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

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January 14, 2022

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.

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1 Time-dependent Schrödinger equation and evolution operators

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

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

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

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

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 $t_0 < t_1 < \cdots < t_n < t_{n+1} = t$

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

Then we have

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

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:

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

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

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

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

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

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

But with time ordering operators, we actually have:

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

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

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

$$|\Psi(t)\rangle = \hat{T}\left(e^{-i\Delta t\left(\sum_{p}\hat{H}(t_{p})\right)}\right)|\Psi(t_{0})\rangle$$

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

$$\begin{split} |\Psi(t)\rangle &= \lim_{\Delta t \to 0} \hat{T} \left(\mathrm{e}^{-\mathrm{i}\Delta t \left(\sum_{p} \hat{H}(t_{p}) \right)} \right) |\Psi(t_{0})\rangle \\ &= \hat{T} \left(\mathrm{e}^{-\mathrm{i} \int_{t_{0}}^{t} \mathrm{d}\tau \hat{H}(\tau)} \right) |\Psi(t_{0})\rangle \end{split}$$

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

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

• 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 operator above. We have

$$\hat{U}(t,t_0) = \mathbf{1} - i \int_{t_0}^t dt_1 \hat{H}(t_1) \hat{U}(t_1,t_0)$$

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

$$\hat{U}(t,t_0) = \mathbf{1} - i \int_{t_0}^t dt_1 \hat{H}(t_1) + (-i)^2 \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \hat{H}(t_1) \hat{H}(t_2) \hat{U}(t_2,t_0)$$

$$= \sum_{k=0}^{\infty} (-i)^k \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{k-1}} dt_k \hat{H}(t_1) \hat{H}(t_2) \cdots \hat{H}(t_k)$$

Note that

$$\int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{k-1}} dt_k \hat{H}(t_1) \hat{H}(t_2) \cdots \hat{H}(t_k) = \frac{1}{k!} \int_{t_0}^t dt_1 \int_{t_0}^t dt_2 \cdots \int_{t_0}^t dt_k \hat{T} \left(\hat{H}(t_1) \hat{H}(t_2) \cdots \hat{H}(t_k) \right)$$

Therefore

$$\hat{U}(t, t_0) = \sum_{k=0}^{\infty} \frac{(-i)^k}{k!} \int_{t_0}^t dt_1 \int_{t_0}^t dt_2 \cdots \int_{t_0}^t dt_k \hat{T} \left(\hat{H}(t_1) \hat{H}(t_2) \cdots \hat{H}(t_k) \right)$$

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

• 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 $\hat{n}(\mathbf{x}) = \hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}(\mathbf{x})$, we have $\hat{n}_H(\mathbf{x},t)$ 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 $\hat{H}(t)$

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

$$= H_0 + H_{\text{int}}$$

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

$$\begin{split} \left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}')\right] &= \hat{\psi}(\boldsymbol{x}) \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}') - \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}) \\ &= \hat{\psi}(\boldsymbol{x}) \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}') \mp \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}) \hat{\psi}(\boldsymbol{x}') = \hat{\psi}(\boldsymbol{x}') \delta(\boldsymbol{x} - \boldsymbol{x}') \\ \left[\hat{\psi}^{\dagger}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}')\right] &= \hat{\psi}^{\dagger}(\boldsymbol{x}) \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}') - \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}') \hat{\psi}^{\dagger}(\boldsymbol{x}) \\ &= \pm \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}^{\dagger}(\boldsymbol{x}) \hat{\psi}(\boldsymbol{x}') - \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}(\boldsymbol{x}') \hat{\psi}^{\dagger}(\boldsymbol{x}) = -\hat{\psi}^{\dagger}(\boldsymbol{x}') \delta(\boldsymbol{x}' - \boldsymbol{x}) \\ \left[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}^{\dagger}(\boldsymbol{x}'') \hat{\psi}(\boldsymbol{x}'') \hat{\psi}(\boldsymbol{x}'') \hat{\psi}(\boldsymbol{x}'') \hat{\psi}(\boldsymbol{x}'') - \hat{\psi}^{\dagger}(\boldsymbol{x}') \hat{\psi}^{\dagger}(\boldsymbol{x}'') \hat{\psi}(\boldsymbol{x}'') \hat{$$

Then we have:

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

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:

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

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:

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

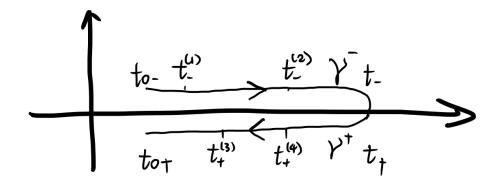


Figure 1: The oriented contour $\gamma = \gamma_- \oplus \gamma_+$

- 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 $z_1, \dots, z_m \in \gamma$

$$\mathcal{T}\left(\hat{A}_{1}(z_{1})\cdots\hat{A}_{m}(z_{m})\right) = \hat{A}_{P(1)}(z_{P(1)})\cdots\hat{A}_{P(m)}(z_{P(m)})$$

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

$$\int_{t}^{t_0} dt_1 \cdots \int_{t}^{t_0} dt_n \int_{t_0}^{t} dt'_1 \cdots \int_{t_0}^{t} dt'_m \bar{T} \left(\hat{H}(t_1) \cdots \hat{H}(t_n) \right) \hat{O}(t) \hat{T} \left(\hat{H}(t'_1) \cdots \hat{H}(t'_m) \right)$$

$$= \int_{\gamma_+} dz_1 \cdots \int_{\gamma_+} dz_n \int_{\gamma_-} dz'_1 \cdots \int_{\gamma_-} dz'_m \mathcal{T} \left(\hat{H}(z_1) \cdots \hat{H}(z_n) \hat{O}(t_{\pm}) \hat{H}(z'_1) \cdots \hat{H}(z'_m) \right)$$

• 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

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

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:

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

This $\tilde{\gamma}$ is referred 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

$$\hat{H} = \sum_{k} E_k^M \ket{\Psi_k} \langle \Psi_k |$$

• 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

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

• 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

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

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:

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

- 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 .

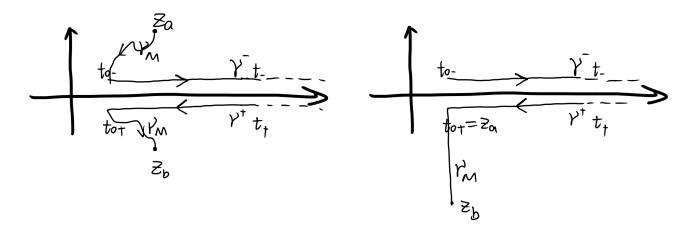


Figure 2: Different choices of z_a, z_b

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

$$\operatorname{Tr}\left(e^{-i\int_{\gamma^M} dz \hat{H}^M} \mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz \hat{H}(z)} \hat{O}(t_{\pm})\right)\right) = \operatorname{Tr}\left(e^{-i\int_{z_a}^{t_0} dz \hat{H}^M} \mathcal{T}\left(e^{-i\int_{\tilde{\gamma}} dz \hat{H}(z)} \hat{O}(t_{\pm})\right) e^{-i\int_{t_0+}^{z_b} dz \hat{H}^M}\right)$$

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

• In general, we have

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

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 :

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

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:

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

The integral is taken along the contour.

• This evolution operator has the following property:

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

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

$$i\frac{\partial}{\partial z}\hat{U}(z,z_{0}) = \mathcal{T}\left(i\frac{\partial}{\partial z}e^{-i\int_{z_{0}}^{z}d\tilde{z}\hat{H}(\tilde{z})}\right) = \mathcal{T}\left(\hat{H}(z)e^{-i\int_{z_{0}}^{z}d\tilde{z}\hat{H}(\tilde{z})}\right) = \hat{H}(z)\hat{U}(z,z_{0})$$

$$i\frac{\partial}{\partial z}\hat{U}(z_{0},z) = \bar{\mathcal{T}}\left(i\frac{\partial}{\partial z}e^{i\int_{z_{0}}^{z}d\tilde{z}\hat{H}(\tilde{z})}\right) = -\bar{\mathcal{T}}\left(\hat{H}(z)e^{i\int_{z_{0}}^{z}d\tilde{z}\hat{H}(\tilde{z})}\right) = -\hat{U}(z_{0},z)\hat{H}(z)$$

• 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:

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

• 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:

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

- 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:

$$\hat{H}^{M} = \int d\mathbf{x} \hat{\psi}^{\dagger}(\mathbf{x}) \hat{h}(\mathbf{x}, z) \hat{\psi}(\mathbf{x}) + \frac{1}{2} \int d\mathbf{x} d\mathbf{x}' \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}^{\dagger}(\mathbf{x}') v(\mathbf{x}, \mathbf{x}') \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x})$$
$$= \hat{H}_{0}^{M} + \hat{H}_{int}^{M}$$

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

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

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 $\theta(z_1, z_2)$:

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

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:

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

 \bullet 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 $\theta(z_1, \dots, z_n)$ is defined as

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

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.

• 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.
- \bullet 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:

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

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

where \tilde{Q}_k means exclude this term from the multiplication.

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

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

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

• 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:

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

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

• Therefore we have:

$$i\frac{\mathrm{d}}{\mathrm{d}z_{k}}\hat{G}_{n}(1,\cdots,n;1',\cdots,n') = \frac{1}{\mathrm{i}^{n}}\mathcal{T}\left(\hat{\psi}_{H}(1)\cdots\left(i\frac{\mathrm{d}}{\mathrm{d}z_{k}}\hat{\psi}_{H}(k)\right)\cdots\hat{\psi}_{H}(n)\psi_{H}^{\dagger}(n')\cdots\psi_{H}^{\dagger}(1')\right) + \sum_{j=1}^{n}(\pm)^{k+j}\delta(k;j')\hat{G}_{n-1}(1,\cdots,\tilde{k},\cdots,n;1',\cdots,\tilde{j}',\cdots,n')$$

Similarly:

$$-i\frac{\mathrm{d}}{\mathrm{d}z_{k}'}\hat{G}_{n}(1,\dots,n;1',\dots,n') = \frac{1}{\mathrm{i}^{n}}\mathcal{T}\left(\hat{\psi}_{H}(1)\dots\left(-i\frac{\mathrm{d}}{\mathrm{d}z_{k}'}\hat{\psi}_{H}(k)\right)\dots\hat{\psi}_{H}(n)\psi_{H}^{\dagger}(n')\dots\psi_{H}^{\dagger}(1')\right)$$
$$+\sum_{j=1}^{n}(\pm)^{k+j}\delta(j;k')\hat{G}_{n-1}(1,\dots,\tilde{j},\dots,n;1',\dots,\tilde{k}',\dots,n')$$

• Recall the equation of motion for field operators:

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

• 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:

$$\frac{1}{\mathrm{i}^{n}} \mathcal{T} \left\{ \hat{\psi}_{H}(1) \dots \left(\mathrm{i} \frac{d}{dz_{k}} \hat{\psi}_{H}(k) \right) \dots \hat{\psi}_{H}(n) \hat{\psi}_{H}^{\dagger} \left(n' \right) \dots \hat{\psi}_{H}^{\dagger} \left(1' \right) \right\}$$

$$= h(k) \hat{G}_{n} \left(1, \dots, n; 1', \dots, n' \right) \pm \frac{1}{\mathrm{i}^{n}} \int d\overline{1} v(k; \overline{1}) \mathcal{T} \left\{ \hat{\psi}_{H}(1) \dots \hat{\psi}_{H}(n) \hat{\psi}_{H}(\overline{1}) \hat{\psi}_{H}^{\dagger} \left(\overline{1}^{+} \right) \hat{\psi}_{H}^{\dagger} \left(n' \right) \dots \hat{\psi}_{H}^{\dagger} \left(1' \right) \right\}$$

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

Therefore we have:

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

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

Similarly, we have:

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

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

7 Martin-Schwinger hierarchy

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

$$G_n(1, \dots, n; 1, \dots, n') = \frac{\operatorname{Tr}\left(e^{-\beta H^M} \hat{G}_n(1, \dots, n; 1, \dots, n')\right)}{\operatorname{Tr}\left(e^{-\beta H^M}\right)}$$
$$= \frac{1}{\mathrm{i}^n} \frac{\operatorname{Tr}\left(\mathcal{T}\left(e^{-\mathrm{i}\int_{\gamma} \mathrm{d}\bar{z}\hat{H}(\bar{z})} \hat{\psi}(1) \dots \hat{\psi}(n) \psi^{\dagger}(n') \dots \psi^{\dagger}(1')\right)\right)}{\operatorname{Tr}\left(\mathcal{T}\left(e^{-\mathrm{i}\int_{\gamma} \mathrm{d}\bar{z}\hat{H}(\bar{z})}\right)\right)}$$

This requires derivation!

• For G_1 , by choosing $z_1 = z$, $z'_1 = z^+$, we have the time dependent ensemble average for $\hat{\psi}^{\dagger}(x'_1)\hat{\psi}(x_1)$, which could be used to calculate the ensemble average of any one-body operator. For example, the density operator:

$$n(\boldsymbol{x},z) = \frac{\operatorname{Tr}\left(e^{-\beta H^M}\hat{\psi}_H^{\dagger}(\boldsymbol{x},z)\hat{\psi}_H(\boldsymbol{x},z)\right)}{\operatorname{Tr}\left(e^{-\beta H^M}\right)} = \pm iG_1(\boldsymbol{x},z;\boldsymbol{x},z^+)$$

and the current density operator:

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

$$= \pm \frac{\nabla - \nabla'}{2m} G_{1}(\boldsymbol{x}, z; \boldsymbol{x}', z^{+})|_{\boldsymbol{x} = \boldsymbol{x}'}$$

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

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

• We have the differential equation for G_n :

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

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

and

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

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

This is called the Martin-Schwinger hierarchy.

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

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

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

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:

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

• If we define Σ as:

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

where

$$V_H(1) = \pm i \int d3v(1;3)G(3,3^+) = \int d\boldsymbol{x}_3 v(\boldsymbol{x}_1,\boldsymbol{x}_3,z_1)n(\boldsymbol{x}_3,z_1)$$

is the well-known Hartree potential. Then we have

$$\left(i\frac{d}{dz_{1}} - h(1)\right)G(1;1') = \delta(1;1') + i\int d2\Sigma(1,2)G(2;1')$$

$$G(1;1')\left(-i\frac{\overleftarrow{d}}{dz_{1}} - h(1')\right) = \delta(1;1') + i\int d2G(1;2)\Sigma(2;1')$$

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:

$$\int d1G_0(2;1) \left[i \frac{d}{dz_1} - h(1) \right] G(1;1')$$

$$= \int d1G_0(2;1) \left[-i \frac{d}{dz_1} - h(1) \right] G(1;1') + i \int dx_1 G_0(2;x_1,z_1) G(x_1,z_1;1') \Big|_{z_1=z_1}^{z_1=z_1}$$

$$= \int d1\delta(2;1)G(1;1') = G(2,1')$$

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

$$G(1;2) = G_0(1;2) + \int d3d4G_0(1;3)\Sigma(3;4)G(4;2)$$

Similarly, we can also get:

$$G(1;2) = G_0(1;2) + \int d3d4G_1(1;3)\Sigma(3;4)G_0(4;2)$$

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

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

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

$$\left(i\frac{\mathrm{d}}{\mathrm{d}z_1} - h(1)\right)G_2(1,2;1',2') = \delta(1;1')G(2,2') \pm \delta(1;2')G(2;1') \pm i\int \mathrm{d}3v(1,3)G_3(1,2,3;1',2',3^+)$$

• 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

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

• If we neglect the higher order term, we have:

$$\left[i\frac{d}{dz_1} - h(1)\right] \left[i\frac{d}{dz_2} - h(2)\right] \Upsilon(1, 2; 1', 2') = iv(1; 2)G_2(1, 2; 1', 2')$$

Therefore

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

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:

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

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:

$$G_{n} = \frac{1}{\mathrm{i}^{n}} \frac{\mathrm{Tr}\left[\mathcal{T}\left\{\mathrm{e}^{-\mathrm{i}\int_{\gamma}\mathrm{d}\bar{z}\hat{H}_{0}(\bar{z})}\mathrm{e}^{-\mathrm{i}\int_{\gamma}\mathrm{d}\bar{z}\hat{H}_{\mathrm{int}}(\bar{z})}\hat{\psi}(1)\dots\hat{\psi}^{\dagger}(1')\right\}\right]}{\mathrm{Tr}\left[\mathcal{T}\left\{\mathrm{e}^{-\mathrm{i}\int_{\gamma}\mathrm{d}\bar{z}\hat{H}_{0}(\bar{z})}\mathrm{e}^{-\mathrm{i}\int_{\gamma}\mathrm{d}\bar{z}\hat{H}_{\mathrm{int}}(\bar{z})}\right\}\right]}$$

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

• If we introduce the notation:

$$\operatorname{Tr}\left[\mathcal{T}\left\{e^{-i\int_{\gamma}d\bar{z}\hat{H}_{0}(\bar{z})}\ldots\right\}\right] = \langle \mathcal{T}\{\ldots\}\rangle_{0}$$

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

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

where \hat{H}_{int} is

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

where

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

• Now we look at the case of one-particle Green's function. Let $a = (x_a, z_a), b = (x_b, z_b)$, we have

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

The numerator could be rewritten as

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

The quantity inside time-ordering operator could be rewritten as

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

which is exactly

$$i^{2k+1}Z_0G_{0,2k+1}(a,1,1',\ldots,k,k';b,1^+,1'^+,\ldots k^+,k'^+)$$

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

$$i^{2k}Z_0G_{0,2k}(1,1',\ldots,k,k';1^+,1'^+,\ldots k^+,k'^+)$$

Therefore we have

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

which could be further written using Wick's theorem

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

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

• Similarly, we have

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

We also have Z/Z_0 , which is just the denominator above

$$\frac{Z}{Z_0} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{\mathrm{i}}{2}\right)^k \int v\left(1;1'\right) \dots v\left(k;k'\right) \begin{vmatrix} G_0\left(1;1^+\right) & G_0\left(1;1'^+\right) & \dots & G_0\left(1;k'^+\right) \\ G_0\left(1';1^+\right) & G_0\left(1';1'^+\right) & \dots & G_0\left(1';k'^+\right) \\ \vdots & \vdots & \ddots & \vdots \\ G_0\left(k';1^+\right) & G_0\left(k';1'^+\right) & \dots & G_0\left(k';k'^+\right) \end{vmatrix}_+$$

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.

 $k\left(z,z'\right) = \operatorname{Tr}\left[\hat{\rho}\hat{k}\left(z,z'\right)\right] = \operatorname{Tr}\left[\hat{\rho}\mathcal{T}\left\{\hat{O}_{1}(z)\hat{O}_{2}\left(z'\right)\right\}\right]$

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

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

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

$$k^{>}\left(z,z'\right) = \operatorname{Tr}\left[\hat{\rho}\hat{O}_{1}(z)\hat{O}_{2}\left(z'\right)\right], \quad k^{<}\left(z,z'\right) = \pm \operatorname{Tr}\left[\hat{\rho}\hat{O}_{2}\left(z'\right)\hat{O}_{1}(z)\right]$$

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

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

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

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

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 $t_0 - i\tau$:

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

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

$$k^{\mathrm{M}}(\tau, \tau') \equiv k (t_0 - i\tau, t_0 - i\tau')$$

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

where

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

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

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

• We also define the retarded and advanced component:

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

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

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

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

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

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:

$$\hat{\mathcal{G}}\left(z_{1},z_{2}
ight)=\int doldsymbol{x}_{1}doldsymbol{x}_{2}\left|oldsymbol{x}_{1}
ight
angle G(1;2)\left\langleoldsymbol{x}_{2}
ight|$$

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:

$$G(1;2) = \sum_{ji} \varphi_{j}(\boldsymbol{x}_{1}) G_{ji}(z_{1}, z_{2}) \varphi_{i}^{*}(\boldsymbol{x}_{2}) = \sum_{ji} \langle \boldsymbol{x}_{1} \mid j \rangle G_{ji}(z_{1}, z_{2}) \langle i \mid \boldsymbol{x}_{2} \rangle$$
$$\hat{\mathcal{G}}(z_{1}, z_{2}) = \sum_{ij} |j\rangle G_{ji}(z_{1}, z_{2}) \langle i|$$

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

$$\left(i\frac{\mathrm{d}}{\mathrm{d}z_{1}}-\hat{h}\left(z_{1}\right)\right)\hat{\mathcal{G}}_{0}\left(z_{1},z_{2}\right)=\delta\left(z_{1},z_{2}\right)$$

For interacting case, we have

$$\left[i\frac{d}{dz_{1}}-\hat{h}\left(z_{1}\right)\right]\hat{\mathcal{G}}\left(z_{1},z_{2}\right)-\int_{\gamma}d\bar{z}\hat{\Sigma}\left(z_{1},\bar{z}\right)\hat{\mathcal{G}}\left(\bar{z},z_{2}\right)=\delta\left(z_{1},z_{2}\right)$$

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

$$G_{ji}^{\mathrm{M}}\left(\tau_{1},\tau_{2}\right)=\frac{1}{\mathrm{i}}\left\{\theta\left(\tau_{1}-\tau_{2}\right)\frac{\mathrm{Tr}\left[e^{\left(\tau_{1}-\tau_{2}-\beta\right)\hat{H}^{\mathrm{M}}}\hat{d}_{j}e^{\left(\tau_{2}-\tau_{1}\right)\hat{H}^{\mathrm{M}}}\hat{d}_{i}^{\dagger}\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^{\mathrm{M}}}\right]}\pm\theta\left(\tau_{2}-\tau_{1}\right)\frac{\mathrm{Tr}\left[e^{\left(\tau_{2}-\tau_{1}-\beta\right)\hat{H}^{\mathrm{M}}}\hat{d}_{i}^{\dagger}e^{\left(\tau_{1}-\tau_{2}\right)\hat{H}^{\mathrm{M}}}\hat{d}_{j}\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}^{\mathrm{M}}}\right]}\right\}$$

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

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

- $G_{ji}^M(\tau_1, \tau_2)$ 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:

$$\hat{\mathcal{G}}^{\mathrm{M}}\left(\tau_{1}, \tau_{2}\right) = \frac{1}{-\mathrm{i}\beta} \sum_{m=-\infty}^{\infty} e^{-\omega_{m}(\tau_{1}-\tau_{2})} \hat{\mathcal{G}}^{\mathrm{M}}\left(\omega_{m}\right)$$

where the Matsubara frequencies are

$$\omega_m = \begin{cases} \frac{i2m\pi}{\beta} & \text{for bosons} \\ \frac{i(2m+1)\pi}{\beta} & \text{for fermions} \end{cases}$$

• 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

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

with the help of

$$\delta(\tau) = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} \left\{ \begin{array}{l} e^{-i\frac{2m\pi}{\beta}\tau} \\ e^{-i\frac{(2m+1)\pi}{\beta}\tau} \end{array} \right. = \frac{1}{\beta} \sum_{m=-\infty}^{\infty} e^{-\omega_m \tau}$$

we get

$$\hat{\mathcal{G}}^{\mathrm{M}}\left(\omega_{m}\right) = \frac{1}{\omega_{m} - \hat{h}^{\mathrm{M}}}$$

Now we discuss lesser/greater Green's function.

• The definition is

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

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

• 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:

$$n_i(t) = \pm i \sum_{ij} O_{ij} G_{ji}^{\leq}(t,t)$$

• 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

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

• In general, G_{ij}^{\leq} 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:

$$i\frac{\mathrm{d}}{\mathrm{d}z}\hat{\mathcal{U}}_L(z) = \hat{h}(z)\hat{\mathcal{U}}_L(z), \quad i\frac{\mathrm{d}}{\mathrm{d}z}\hat{\mathcal{U}}_R(z) = -\hat{\mathcal{U}}_R(z)\hat{h}(z)$$

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

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

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

$$i\frac{\mathrm{d}}{\mathrm{d}z_{1}}\hat{\mathcal{F}}\left(z_{1},z_{2}\right)=\delta\left(z_{1},z_{2}\right),\quad -i\frac{\mathrm{d}}{\mathrm{d}z_{2}}\hat{\mathcal{F}}\left(z_{1},z_{2}\right)=\delta\left(z_{1},z_{2}\right)$$

• We have

$$\hat{\mathcal{F}}\left(z_{1},z_{2}\right)=\theta\left(z_{1},z_{2}\right)\hat{\mathcal{F}}^{>}+\theta\left(z_{2},z_{1}\right)\hat{\mathcal{F}}^{<}$$

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

$$\hat{\mathcal{F}}^{<} = \pm \hat{\mathcal{U}}_{L} (t_{0} - i\beta) \,\hat{\mathcal{F}}^{>} = \pm e^{-\beta \hat{h}^{M}} \hat{\mathcal{F}}^{>} \quad \left\{ \begin{array}{l} + \text{ for bosons} \\ - \text{ for fermions} \end{array} \right.$$

Then

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

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

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

Then we have

$$\hat{\mathcal{G}}^{\mathrm{M}}\left(\tau_{1},\tau_{2}\right)=-\mathrm{i}\left[\theta\left(\tau_{1}-\tau_{2}\right)\bar{f}\left(\hat{h}^{\mathrm{M}}\right)\pm\theta\left(\tau_{2}-\tau_{1}\right)f\left(\hat{h}^{\mathrm{M}}\right)\right]e^{-\left(\tau_{1}-\tau_{2}\right)\hat{h}^{\mathrm{M}}}$$

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

$$\hat{\mathcal{G}}^{\mathrm{M}}\left(\tau_{1}, \tau_{2}\right) = \frac{1}{-\mathrm{i}\beta} \sum_{m=-\infty}^{\infty} \frac{e^{-\omega_{m}(\tau_{1}-\tau_{2})}}{\omega_{m} - \hat{h}^{\mathrm{M}}}$$

• We can prove they are equivalent.

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:

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

• 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

$$n(\boldsymbol{x},t) = \pm \mathrm{i} G^{<}(\boldsymbol{x},t;\boldsymbol{x},t)$$

• If the Hamiltonian is constant, we have

$$\hat{\mathcal{G}}^{<}(t_1, t_2) = \mp i f(\hat{h}^M) e^{-i\hat{h}(t_1 - t_2)}$$

$$\hat{\mathcal{G}}^{>}(t_1, t_2) = -i\bar{f}(\hat{h}^M)e^{-i\hat{h}(t_1 - t_2)}$$

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

• We can define the Fourier transform:

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

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

We can directly see that

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

Now let's discuss other components.

• The retarded Green's function is

$$\hat{\mathcal{G}}^{R}(t_{1}, t_{2}) = \theta(t_{1} - t_{2}) \left(\hat{\mathcal{G}}^{>}(t_{1}, t_{2}) - \hat{\mathcal{G}}^{<}(t_{1}, t_{2}) \right)$$

$$= -i\theta(t_{1} - t_{2})\hat{\mathcal{U}}(t_{1})\hat{\mathcal{U}}^{\dagger}(t_{2}) = -i\theta(t_{1} - t_{2})T \left(e^{-i\int_{t_{2}}^{t_{1}} d\bar{t}\hat{h}(\bar{t})} \right)$$

• The advanced Green's function is

$$\hat{\mathcal{G}}^{A}(t_{1}, t_{2}) = i\theta(t_{2} - t_{1})\bar{T}\left(e^{i\int_{t_{2}}^{t_{1}} d\bar{t}\hat{h}(\bar{t})}\right) = \left(\hat{\mathcal{G}}^{R}(t_{2}, t_{1})\right)^{\dagger}$$

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

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

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

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

• 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:

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

• Therefore

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

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

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

And because

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

we have

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

• 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:

$$\begin{split} \hat{\mathcal{G}}^{\uparrow}(t,\tau) &= \mp \mathrm{i} \hat{\mathcal{U}}(t) f\left(\hat{h}^{\mathrm{M}}\right) e^{\tau \hat{h}^{\mathrm{M}}} = \mathrm{i} \hat{\mathcal{G}}^{\mathrm{R}}\left(t,t_{0}\right) \hat{\mathcal{G}}^{\mathrm{M}}(0,\tau) \\ \\ \hat{\mathcal{G}}^{\uparrow}(\tau,t) &= -\mathrm{i} e^{-\tau \hat{h}^{\mathrm{M}}} \bar{f}\left(\hat{h}^{\mathrm{M}}\right) \hat{\mathcal{U}}^{\dagger}(t) = -\mathrm{i} \hat{\mathcal{G}}^{\mathrm{M}}(\tau,0) \hat{\mathcal{G}}^{\mathrm{A}}\left(t_{0},t\right) \end{split}$$

• We have time-ordered Green's function

$$\hat{\mathcal{G}}^{\mathrm{T}}\left(t_{1},t_{2}\right)=-\mathrm{i}\hat{\mathcal{U}}\left(t_{1}\right)\left[\theta\left(t_{1}-t_{2}\right)\bar{f}\left(\hat{h}^{\mathrm{M}}\right)\pm\theta\left(t_{2}-t_{1}\right)f\left(\hat{h}^{\mathrm{M}}\right)\right]\hat{\mathcal{U}}^{\dagger}\left(t_{2}\right)$$

and we have

$$\hat{\mathcal{G}}^{\mathrm{T}}\left(t_{1},t_{2}\right)=\int\frac{d\omega}{2\pi}e^{-\mathrm{i}\omega\left(t_{1}-t_{2}\right)}\underbrace{\left[\frac{\bar{f}\left(\hat{h}^{\mathrm{M}}\right)}{\omega-\hat{h}+\mathrm{i}\eta}\mp\frac{f\left(\hat{h}^{\mathrm{M}}\right)}{\omega-\hat{h}-\mathrm{i}\eta}\right]}_{\hat{\mathcal{G}}^{\mathrm{T}}\left(\omega\right)}$$

• 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

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

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

$$G_{ji}^{\leq}\left(t,t'\right) = \mp i \sum_{k} \rho_{k} \left\langle \Psi_{k} \left| \hat{d}_{i}^{\dagger} e^{-i\left(\hat{H} - E_{k}\right)\left(t' - t\right)} \hat{d}_{j} \right| \Psi_{k} \right\rangle$$

$$G_{ji}^{\geq}\left(t,t'\right) = -i \sum_{k} \rho_{k} \left\langle \Psi_{k} \left| \hat{d}_{j} e^{-i\left(\hat{H} - E_{k}\right)\left(t - t'\right)} \hat{d}_{i}^{\dagger} \right| \Psi_{k} \right\rangle$$

• Lehmann representation:

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

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

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:

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

and

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

and we have the property

$$iG_{ii}^{>}(\omega) \geq 0$$

$$iG_{jj}^{\leq}(\omega) \geq 0$$
 for bosons; $iG_{jj}^{\leq}(\omega) \leq 0$ for fermions

• For retarded and advanced function, we have

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

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

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

• For thermodynamic equilibrium,

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

we have

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

• 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

$$G_{ji}^{\Gamma}\left(\tau,t'\right) = -\mathrm{i}\sum_{k}\rho_{k}\left\langle\Psi_{k}\middle|\underbrace{e^{\mathrm{i}(\hat{H}-\mu\hat{N})(-\mathrm{i}\tau)}\hat{d}_{j}e^{-\mathrm{i}(\hat{H}-\mu\hat{N})(-\mathrm{i}\tau)}}_{\hat{d}_{j,H}(t_{0}-\mathrm{i}\tau)}\underbrace{e^{\mathrm{i}\hat{H}(t'-t_{0})}\hat{d}_{i}^{\dagger}e^{-\mathrm{i}\hat{H}(t'-t_{0})}}_{d_{i,H}^{\dagger}(t')}\middle|\Psi_{k}\right\rangle$$

$$= -\mathrm{i}e^{\mu\tau}\sum_{k}\rho_{k}\left\langle\Psi_{k}\middle|\hat{d}_{j}e^{-\mathrm{i}(\hat{H}-E_{k})(t_{0}-\mathrm{i}\tau-t')}\hat{d}_{i}^{\dagger}\middle|\Psi_{k}\right\rangle$$

then

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

Similarly

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

• For system in thermodynamic equilibrium, we have

$$G_{ji}^{M}(\tau_{1},\tau_{2}) = \frac{1}{\mathrm{i}} \sum_{kn} \rho_{p} \left[\theta \left(\tau_{1} - \tau_{2} \right) e^{\beta \left(E_{p}^{\mathrm{M}} - E_{k}^{\mathrm{M}} \right)} \pm \theta \left(\tau_{2} - \tau_{1} \right) \right] e^{-(\tau_{1} - \tau_{2}) \left(E_{p}^{\mathrm{M}} - E_{k}^{\mathrm{M}} \right)} \Phi_{kp}(j) \Phi_{kp}^{*}(i)$$

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

$$G_{ji}^{\mathrm{M}}\left(\tau_{1},\tau_{2}\right) = \frac{1}{-\mathrm{i}\beta} \sum_{m=-\infty}^{\infty} e^{-\omega_{m}(\tau_{1}-\tau_{2})} \underbrace{\sum_{kp} \frac{\rho_{p}}{f\left(E_{p}^{\mathrm{M}}-E_{k}^{\mathrm{M}}\right)} \frac{\Phi_{kp}(j)\Phi_{kp}^{*}(i)}{\omega_{m}-E_{p}^{\mathrm{M}}+E_{k}^{\mathrm{M}}}}_{G_{ij}^{\mathrm{M}}(\omega_{m})}.$$

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

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

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

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

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 $|\Psi_{N\pm 1,m}\rangle$ 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

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

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

$$G_{ji}^{<}(t,t') = \mp i \sum_{m} Q_{m}(j) Q_{m}^{*}(i) e^{-i(E_{N-1,m} - E_{N,0})(t'-t)}$$

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

• The Fourier transform of these functions are

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

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

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

• We define

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

• We have

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

• It is not difficult to verify that:

$$\int \frac{d\omega}{2\pi} A_{ji}(\omega) = \delta_{ji}$$

• We have

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

• We have

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

14 Galitskii-Migdal formula

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

$$\hat{H}_{\mathrm{S}}\left(t_{1}\right) \equiv \hat{H}\left(t_{1}\right) - q \int \mathrm{d}\boldsymbol{x}_{1}\hat{n}\left(\boldsymbol{x}_{1}\right)\delta V(1), \quad \delta V(1) = V\left(\boldsymbol{r}_{1},t_{1}\right) - V\left(\boldsymbol{r}_{1}\right)$$

• Then we have

$$\begin{split} E_{\mathrm{S}}\left(z_{1}\right) &= \\ \sum_{k} \rho_{k} \left\langle \Psi_{k} \middle| \hat{U}\left(t_{0-}, z_{1}\right) \left[\int \mathrm{d}\boldsymbol{x}_{1} \mathrm{d}\boldsymbol{x}_{2} \hat{\psi}^{\dagger}\left(\boldsymbol{x}_{1}\right) \left\langle \boldsymbol{x}_{1} \middle| \hat{h}_{\mathrm{S}}\left(z_{1}\right) \middle| \boldsymbol{x}_{2}\right\rangle \hat{\psi}\left(\boldsymbol{x}_{2}\right) + \frac{1}{2} \int \mathrm{d}\boldsymbol{x}_{1} \mathrm{d}\boldsymbol{x}_{2} v\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}\right) \hat{\psi}^{\dagger}\left(\boldsymbol{x}_{1}\right) \hat{\psi}^{\dagger}\left(\boldsymbol{x}_{2}\right) \hat{\psi}\left(\boldsymbol{x}_{2}\right) \right] \hat{U}\left(z_{1}, t_{0-}\right) \left| \Psi_{k} \right\rangle \\ \text{where } \hat{h}_{\mathrm{S}}\left(z_{1}\right) &= \hat{h}\left(z_{1}\right) - q\delta V\left(\hat{\boldsymbol{r}}_{1}, z_{1}\right). \end{split}$$

• In contour formalism, we have

$$E_{S}(z_{1}) = \pm i \int d\boldsymbol{x}_{1} d2h_{S}(1;2)G(2;1^{+}) - \frac{1}{2} \int d\boldsymbol{x}_{1} d2v(1;2)G_{2}(1,2;1^{+},2^{+})$$

• Since we have

$$\left[\left(i \frac{d}{dz_1} - i \frac{d}{dz_2} \right) G(1;2) \right]_{2=1^+} - \int d3 \left[h(1;3)G(3;1^+) + G(1;3^+) h(3;1) \right] = \pm 2i \int d3v(1;3)G_2(1,3;1^+,3^+) d3v(1;3)G_2(1,3;1^+) d3v(1;3)G_2(1,3;1^+)$$

• 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

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

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

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

• If $\hat{H}(t) = \hat{H}$, then

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

This is called the Galitskii–Migdal formula.

• For noninteracting system, the above formula becomes

$$E_{\rm S} = \sum_{\lambda} f\left(\epsilon_{\lambda}^{\rm M}\right) \epsilon_{\lambda}$$