Keldysh Formalism: Non-equilibrium Green's Function

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A review of Non-equilibrium Green's Function (NEGF), also named as Keldysh Formalism, is presented here. Perturbation theory is also builded up step by step on the basis of non-interacting NEGF, and then leads to the Dyson's Equation. Finally, application of NEGF on tight-binding model with random impurity is explicitly calculated as an example.

I. DEFINITION, FREE FIELD AND PERTURBATION

When only the properties of ground state is concerned, Zero-temperature (single- and many-particle) Green's function together with its perturbation theory principally gives all the information. Also if the equilibrium thermal distribution is concerned, we can turn to Matsubara Green's function and its perturbation theory[2]. However, we may need to consider some more general states, such as a stationary non-equilibrium state – for example – a state with nonzero current, or even an arbitrary state ρ, how to get correlation function for such system and then how to do the corresponding perturbation expansion? In experiments of conductivity, there are such non-equilibrium system, which has non-zero current and includes interaction between particles.

So in this note I will shortly review the idea and technics of Non-equilibrium Green's function, also known as Keldysh Formalism. All the formulas defined in this note is only for fermions, although it is not hard to make them to also cover bosons.

Generally we need to calculate the Green's function

$$G\left(x,t;x',t'\right)=-\frac{i}{\hbar}Tr\left(T\left\{\psi_H\left(x,t\right)\psi_H^{\dagger}\left(x',t'\right)\right\}\rho_H\right), \tag{1}$$

where $\psi_H\left(x,t\right)$ is the annihilation operator in Heisenberg picture, and ρ is the density matrix also in Heisenberg picture. We will set $\hbar=1$ for a while. We also assume ρ is diagonal under particle number basis, $[N,\rho]=0$. More general density matrix could be possible, but not used anywhere yet.

For free field, this can be calculated quite strait forward, that

$$\left\{\begin{array}{l}\psi_H\left(x,t\right)=\sum_k e^{-i\omega(k)t+ikx}c_k\\ \psi_H^{\dagger}\left(x,t\right)=\sum_k e^{i\omega(k)t-ikx}c_k^{\dagger}\end{array}\right., \tag{2}$$

then

$$\begin{array}{rcl}G^0\left(x,t;x',t'\right) & = & -i\theta\left(t-t'\right)\sum_k\left\langle 1-n_k\right\rangle e^{-i\omega(k)\left(t-t'\right)+ik\left(x-x'\right)}\\ & & -i\theta\left(t'-t\right)\sum_k\left\langle n_k\right\rangle e^{-i\omega(k)\left(t-t'\right)+ik\left(x-x'\right)}\end{array} \tag{3}$$

Following the roadmap of zero-temperature Green's function, next step would be to turn $\psi_H\left(x,t\right)$ into interaction picture $\psi_I\left(x,t\right)$ and to somehow replace the real state ρ_H with state of non-interacting system ρ_H^0.

Let's first organize the above mapping for zero-temperature Green's function and then see if the same procedure can be applied onto NEGF. Zero-temperature Green's function is defined as a special case of eq(1), $\rho_H=\left|\Omega\right\rangle\left\langle\Omega\right|$,

$$G\left(x,t;x',t'\right)=-i\left\langle\Omega\right|T\left\{\psi_H\left(x,t\right)\psi_H^{\dagger}\left(x',t'\right)\right\}\left|\Omega\right\rangle, \tag{4}$$

First, express $T\left\{A_H\left(t_1\right)B_H\left(t_2\right)\right\}$ in interaction picture.

$$H=H_0+e^{-\epsilon|t-t_0|}H_1, \tag{5}$$

and

$$A_H\left(t\right)=e^{iH(t-t_0)}e^{-iH_0(t-t_0)}A_I\left(t\right)e^{iH_0(t-t_0)}e^{-iH(t-t_0)}. \tag{6}$$

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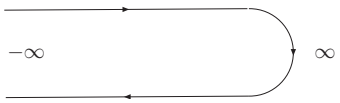


FIG. 1: The time-loop integration path.

Define unitary operator

$$U(t,t') = e^{iH_0(t-t_0)}e^{-iH(t-t_0)}e^{-iH_0\left(t'-t_0\right)}, \tag{7}$$

which is the formal solution of

$$i\frac{\partial}{\partial t}U(t,t') = H_I(t)\,U(t,t'), \tag{8}$$

where $H_I(t) = e^{iH_0(t-t_0)}H_1e^{-iH_0(t-t_0)}$. Or the explicit form is

$$U(t,t') = T\exp^{-i\int_{t'}^{t}dtH^I(t)}. \tag{9}$$

Then for $t_1 > t_2$ the time-ordered operators,

$$\begin{array}{rcl} T\{A_H(t_1)B_H(t_2)\} & = & A_H(t_1)B_H(t_2) \\ & = & U^\dagger(t_1,t_0)A_I(t_1)U(t_1,t_0)U^\dagger(t_2,t_0)B_I(t_2)U(t_2,t_0) \\ & = & U(t_0,t_1)A_I(t_1)U(t_1,t_2)B_I(t_2)U(t_2,t_0) \\ & = & U(t_0,\infty)U(\infty,t_1)A_I(t_1)U(t_1,t_2)B_I(t_2)U(t_2,-\infty)U(-\infty,t_0) \end{array}. \tag{10}$$

Next for true ground state $|\Omega\rangle$, we can relate it with $|0\rangle$, the ground state of non-interacting field,

$$U(t_0,-\infty)|0\rangle = \lim_{T\to\infty}e^{iH(-T-t_0)}e^{-iH_0(-T-t_0)}|0\rangle = \lim_{T\to\infty}e^{-iH(T+t_0)}|0\rangle. \tag{11}$$

According to Gell-Mann and Low Theorem, for adiabatic coupling, back in Schrödinger picture, ground state is stable, $|\phi_0(t_f)\rangle \propto U(t_f,t_i)|\phi_0(t_i)\rangle$. In our case, $|\Omega(t_0)\rangle \propto U(t_0,-T)|0(-T)\rangle$, so up to some constant,

$$U(t_0,-\infty)|0\rangle \propto |\Omega\rangle \Rightarrow U(-\infty,t_0)|\Omega\rangle \propto |0\rangle, \tag{12}$$

and similarly, $U(\infty,t_0)|\Omega\rangle \propto |0\rangle$. Therefore, when $t_1 > t_2$

$$\langle\Omega|T\left\{\psi_H(x,t)\psi_H^\dagger(x',t')\right\}|\Omega\rangle \propto \langle 0|U(\infty,t_1)A_I(t)U(t_1,t_2)B_I(t)U(t_2,-\infty)|0\rangle. \tag{13}$$

Finally, the constant can be eliminated as

$$G(x,t;x',t') = -i\frac{\langle 0|T\left\{\psi_I(x,t)\psi_I^\dagger(x',t')U(\infty,-\infty)\right\}|0\rangle}{\langle 0|U(\infty,-\infty)|0\rangle}, \tag{14}$$

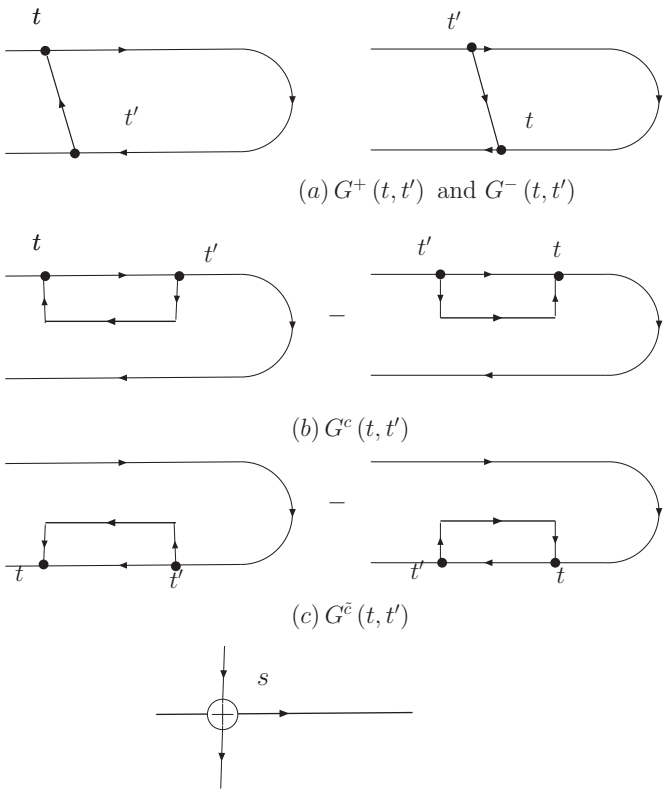
where now all the quantities are from free field, and therefore can be calculated order by order by perturbation.

However, when we apply the same procedure to general ρ_H, we require the Gell-Mann and Low theorem holds for excited states for both $t = \pm\infty$. This condition is too strong. The idea to solve above problem is to remove some special points from the three special points $t = (-\infty, t_0, \infty)$, for example by setting $t_0 \to \infty$. In this way we require that only $|\phi_0(-\infty)\rangle = |0\rangle$ instead of both $|\phi_0(\pm\infty)\rangle = |0\rangle$. The path is to start along $t = -\infty$ to $t = t_0$ and then come back along $t = t_0$ to $t = -\infty$. And finally let $t_0 \to \infty$, at pictured in fig(1). As inthe case of usual Green's function, let firstly reorganize $T\{A(t_1)B(t_2)\}$, and then the relation between ρ_H and ρ_H^0. For $t_1 > t_2$, insert $U(-\infty,\infty)$ into eq(10),

$$\begin{array}{rcl} T\{A_H(t_1)B_H(t_2)\} & = & U(t_0,-\infty)\{U(-\infty,\infty)U(\infty,t_1)A_I(t_1) \\ & & U(t_1,t_2)B_I(t_2)U(t_2,-\infty)\}U(-\infty,t_0). \end{array} \tag{15}$$

Then both sides relates only with $U(-\infty,t_0)$, which still link the true eigenstates $|n\rangle$ with free-field eigenstates $\left|n^0\right\rangle$, that

$$U(-\infty,t_0)|n\rangle \propto \left|n^0\right\rangle. \tag{16}$$



$(a)\, G^{+}(t,t')$ and $G^{-}(t,t')$

$(b)\, G^{c}(t,t')$

$(c)\, G^{\tilde{c}}(t,t')$

(d) Impurity Scattering

FIG. 2: One possible Feynman rules for NEGF.

Therefore, we arrive

$$\begin{aligned} G(x,t;x',t') &= -i\frac{Tr\left(U(-\infty,\infty)T\left\{\psi_I(x,t)\psi_I^{\dagger}(x',t')U(\infty,-\infty)\right\}\rho_H^0\right)}{Tr\left(U(-\infty,-\infty)\rho_H^0\right)} \\ &= -i\frac{Tr\left(T_c\left\{\psi_I(x,t)\psi_I^{\dagger}(x',t')U(-\infty,-\infty)\right\}\rho_H^0\right)}{Tr\left(U(-\infty,-\infty)\rho_H^0\right)} \end{aligned}, \tag{17}$$

where T_c is the loop order as shown in fig(1) to order the time along the loop from $-\infty$ to $-\infty$. For example, at the above branch it's the same with time order $T_c = T$, while at the lower branch it's anti-time order $T_c = \tilde{T}$. And

$$U(-\infty,-\infty) = T_c \exp^{-i\int_{-\infty}^{-\infty} dt H^I(t)}. \tag{18}$$

One thing need to be noticed that in the final expression of Green's function, all the time spots should be treated as points at above branch (also call positive branch). However, later on, we will see that when we try to calculate such Green's function, we will need to do integral also over the lower branch (also call negative branch). This means generally not all the time spots are at the positive branch, and the second line of eq(17) could not be separated as $U(-\infty,\infty)$ and $U(\infty,-\infty)$ outside and inside usual time order T. Therefore, generally we need to define Green's function according to the branches of t and t'. There are four different configurations of them, as pictured in fig(2).

They are "less" and "greater" Green's function[1],

$$\begin{cases} G^{+}(x,t;x',t') = -iTr\left(\rho_H T_c\left\{\psi_H(x,t_+)\psi_H^{\dagger}(x',t'_-)\right\}\right) = iTr\left(\rho_H\psi_H^{\dagger}(x',t')\psi_H(x,t)\right) \\ G^{-}(x,t;x',t') = -iTr\left(\rho_H T_c\left\{\psi_H(x,t_-)\psi_H^{\dagger}(x',t'_+)\right\}\right) = -iTr\left(\rho_H\psi_H(x,t)\psi_H^{\dagger}(x',t')\right) \end{cases}, \tag{19}$$

where $t_{\pm}$ means the time t is on positive/negative branch; "time ordered" and "anti-time ordered" Green's function,

$$\begin{cases} G^{c}(x,t;x',t') = -iTr\left(\rho_H T_c\left\{\psi_H(x,t_+)\psi_H^{\dagger}(x',t'_+)\right\}\right) = -iTr\left(\rho_H T\left\{\psi_H(x,t)\psi_H^{\dagger}(x',t')\right\}\right) \\ G^{\tilde{c}}(x,t;x',t') = -iTr\left(\rho_H T_c\left\{\psi_H(x,t_-)\psi_H^{\dagger}(x',t'_-)\right\}\right) = -iTr\left(\rho_H \tilde{T}\left\{\psi_H(x,t)\psi_H^{\dagger}(x',t')\right\}\right) \end{cases}; \tag{20}$$

and "retarded" and "advanced" Green's function,

$$\begin{cases} G^r(x,t;x',t') = -i\theta(t-t')\,Tr\left(\rho_H\left\{\psi_H(x,t),\psi_H^\dagger(x',t')\right\}\right) \\ G^a(x,t;x',t') = i\theta(t'-t)\,Tr\left(\rho_H\left\{\psi_H(x,t),\psi_H^\dagger(x',t')\right\}\right) \end{cases}. \tag{21}$$

Only three of them are independent,

$$G^r = G^c - G^+ = G^- - G^{\tilde{c}}, G^a = G^c - G^- = G^+ - G^{\tilde{c}}. \tag{22}$$

This can be seen easily by separating $G^\pm$ as four parts, $\theta(t-t')G^\pm$ and $\theta(-t+t')G^\pm$. Then

$$\begin{cases} G^c = \theta(-t+t')G^+ + \theta(t-t')G^- \\ G^{\tilde{c}} = \theta(t-t')G^+ + \theta(-t+t')G^- \end{cases} \tag{23}$$

So $G^c + G^{\tilde{c}} = G^+ + G^-$. Notice for "greater/less" Green's function, different definitions and notations are used in literature, for example, $G^> \triangleq G^-$ and $G^< \triangleq G^+$ in [2]. Before we go further to perturbation calculation of interacting field, let's first list all the free-field Non-equilibrium Green's functions.

$$\begin{array}{l} G^{0,+}(x,t;x',t') = i\sum_k \langle n_k\rangle e^{-i\omega(k)\left(t-t'\right)+ik\left(x-x'\right)} \\ G^{0,-}(x,t;x',t') = -i\sum_k \langle 1-n_k\rangle e^{-i\omega(k)\left(t-t'\right)+ik\left(x-x'\right)} \\ G^{0,c}(x,t;x',t') = -i\sum_k \langle \theta(t-t')-n_k\rangle e^{-i\omega(k)\left(t-t'\right)+ik\left(x-x'\right)} \\ G^{0,\tilde{c}}(x,t;x',t') = -i\sum_k \langle \theta(t'-t)-n_k\rangle e^{-i\omega(k)\left(t-t'\right)+ik\left(x-x'\right)} \\ G^{0,r}(x,t;x',t') = i\theta(t-t')\sum_k e^{-i\omega(k)\left(t-t'\right)+ik\left(x-x'\right)} \\ G^{0,a}(x,t;x',t') = i\theta(t'-t)\sum_k e^{-i\omega(k)\left(t-t'\right)+ik\left(x-x'\right)} \end{array} \tag{24}$$

About Eq(16), the expression similar with of Gell-Mann and Low Theorem, it should be understood in a kind inverse logic order. For an interacting field $H = H_0 + H_1$, the non-equilibrium density matrix ρ_H is not clearly defined, while ρ_H^0 of the corresponding free filed H_0 could be well defined. Then the meaning of eq(16) is that we start from ρ_H^0 at $t = -\infty$ and arrive a state at $t = t_0$, and then just use this new state as ρ_H. It's not guaranteed that this treatment will correspond to the true non-equilibrium distribution ρ_H. So for NEGF, even conceptually instead of starting from the true ρ_H, we build up the theory from ρ_H^0. This could be a disadvantage of NEGF. Also several advantages need to be noticed. First, this NEGF can be used for system at thermal equilibrium state, which is usually the subject of Matsubara Green's function. We will use as an example in §III. Second, even H_1 explicitly depends on t, this NEFG is still applicable, because we only set one end as $H_1(-\infty) = 0$, $H_1(\infty)$ could be arbitrary. At last, for non-equilibrium system as long as a unambiguous free-field corresponding non-equilibrium state could be defined, we could always do the perturbation calculation order by order.

II. SELF-ENERGY AND DYSON'S EQUATION

In order to arrive at the Dyson's equation, we would firstly go to a little practice of first and second order calculation. Consider an example with $V = \sum_{\alpha\beta} M_{\alpha\beta} C_\alpha^\dagger C_\beta$[2]. Then the first order perturbation gives,

$$G^+(\mu,t;\nu,t') = G^{0,+}(\mu,t;\nu,t') - \sum_{\alpha\beta}\int ds M_{\alpha\beta} Tr\left(T_c\left\{C_\mu(t)C_\nu^\dagger(t')C_\alpha^\dagger(s)C_\beta(s)\right\}\right). \tag{25}$$

The second term has one disconnected term and one non-zero connected term, which includes

$$\begin{array}{l} \sum_{\alpha\beta}\int ds M_{\alpha\beta}\left\langle T_c\left\{C_\mu(t)C_\alpha^\dagger(s)\right\}\right\rangle\left\langle T_c\left\{C_\nu^\dagger(t')C_\beta(s)\right\}\right\rangle \\ = \sum_{\alpha\beta}\left[\int_{-\infty}^{\infty} ds G^{0,c}(\mu,t;\alpha,s)M_{\alpha\beta}G^{0,+}(\beta,s;\nu,t') + \int_{\infty}^{-\infty} ds G^{0,+}(\mu,t;\alpha,s)M_{\alpha\beta}G^{0,\tilde{c}}(\beta,s;\nu,t')\right] \end{array} \tag{26}$$

At the next order, more terms will be coupled into this expansion series. Similarly G^- also couples with all other Gs. We will work out explicitly a special case of this interaction in the next section §III. Skipping some detailed calculation here, overall these expansion series could be represented by a matrix equation, in the form of

$$\hat{G} = \hat{G}^0\Sigma\hat{G}^0 + \hat{G}^0\Sigma\hat{G}^0\Sigma\hat{G}^0 + \cdots = \hat{G}^0\left(1+\Sigma\hat{G}\right) \tag{27}$$

Like the example about disordered system in lecture notes[3], concept of self-energy Σ can be introduced. Then the Dyson's equation of NEGF could be organized as

$$\hat{G}(t,t') = \hat{G}^0(t,t') + \iint_{-\infty}^{\infty} dt_1 dt_2 \hat{G}^0(t,t_1)\,\hat{\Sigma}(t_1,t_2)\,\hat{G}(t_2,t'), \tag{28}$$

where

$$\hat{G} = \begin{pmatrix} \hat{G}^c & \hat{G}^- \\ \hat{G}^+ & \hat{G}^{\tilde{c}} \end{pmatrix}, \tag{29}$$

and $\hat{G}(t,t')$ is the operator form of $G(x,t;x',t') = \langle x|\,\hat{G}(t,t')\,|x'\rangle$; $\hat{G}^0 = \hat{D}$ is the free-field NEGF; and $\hat{\Sigma}$ is the self-energy term coming from interaction,

$$\hat{\Sigma} = \begin{pmatrix} \hat{\Sigma}^c & \hat{\Sigma}^- \\ \hat{\Sigma}^+ & \hat{\Sigma}^{\tilde{c}} \end{pmatrix}. \tag{30}$$

We will explain both theoretically and by examples how to get the self-energy term from interaction later. Let's temporally suppose they are known.

Because only three are independent of these six NEGFs, the above formula can be simplified further by choosing the right three independent ones. Let's use $\hat{G}^a, \hat{G}^r$ and

$$\hat{F} = \hat{G}^c + \hat{G}^{\tilde{c}}. \tag{31}$$

From eq(22) it is easy to see that this transformation is unitary,

$$U \begin{pmatrix} \hat{G}^c & \hat{G}^- \\ \hat{G}^+ & \hat{G}^{\tilde{c}} \end{pmatrix} U^\dagger = \begin{pmatrix} 0 & \hat{G}^a \\ \hat{G}^r & \hat{F} \end{pmatrix} \triangleq \check{G}, \tag{32}$$

where

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \tag{33}$$

Induced by this transformation, the self-energy term will transform as

$$\check{\Sigma} \triangleq U \begin{pmatrix} \hat{\Sigma}^c & \hat{\Sigma}^- \\ \hat{\Sigma}^+ & \hat{\Sigma}^{\tilde{c}} \end{pmatrix} U^\dagger, \tag{34}$$

And finally, as we will see from the example in section §III, because generally $\Sigma^c + \Sigma^{\tilde{c}} = -(\Sigma^+ + \Sigma^-)$,

$$\check{\Sigma} \triangleq \begin{pmatrix} \Omega & \Sigma^r \\ \Sigma^a & 0 \end{pmatrix}, \tag{35}$$

Therefore, eq(28) still holds, but in a new form, or simply denoted as,

$$\check{G} = \check{G}^0 + \check{G}^0 \check{\Sigma} \check{G}. \tag{36}$$

Then the calculation of Green's function becomes calculation of self-energy, where different approximations, such as Born or Self-Consistent Born approximation, could be used.

III. EXAMPLE

Let's apply the general procedure above onto the following problem, the random impurity, a special case of the example in section §II,

$$H = \sum_k \epsilon(k)\, C_k^\dagger C_k + \sum_{k,q,X} \frac{M(q)}{V} e^{-iq\cdot X} C_{k+q}^\dagger C_k, \tag{37}$$

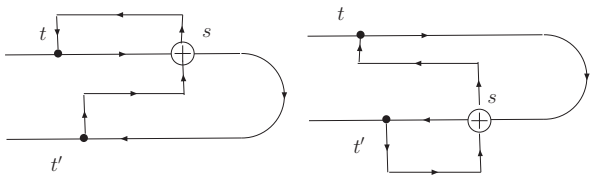


FIG. 3: First order expansion on loop path, LHS for s on positive branch, RHS for s on negative branch. Both of them are zero if $M(0)=0$.

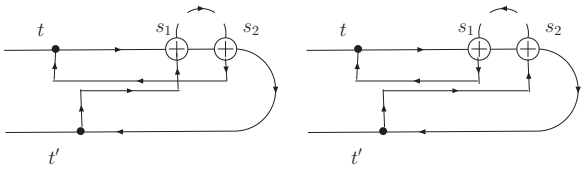


FIG. 4: Second order expansion of G^{+} on loop path, for s_1, s_2 both on positive branch.

with $M(0)=0$ means average effect of impurity is zero. X is uniformly distributed so that k is still a good quantum number, so $G^0(k,t;k',t')=G^0(k,t;k,t')\,\delta(k-k')$ and $G(k,t;k',t')=G(k,t;k,t')\,\delta(k-k')$. Let's first work in time domain, later on we will do the Fourier transformation to work in the frequency domain. First order expansion of G^{+}, eq(26) for our special case will be

$$\sum_X \frac{1}{V}\left[\int_{-\infty}^{\infty} dsG^{0,c}(k,t;k,s)\,M(0)\,G^{0,+}(k,s;k,t')+\int_{\infty}^{-\infty} dsG^{0,+}(k,t;k,s)\,M(0)\,G^{0,\tilde{c}}(k,s;k,t')\right]=0. \tag{38}$$

Or equivalently by Feynman Diagram, as in fig(3). The second order expansion of G^{+} is,

$$\begin{array}{c}\dfrac{i}{2V^2}\iint_C ds_1 ds_2 \sum_{k_1,q_1,X_1}\sum_{k_2,q_2,X_2} e^{-iq_1\cdot X_1-iq_2\cdot X_2}M(q_1)\,M(q_2)\cdot \\ Tr\left(T_c\left\{C_k(t)\,C_k^{\dagger}(t')\,C_{k_1+q_1}^{\dagger}(s_1)\,C_{k_1}(s_1)\,C_{k_2+q_2}^{\dagger}(s_2)\,C_{k_2}(s_2)\right\}\right)\end{array}, \tag{39}$$

where by Wick's Theorem,

$$\begin{aligned} &Tr\left(T_c\left\{C_k(t)\,C_k^{\dagger}(t')\,C_{k_1+q_1}^{\dagger}(s_1)\,C_{k_1}(s_1)\,C_{k_2+q_2}^{\dagger}(s_2)\,C_{k_2}(s_2)\right\}\right)\\ =&\,Tr\left(T_c\left\{C_k(t)\,C_{k_2+q_2}^{\dagger}(s_2)\right\}\right)Tr\left(T_c\left\{C_{k_1}(s_1)\,C_k^{\dagger}(t')\right\}\right)Tr\left(T_c\left\{C_{k_2}(s_2)\,C_{k_1+q_1}^{\dagger}(s_1)\right\}\right).\\ +&Tr\left(T_c\left\{C_k(t)\,C_{k_1+q_1}^{\dagger}(s_1)\right\}\right)Tr\left(T_c\left\{C_{k_2}(s_2)\,C_k^{\dagger}(t')\right\}\right)Tr\left(T_c\left\{C_{k_1}(s_1)\,C_{k_2+q_2}^{\dagger}(s_2)\right\}\right)\end{aligned} \tag{40}$$

This has to be calculated for the four configurations of s_1, s_2. For example, here let's work out for case of both s_1, s_2 on positive branch.

$$\begin{aligned} &\frac{i}{2V^2}\iint_{-\infty}^{\infty} ds_1 ds_2 \sum_{q_1,X_1,X_2}|M(q_1)|^2\,e^{-iq_1\cdot X_1+iq_1\cdot X_2}G^{0,c}(k,t;k,s_2)\,G^{0,+}(k,s_1;k,t')\,G^{0,c}(k+q_1,s_2;k+q_1,s_1)\\ +&\frac{i}{2V^2}\iint_{-\infty}^{\infty} ds_1 ds_2 \sum_{q_2,X_1,X_2}|M(q_2)|^2\,e^{iq_2\cdot X_1-iq_2\cdot X_2}G^{0,c}(k,t;k,s_1)\,G^{0,+}(k,s_2;k,t')\,G^{0,c}(k+q_2,s_1;k+q_2,s_2).\\ =&\frac{i}{V^2}\iint_{-\infty}^{\infty} ds_1 ds_2 \sum_{q,X_1,X_2}|M(q)|^2\,e^{iq\cdot X_1-iq\cdot X_2}G^{0,c}(k,t;k,s_1)\,G^{0,+}(k,s_2;k,t')\,G^{0,c}(k+q,s_1;k+q,s_2)\end{aligned} \tag{41}$$

Those two term give the same contribution because of the integration and summation over $s_1, s_2, q_{1,2}$. Except that here G^{+} couples with $G^{0,c}$ and etc, this expression has exactly the same form with the second order of the usual

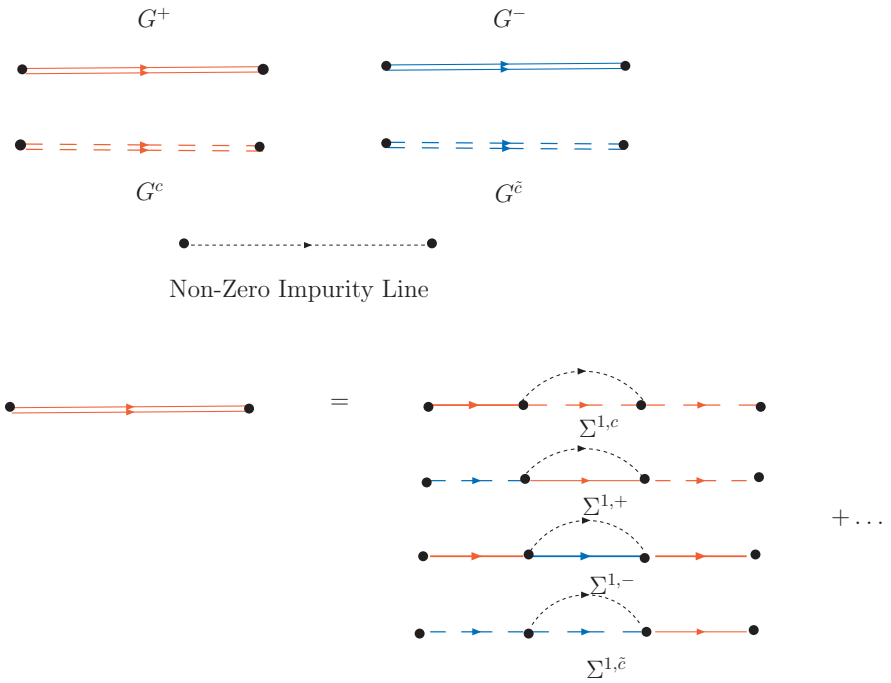


FIG. 5: Another set of Feynman rules for NEGF, second order expansion is shown as example to express in these new rules. Further perturbation could be done in this diagram form.

Green's function with impurity. Similarly, G^+ also coupled with $G^{0,-}$, $G^{0,\tilde{c}}$ and obviously $G^{0,+}$ itself. So part of the first order of self-energy term could be defined as

$$\Sigma^c\left(k;s_2,s_1\right) \propto \frac{i}{2V^2}\iint_{-\infty}^{\infty}\sum_{q_1,X_1,X_2}\left|M\left(q_1\right)\right|^2 e^{-iq_1\cdot X_1+iq_1\cdot X_2}G^{0,c}\left(k+q,s_2;k+q,s_1\right). \tag{42}$$

So we get a term of G^+ at the second order in the form of

$$G^{2,+} = G^{0,+}\Sigma^{1,c}G^{0,c} + \ldots \tag{43}$$

If we check the term about G^+ in eq(28), we will get

$$G^{2,+} = G^{0,+}\Sigma^{1,c}G^{0,c} + G^{0,\tilde{c}}\Sigma^{1,+}G^{0,c} + G^{0,+}\Sigma^{1,-}G^{0,+} + G^{0,\tilde{c}}\Sigma^{1,\tilde{c}}G^{0,+}, \tag{44}$$

which does include the above term we already calculated. The diagram expression of all those four terms are shown in the follow fig(5). A detail calculation include all the configuration of s_1, s_2 will give us the left three terms. Similarly we can do the second order expansion of $G^{-,c\tilde{c}}$. Then the third order expansion will give us more self-energy terms. Finally, we can get the Dyson's equation, which after Fourier transformation will lead us to frequency domain Dyson's equation.

In the Feynman diagrams in fig(2), where the time loop is explicitly down to be an indicator of the type of Green's function. Besides this, considering the character of our specific case, $M\left(0\right) = 0$, we may just use different lines to represent different Green's functions, so that the diagrams could be simpler, Here we skip the boring derivation of eq(36), the matrix form Dyson's equation, hopefully this will not stop one understanding the general picture of NEGF.

IV. SUMMARY

Keldysh NEGF Formula is a generalization of the usual zero and non-zero temperature Green's function. It can be applied onto the usual equilibrium cases and non-equilibrium case. The way we derive such formula here is to construct a loop from $-\infty$ to ∞ and back to $-\infty$, and introducing Green's functions $G\left(t,t'\right)$ corresponding to the different configuration of (t,t') over branches. Formally the structure of Green's function and their Dyson's Equation

looks equivalent with the one for usual Green's Function. So all the perturbation calculation is quite straightforward. However, in order to do the perturbation, a well-defined non-interacting state and Green's function is a necessary starting point. Whether such starting point leads to the real non-equilibrium state is questionable, and relies on the comparison between calculation and experiments. There is another way to get this formula in [4], where the authors use contour path over complex plan to replace above loop path. The derivation is more elegant in a sense, but the problem of picking up the right starting point still exists, although the authors claim their treatment is exact more or less.

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