac{\Phi_{kp}(j)\Phi_{kp}^*(i)}{\omega_m - E_p^{\mathrm{M}} + E_k^{\mathrm{M}}}}_{G_{ji}^{\mathrm{M}}(\omega_m)}.$$

we have

$$\frac{\rho_p}{f\left(E_p^{\mathrm{M}}-E_k^{\mathrm{M}}\right)} = \rho_p\left(e^{\beta\left(E_p^{\mathrm{M}}-E_k^{\mathrm{M}}\right)} \mp 1\right) = \rho_k \mp \rho_p$$

and

$$E_p^{\mathrm{M}} - E_k^{\mathrm{M}} = E_p - E_k - \mu\left(N_p - N_k\right) = E_p - E_k - \mu$$

therefore we have

$$G_{ji}^{\mathrm{M}}\left(\omega_m\right) = \sum_{kp}\frac{\Phi_{kp}(j)\Phi_{kp}^*(i)}{\omega_m + \mu - E_p + E_k}\left[\rho_k \mp \rho_p\right]$$

therefore

$$\hat{\mathcal{G}}^{\mathrm{M}}(\zeta) = \begin{cases} \hat{\mathcal{G}}^{\mathrm{R}}(\zeta + \mu) & \text{for } \mathrm{Im}[\zeta] > 0 \\ \hat{\mathcal{G}}^{\mathrm{A}}(\zeta + \mu) & \text{for } \mathrm{Im}[\zeta] < 0 \end{cases}$$

Thus $\mathcal{G}^M(\zeta)$ is analytic everywhere except along the real axis where it can have poles or branch points.

- As a result,

$$\hat{\mathcal{G}}^{\mathrm{M}}(\omega \pm \mathrm{i}\eta) = \hat{\mathcal{G}}^{\mathrm{R/A}}(\omega + \mu)$$

which means that $\mathcal{G}^M$ has a discontinuity given by the difference $\mathcal{G}^R - \mathcal{G}^A$ when the complex frequency crosses the real axis.

13 Spectral function

- For systems that are initially in a pure state $\hat{\rho} = |\Psi_{N,0}\rangle\langle\Psi_{N,0}|$, We denote by $|\Psi_{N\pm1,m}\rangle$ the eigenstates of $\hat{H}$ with $N \pm 1$ particles and define the quasi-particle wavefunctions P_m and the quasi-hole wavefunctions Q_m according to

$$P_m(i) = \left\langle \Psi_{N,0} \left| \hat{d}_i \right| \Psi_{N+1,m} \right\rangle, \quad Q_m(i) = \left\langle \Psi_{N-1,m} \left| \hat{d}_i \right| \Psi_{N,0} \right\rangle$$

- Then, the lesser and greater Green's functions become

$$G_{ji}^{<}\left(t, t'\right) = \mp \mathrm{i} \sum_m Q_m(j) Q_m^*(i) e^{-\mathrm{i}\left(E_{N-1,m} - E_{N,0}\right)(t'-t)}$$

$$G_{ji}^{>}\left(t, t'\right) = -\mathrm{i} \sum_m P_m(j) P_m^*(i) e^{-\mathrm{i}\left(E_{N+1,m} - E_{N,0}\right)(t-t')}$$

- The Fourier transform of these functions are

$$G_{ji}^{<}(\omega) = \mp 2\pi\mathrm{i} \sum Q_m(j) Q_m^*(i) \delta\left(\omega - [E_{N,0} - E_{N-1,m}]\right)$$

$$G_{ji}^{>}(\omega) = -2\pi\mathrm{i} \sum P_m(j) P_m^*(i) \delta\left(\omega - [E_{N+1,m} - E_{N,0}]\right)$$

$G^{<}$ is peaked at the removal energies, and $G^{>}$ is peaked at the addition energies.

- We define
$$\hat{A}(\omega) = \mathrm{i}\left[\hat{\mathcal{G}}^{>}(\omega) - \hat{\mathcal{G}}^{<}(\omega)\right] = \mathrm{i}\left[\hat{\mathcal{G}}^{\mathrm{R}}(\omega) - \hat{\mathcal{G}}^{\mathrm{A}}(\omega)\right]$$

- We have

$$A_{jj}(\omega) = 2\pi\left[\sum_m |P_m(j)|^2 \delta\left(\omega - [E_{N+1,m} - E_{N,0}]\right) \mp \sum_m |Q_m(j)|^2 \delta\left(\omega - [E_{N,0} - E_{N-1,m}]\right)\right]$$

- It is not difficult to verify that:
$$\int \frac{d\omega}{2\pi} A_{ji}(\omega) = \delta_{ji}$$

- We have
$$\hat{\mathcal{G}}^{\mathrm{R}}(\omega) = \int \frac{d\omega'}{2\pi} \frac{\hat{A}(\omega')}{\omega - \omega' + \mathrm{i}\eta}, \quad \hat{\mathcal{G}}^{\mathrm{A}}(\omega) = \int \frac{d\omega'}{2\pi} \frac{\hat{A}(\omega')}{\omega - \omega' - \mathrm{i}\eta}$$

- We have
$$\hat{\mathcal{G}}^{<}(\omega) = \mp\mathrm{i}f(\omega - \mu)\hat{A}(\omega), \quad \hat{\mathcal{G}}^{>}(\omega) = -\mathrm{i}\bar{f}(\omega - \mu)\hat{A}(\omega)$$

14 Galitskii–Migdal formula

- For systems of interacting identical particles with Hamiltonian $\hat{H}(t) = \hat{H}_0(t) + \hat{H}_{\text{int}}$, the time-dependent energy $E_S(t_1)$ is considered as the ensemble average of $\hat{H}_S(t_1)$:

$$\hat{H}_S(t_1) \equiv \hat{H}(t_1) - q \int d\boldsymbol{x}_1 \hat{n}(\boldsymbol{x}_1) \delta V(1), \quad \delta V(1) = V(\boldsymbol{r}_1, t_1) - V(\boldsymbol{r}_1)$$

- Then we have

$$E_S(z_1) =$$

$$\sum_k \rho_k \langle \Psi_k | \hat{U}(t_{0-}, z_1) \left[\int d\boldsymbol{x}_1 d\boldsymbol{x}_2 \hat{\psi}^\dagger(\boldsymbol{x}_1) \langle \boldsymbol{x}_1 | \hat{h}_S(z_1) | \boldsymbol{x}_2 \rangle \hat{\psi}(\boldsymbol{x}_2) + \frac{1}{2} \int d\boldsymbol{x}_1 d\boldsymbol{x}_2 v(\boldsymbol{x}_1, \boldsymbol{x}_2) \hat{\psi}^\dagger(\boldsymbol{x}_1) \hat{\psi}^\dagger(\boldsymbol{x}_2) \hat{\psi}(\boldsymbol{x}_2) \hat{\psi}(\boldsymbol{x}_1) \right] \hat{U}(z_1, t_{0-}) | \Psi_k \rangle$$

  where $\hat{h}_S(z_1) = \hat{h}(z_1) - q\delta V(\hat{\boldsymbol{r}}_1, z_1)$.

- In contour formalism, we have

$$E_S(z_1) = \pm i \int d\boldsymbol{x}_1 d2\, h_S(1; 2) G(2; 1^+) - \frac{1}{2} \int d\boldsymbol{x}_1 d2\, v(1; 2) G_2(1, 2; 1^+, 2^+)$$

- Since we have

$$\left[\left(i\frac{d}{dz_1} - i\frac{d}{dz_2} \right) G(1; 2) \right]_{2=1^+} - \int d3 \left[h(1; 3) G(3; 1^+) + G(1; 3^+) h(3; 1) \right] = \pm 2i \int d3\, v(1; 3) G_2(1, 3; 1^+, 3^+)$$

- Then, we have

$$E_S(z_1) =$$

$$\pm i \int d\boldsymbol{x}_1 \left\langle \boldsymbol{x}_1 \left| \left[\hat{h}_S(z_1) - \frac{1}{2} \hat{h}(z_1) \right] \hat{\mathcal{G}}(z_1, z_1^+) \right| \boldsymbol{x}_1 \right\rangle \pm \frac{i}{4} \int d\boldsymbol{x}_1 \left[\left(i\frac{d}{dz_1} - i\frac{d}{dz_2} \right) \left\langle \boldsymbol{x}_1 \left| \hat{\mathcal{G}}(z_1, z_2) \right| \boldsymbol{x}_1 \right\rangle \right]_{z_2 = z_1^+}$$

- For $z_1 = t_0 - i\tau_1$, $h_S(z_1) = h(z_1) = h^M$, then the initial energy E_S^M is

$$E_S^M = \pm \frac{i}{2} \frac{1}{-i\beta} \sum_m e^{\eta \omega_m} \int d\boldsymbol{x} \left\langle \boldsymbol{x} \left| \left(\omega_m + \hat{h}^M \right) \hat{\mathcal{G}}^M(\omega_m) \right| \boldsymbol{x} \right\rangle$$

- For $z_1 = t_\pm$, we have $\hat{h}_S(t) = \hat{h}(t) - q\delta V(\hat{\boldsymbol{r}}, t)$, then

$$E_S(t) = \pm \frac{i}{4} \int d\boldsymbol{x} \left\langle \boldsymbol{x} \left| \left(i\frac{d}{dt} - i\frac{d}{dt'} + 2\hat{h}(t) \right) \hat{\mathcal{G}}^<(t, t') \right| \boldsymbol{x} \right\rangle \bigg|_{t'=t} - q \int d\boldsymbol{x}\, n(\boldsymbol{x}, t) \delta V(\mathbf{r}, t)$$

- If $\hat{H}(t) = \hat{H}$, then

$$E_S = \pm \frac{i}{2} \int \frac{d\omega}{2\pi} \int d\boldsymbol{x} \left\langle \boldsymbol{x} \left| (\omega + \hat{h}) \hat{\mathcal{G}}^<(\omega) \right| \boldsymbol{x} \right\rangle$$

  This is called the Galitskii–Migdal formula.

- For noninteracting system, the above formula becomes

$$E_S = \sum_\lambda f\left(\epsilon_\lambda^M \right) \epsilon_\lambda$$