Calculation of the total energy

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1 Calculation of the total energy

For more details about the methods used in this section, see Ref. [1, 2]. Our model Hamiltonian in momentum space is

$$\begin{aligned}
\hat{H} &= \hat{H}_0 + \hat{H}_I \qquad (1)\\
\hat{H}_0 &= \sum_{\boldsymbol{k},\sigma} \begin{pmatrix} \hat{c}^\dagger_{\boldsymbol{k}\sigma} & \hat{f}^\dagger_{\boldsymbol{k}\sigma} \end{pmatrix} \cdot \begin{pmatrix} \epsilon_{\boldsymbol{k}} & V \\ V & \epsilon_f \end{pmatrix} \cdot \begin{pmatrix} \hat{c}_{\boldsymbol{k}\sigma} \\ \hat{f}_{\boldsymbol{k}\sigma} \end{pmatrix} + \sum_{\boldsymbol{k}} \omega_0 \hat{a}^\dagger_{\boldsymbol{k}} \hat{a}_{\boldsymbol{k}}\\
\hat{H}_I &= \sum_{\boldsymbol{kq}\sigma} g \hat{c}^\dagger_{\boldsymbol{k}+\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k}\sigma} \hat{\phi}_{\boldsymbol{q}} + U \sum_{\boldsymbol{kpq}} \hat{f}^\dagger_{\boldsymbol{p}\uparrow} \hat{f}_{\boldsymbol{k}\uparrow} \hat{f}^\dagger_{\boldsymbol{q}\downarrow} \hat{f}_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k},\downarrow}\\
\hat{\phi}_{\boldsymbol{q}} &= \hat{a}_{\boldsymbol{q}} + \hat{a}^\dagger_{-\boldsymbol{q}}
\end{aligned}$$

We are going to use the path integral method to integrate out the phonons and obtain a Hamiltonian which includes the retarded density-density interactions between electrons. From this Hamiltonian, we can calculate the total energy of the system. With path integrals, the partition function can be written as

$$Z = \int \mathcal{D}[\bar{c}, c]\mathcal{D}[\bar{f}, f]\mathcal{D}[\bar{a}, a] e^{-S} \qquad (2)$$

Here, S is the action which is

$$\begin{aligned}
S &= \int_0^\beta d\tau \sum_{\boldsymbol{k},\sigma} \begin{pmatrix} \bar{c}_{\boldsymbol{k}\sigma} & \bar{f}_{\boldsymbol{k}\sigma} \end{pmatrix} \cdot \begin{pmatrix} \partial_\tau + \epsilon_{\boldsymbol{k}} & V \\ V & \partial_\tau + \epsilon_f \end{pmatrix} \cdot \begin{pmatrix} c_{\boldsymbol{k}\sigma} \\ f_{\boldsymbol{k}\sigma} \end{pmatrix} \qquad (3)\\
&+ \int_0^\beta d\tau \sum_{\boldsymbol{k}} \bar{a}_{\boldsymbol{k}} (\partial_\tau + \omega_0) a_{\boldsymbol{k}} + \int_0^\beta d\tau \sum_{\boldsymbol{kq}\sigma} g \bar{c}_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k}\sigma} (a_{\boldsymbol{q}} + \bar{a}_{-\boldsymbol{q}})\\
&- U \int_0^\beta d\tau \sum_{\boldsymbol{kpq}} \bar{f}_{\boldsymbol{p}\uparrow} \bar{f}_{\boldsymbol{q}\downarrow} f_{\boldsymbol{k}\uparrow} f_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k},\downarrow}
\end{aligned}$$

The part of the action that involves the phonons is

$$S_\phi = \int_0^\beta d\tau \sum_{\boldsymbol{k}} \bar{a}_{\boldsymbol{k}}(\partial_\tau + \omega_0)a_{\boldsymbol{k}} + \int_0^\beta d\tau \sum_{\boldsymbol{kq}\sigma} g\bar{c}_{\boldsymbol{k}+\boldsymbol{q},\sigma}c_{\boldsymbol{k}\sigma}(a_{\boldsymbol{q}} + \bar{a}_{-\boldsymbol{q}}) \tag{4}$$

Integration with respect to phonons yields

$$\begin{aligned} Z_{eff} &= \int \mathcal{D}[\bar{a}, a]e^{-S_\phi} \\ &= Z_{\text{Bare\_phonons}} \exp\left(-\sum_{\boldsymbol{q},m} \bar{J}_{\boldsymbol{q},m} \frac{1}{i\nu_m - \omega_0} J_{\boldsymbol{q},m} \right) \end{aligned} \tag{5}$$

Here, the partition function for bare phonons is

$$Z_{\text{Bare\_phonons}} = \prod_{\boldsymbol{q}} \frac{1}{1 - e^{-\beta\omega_0}}, \tag{6}$$

and the current $J_{\boldsymbol{q},m}$ is defined as

$$\begin{aligned} J_{\boldsymbol{q},m} &= \beta^{-1/2} g \sum_{\boldsymbol{k},\sigma} \sum_{i\omega_n} \bar{c}_{\boldsymbol{k}-\boldsymbol{q},\sigma}(i\omega_n - i\nu_m)c_{\boldsymbol{k},\sigma}(i\omega_n) \\ &= g\beta^{-1/2} \int_0^\beta d\tau e^{i\nu_m\tau} \sum_{\boldsymbol{k},\sigma} \bar{c}_{\boldsymbol{k}-\boldsymbol{q},\sigma}(\tau)c_{\boldsymbol{k},\sigma}(\tau) \end{aligned} \tag{7}$$

Its conjugate is

$$\bar{J}_{\boldsymbol{q},m} = g\beta^{-1/2} \int_0^\beta d\tau e^{-i\nu_m\tau} \sum_{\boldsymbol{k}\sigma} \bar{c}_{\boldsymbol{k}\sigma}(\tau)c_{\boldsymbol{k}-\boldsymbol{q}}(\tau) \tag{8}$$

After integrating out the phonons, we have an effective action

$$S_{eff} = \sum_{\boldsymbol{q},m} \bar{J}_{\boldsymbol{q},m} \frac{1}{i\nu_m - \omega_0} J_{\boldsymbol{q},m} \tag{9}$$

An important property of $J_{\boldsymbol{q},m}$ is that $J_{-\boldsymbol{q},-m} = \bar{J}_{\boldsymbol{q},m}$. Thus, the effective action can be rewritten as

$$\begin{aligned} S_{eff} &= \sum_{\boldsymbol{q},m} \bar{J}_{\boldsymbol{q},m} \frac{1}{i\nu_m - \omega_0} J_{\boldsymbol{q},m} \\ &= \sum_{-\boldsymbol{q},-m} \bar{J}_{-\boldsymbol{q},-m} \frac{1}{-i\nu_m - \omega_0} J_{-\boldsymbol{q},-m} \\ &= \sum_{\boldsymbol{q},m} J_{\boldsymbol{q},m} \frac{1}{-i\nu_m - \omega_0} \bar{J}_{\boldsymbol{q},m} \\ &= \sum_{\boldsymbol{q},m} \bar{J}_{\boldsymbol{q},m} \frac{1}{-i\nu_m - \omega_0} J_{\boldsymbol{q},m} \\ &= \frac{1}{2} \sum_{\boldsymbol{q},m} \bar{J}_{\boldsymbol{q},m} \frac{-2\omega_0}{\omega_0^2 - (i\nu_m)^2} J_{\boldsymbol{q},m} \end{aligned} \tag{10}$$

Fourier transforming back to τ space, we have

$$S_{eff} = \frac{1}{2}g^2 \sum_{\boldsymbol{q}} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{\boldsymbol{k},\sigma} \bar{c}_{\boldsymbol{k},\sigma}(\tau_1) c_{\boldsymbol{k}-\boldsymbol{q},\sigma}(\tau_1) D^0(\tau_1 - \tau_2) \sum_{\boldsymbol{p},s} \bar{c}_{\boldsymbol{p}-\boldsymbol{q},s}(\tau_2) c_{\boldsymbol{p},s}(\tau_2) \tag{11}$$

Here, we have introduced the bare phonon propagator in the effective action,

$$\begin{aligned} D^0(\tau_1 - \tau_2) &= \frac{1}{\beta} \sum_{i\nu_m} \frac{2\omega_0}{(i\nu_m)^2 - \omega_0^2} e^{-i\nu_m(\tau_1 - \tau_2)} \\ &= -\frac{1}{1 - e^{-\beta\omega_0}} (e^{-\omega_0|\tau_1 - \tau_2|} + e^{-(\beta - |\tau_1 - \tau_2|)\omega_0}) \end{aligned} \tag{12}$$

The effective action S_{eff} represents the time-retarded density-density interaction between two c electrons mediated by the exchange of a virtual phonon. This interaction differs from the instantaneous Hubbard interaction not only in that it is time-retarded, but also in that the spins of the two electrons do not have to be opposite, as required for on-site Hubbard interactions.

With this observation, the original partition function can be recast into the form

$$Z = Z_{\text{Bare\_phonons}} \int \mathcal{D}[\bar{c}, c] \mathcal{D}[\bar{f}, f] e^{-S}, \tag{13}$$

where, the action is

$$\begin{aligned} S &= \int_0^\beta d\tau \sum_{\boldsymbol{k},\sigma} \begin{pmatrix} \bar{c}_{\boldsymbol{k}\sigma} & \bar{f}_{\boldsymbol{k}\sigma} \end{pmatrix} \cdot \begin{pmatrix} \partial_\tau + \epsilon_{\boldsymbol{k}} & V \\ V & \partial_\tau + \epsilon_f \end{pmatrix} \cdot \begin{pmatrix} c_{\boldsymbol{k}\sigma} \\ f_{\boldsymbol{k}\sigma} \end{pmatrix} \\ &+ \frac{1}{2}g^2 \sum_{\boldsymbol{q}} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{\boldsymbol{k},\sigma} \bar{c}_{\boldsymbol{k},\sigma}(\tau_1) c_{\boldsymbol{k}-\boldsymbol{q},\sigma}(\tau_1) D^0(\tau_1 - \tau_2) \sum_{\boldsymbol{p},s} \bar{c}_{\boldsymbol{p}-\boldsymbol{q},s}(\tau_2) c_{\boldsymbol{p},s}(\tau_2) \\ &- U \int_0^\beta d\tau \sum_{\boldsymbol{kpq}} \bar{f}_{\boldsymbol{p}\uparrow} \bar{f}_{\boldsymbol{q}\downarrow} f_{\boldsymbol{k}\uparrow} f_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k},\downarrow} \end{aligned} \tag{14}$$

The effective Hamiltonian describing the retarded density-density electron interaction can be obtained by taking the derivative of S_{eff} with respect to β, that is,

$$\begin{aligned} H_{eff} &= \frac{\partial S_{eff}}{\partial \beta} \\ &= \frac{g^2}{2} \sum_{\boldsymbol{q}} \sum_{\boldsymbol{k},\sigma} \bar{c}_{\boldsymbol{k},\sigma}(0) c_{\boldsymbol{k}-\boldsymbol{q},\sigma}(0) \int_0^\beta D^0(\tau_2) \sum_{\boldsymbol{p},s} \bar{c}_{\boldsymbol{p},s}(\tau_2) c_{\boldsymbol{p}+\boldsymbol{q},s}(\tau_2) d\tau_2 \\ &+ \frac{g^2}{2} \sum_{\boldsymbol{q}} \int_0^\beta d\tau_1 \sum_{\boldsymbol{k},\sigma} \bar{c}_{\boldsymbol{k},\sigma}(\tau_1) c_{\boldsymbol{k}-\boldsymbol{q},\sigma}(\tau_1) D^0(\tau_1) \sum_{\boldsymbol{p},s} \bar{c}_{\boldsymbol{p},s}(0) c_{\boldsymbol{p}+\boldsymbol{q},s}(0) \\ &+ \frac{g^2}{2} \sum_{\boldsymbol{q}} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{\boldsymbol{k},\sigma} \sum_{\boldsymbol{p},s} \bar{c}_{\boldsymbol{k},\sigma}(\tau_1) c_{\boldsymbol{k}-\boldsymbol{q},\sigma}(\tau_1) \frac{\partial D^0(\tau_1 - \tau_2)}{\partial \beta} \bar{c}_{\boldsymbol{p},s}(\tau_2) c_{\boldsymbol{p}+\boldsymbol{q},s}(\tau_2) \end{aligned} \tag{15}$$

Here, we have taken advantage of the fact that $c(\beta) = -c(0)$, $D^0(\tau - \beta) = D^0(\tau)$ and $D^0(-\tau) = D^0(\tau)$. In order to get the Hamiltonian in operator notation, we are to rewrite the above effective Hamiltonian as

$$\begin{aligned}
H_{eff} &= -\frac{g^2}{2}\sum_q\sum_{k,\sigma}\sum_{p,s}\int_0^\beta d\tau_2 \bar{c}_{k,\sigma}(0)\bar{c}_{p,s}(\tau_2)D^0(\tau_2)c_{k-q,\sigma}(0)c_{p+q,s}(\tau_2) \\
&- \frac{g^2}{2}\sum_q\sum_{k,\sigma}\sum_{p,s}\int_0^\beta d\tau_1 \bar{c}_{k,\sigma}(\tau_1)\bar{c}_{p,s}(0)D^0(\tau_1)c_{k-q,\sigma}(\tau_1)c_{p+q,s}(0) \\
&- \frac{g^2}{2}\sum_q\sum_{k,\sigma}\sum_{p,s}\int_0^\beta d\tau_1\int_0^\beta d\tau_2 \bar{c}_{k,\sigma}(\tau_1)\bar{c}_{p,s}(\tau_2)\frac{\partial D^0(\tau_1-\tau_2)}{\partial\beta}c_{k-q,\sigma}(\tau_1)c_{p+q,s}(\tau_2)
\end{aligned} \tag{16}$$

In operator notation, the effective Hamiltonian would be

$$\begin{aligned}
\hat{H}_{eff} &= -\frac{g^2}{2}\sum_q\sum_{k,\sigma}\sum_{p,s}\int_0^\beta d\tau_2 \hat{c}^\dagger_{k,\sigma}(0)\hat{c}^\dagger_{p,s}(\tau_2)D^0(\tau_2)\hat{c}_{k-q,\sigma}(0)\hat{c}_{p+q,s}(\tau_2) \\
&- \frac{g^2}{2}\sum_q\sum_{k,\sigma}\sum_{p,s}\int_0^\beta d\tau_1 \hat{c}^\dagger_{k,\sigma}(\tau_1)\hat{c}^\dagger_{p,s}(0)D^0(\tau_1)\hat{c}_{k-q,\sigma}(\tau_1)\hat{c}_{p+q,s}(0) \\
&- \frac{g^2}{2}\sum_q\sum_{k,\sigma}\sum_{p,s}\int_0^\beta d\tau_1\int_0^\beta d\tau_2 \hat{c}^\dagger_{k,\sigma}(\tau_1)\hat{c}^\dagger_{p,s}(\tau_2)\frac{\partial D^0(\tau_1-\tau_2)}{\partial\beta}\hat{c}_{k-q,\sigma}(\tau_1)\hat{c}_{p+q,s}(\tau_2)
\end{aligned} \tag{17}$$

1.1 Schwinger-Dyson equation method for derivation of equation of motion for a simplified Holstein model

Schwinger-Dyson equation is a method that furnishes us with the equation of motion of a system represented in path integrals. To see this, let us consider this simplified Holstein model.

$$\hat{H} = \epsilon\hat{c}^\dagger\hat{c} + \omega\hat{a}^\dagger\hat{a} + g\hat{c}^\dagger\hat{c}(\hat{a} + \hat{a}^\dagger) \tag{18}$$

The action for this model is

$$S = \int_0^\beta d\tau\Big(\bar{c}(\partial_\tau + \epsilon)c + \bar{a}(\partial_\tau + \omega)a + g\bar{c}c(a + \bar{a})\Big) \tag{19}$$

Definition of electron Green function is

$$\begin{aligned}
G(\tau' - \tau) &= -\langle T\hat{c}(\tau')\hat{c}^\dagger(\tau)\rangle \\
&= -\frac{1}{Z}\int \mathcal{D}[\bar{c}, c]\mathcal{D}[\bar{a}, a]c(\tau')\bar{c}(\tau)e^{-S}
\end{aligned} \tag{20}$$

Now we are going to derive the equation of motion for the electron's Green function using both operator notation and path integral formulation, and show that these two methods yield identical result.

1.1.1 Operator formulation

Take the derivative of Green function with respect to imaginary time, we have

$$\frac{\partial G(\tau',\tau)}{\partial \tau'} = -\delta(\tau'-\tau) + \epsilon\langle T\hat{c}(\tau')\hat{c}^\dagger(\tau)\rangle + g\langle T\hat{c}(\tau')\hat{\phi}(\tau')\hat{c}^\dagger(\tau)\rangle \tag{21}$$

That is,

$$(\partial_{\tau'} + \epsilon)G(\tau',\tau) = -\delta(\tau'-\tau) + g\langle T\hat{c}(\tau')\hat{\phi}(\tau')\hat{c}^\dagger(\tau)\rangle \tag{22}$$

1.1.2 Path integral formulation

For the derivation of equation of motion in the path integral formulation, we are to use the Schwinger-Dyson method. In this method, the Grassmann numbers c and $\bar{c}$ are replaced with the shifted ones, that is,

$$\begin{aligned} c &\to c' = c + \delta c, \\ \bar{c} &\to \bar{c}' = \bar{c} + \delta\bar{c}, \end{aligned} \tag{23}$$

and everything is expanded to first order in δc and $\delta\bar{c}$. Consider this quantity,

$$\int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a]\bar{c}(\tau)e^{-S[\bar{c},c;\bar{a},a]} = \int \mathcal{D}[\bar{c}',c']\mathcal{D}[\bar{a},a]\bar{c}'(\tau)e^{-S[\bar{c}',c';\bar{a},a]} \tag{24}$$

The action S represented in $\bar{c}', c'$ is

$$\begin{aligned} S[\bar{c}',c';\bar{a},a] &= S[\bar{c},c;\bar{a},a] \\ &+ \int_0^\beta d\tau \Big(\delta\bar{c}(\partial_\tau+\epsilon)c + \bar{c}(\partial_\tau+\epsilon)\delta c + g\delta\bar{c}c(a+\bar{a}) + g\bar{c}\delta c(a+\bar{a})\Big) \\ &=: S[\bar{c},c;\bar{a},a] + \delta S \end{aligned} \tag{25}$$

Thus, we have (we have taken advantage of the fact that $\mathcal{D}[\bar{c},c] = \mathcal{D}[\bar{c}',c']$)

$$\begin{aligned} \int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a]\bar{c}(\tau)e^{-S[\bar{c},c;\bar{a},a]} &= \int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a](\bar{c}(\tau)+\delta\bar{c}(\tau))e^{-S[\bar{c},c;\bar{a},a]-\delta S} \\ &= \int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a](\bar{c}(\tau)+\delta\bar{c}(\tau))e^{-S}(1-\delta S) \\ &= \int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a]\bar{c}(\tau)e^{-S[\bar{c},c;\bar{a},a]} + \int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a]e^{-S}(\delta\bar{c}(\tau) - \bar{c}(\tau)\delta S) \end{aligned} \tag{26}$$

So we have the Schwinger-Dyson equation

$$0 = \int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a]e^{-S}(\delta\bar{c}(\tau) - \bar{c}(\tau)\delta S) \tag{27}$$

In order to get the equation of motion for Green function, we set $\delta c = 0$, and thus

$$\begin{aligned}
& \delta\bar{c}(\tau) - \bar{c}(\tau)\delta S \qquad (28)\\
= \; & \delta\bar{c}(\tau) - \bar{c}(\tau)\int_0^\beta d\tau'(\delta\bar{c}(\partial_{\tau'}+\epsilon)c + g\delta\bar{c}c(a+\bar{a}))\\
= \; & \int_0^\beta d\tau'\Big(\delta(\tau'-\tau)\delta\bar{c}(\tau') - \delta\bar{c}(\tau')(\partial_{\tau'}+\epsilon)c(\tau')\bar{c}(\tau) - g\delta\bar{c}(\tau')c(\tau')(a+\bar{a})\bar{c}(\tau)\Big)
\end{aligned}$$

Plug this back into the Schwinger-Dyson equation, we have

$$\begin{aligned}
& \int_0^\beta d\tau'\Bigg[\delta(\tau-\tau') - (\partial_{\tau'}+\epsilon)\frac{1}{Z}\int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a]e^{-S}c(\tau')\bar{c}(\tau) \qquad (29)\\
- \; & g\frac{1}{Z}\int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a]e^{-S}c(\tau')\phi(\tau')\bar{c}(\tau)\Bigg]\delta\bar{c}(\tau') = 0
\end{aligned}$$

Since this equation holds for any $\delta\bar{c}$, we thus, from the definition of Green function in path integral formulation, have

$$(\partial_{\tau'}+\epsilon)G(\tau',\tau) - g\langle T\hat{c}(\tau')\hat{\phi}(\tau')\hat{c}^\dagger(\tau)\rangle = -\delta(\tau-\tau') \qquad (30)$$

This is identically the same with the equation of motion that was derived using operator notation.

1.2 Schwinger-Dyson equation for simplified Holstein model: with phonons integrated out

The advantage of Schwinger-Dyson equation method for derivation of equation of motion for Green function is that all we need is the action, rather than the Hamiltonian. Sometimes, the system can be only represented using path integral formulation, but not Hamiltonian. In this case, the Schwinger-Dyson equation is the only method available for the derivation of equation of motion. One such case when the system can be only represented in path integrals is the Holstein model with phonons integrated out, resulting in a time-retarded electronic density interactions. As already stated, the simplified Holstein model is represented by the action

$$S = \int_0^\beta d\tau\bar{c}(\tau)(\partial_\tau+\epsilon)c(\tau) + S_\phi, \qquad (31)$$

where S_ϕ is the part of the action for phonons, that is,

$$S_\phi = \int_0^\beta d\tau\Big(\bar{a}(\partial_\tau+\omega)a + g\bar{c}c(a+\bar{a})\Big) \qquad (32)$$

The partition function for this model is

$$\begin{aligned}
S \; &= \; \int \mathcal{D}[\bar{c},c]\mathcal{D}[\bar{a},a]e^{-S} \qquad (33)\\
&= \; Z_\phi\int \mathcal{D}[\bar{c},c]e^{-S_{eff}}
\end{aligned}$$

Here, Z_ϕ is the partition function for bare phonons, that is, $Z_\phi = \left(1 - e^{-\beta\omega}\right)^{-1}$, and S_{eff} is the effective action obtained after integrating out the phonons. The full expression for the effective action is

$$S_{eff} = \int_0^\beta d\tau \bar{c}(\partial_\tau + \epsilon)c + \frac{1}{2}g^2 \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \bar{c}(\tau_1)c(\tau_1)D^0(\tau_1 - \tau_2)\bar{c}(\tau_2)c(\tau_2) \tag{34}$$

Define a quantity that is invariant under the transformation $c \to c' = c + \delta c, \bar{c} \to \bar{c}' + \delta\bar{c}'$, that is,

$$\int \mathcal{D}[\bar{c}, c]e^{-S_{eff}[\bar{c},c]}\bar{c}(\tau) = \int \mathcal{D}[\bar{c}', c']e^{-S_{eff}[\bar{c}',c']}\bar{c}'(\tau) \tag{35}$$

From this equation, after expanding to first order, we have

$$0 = \int \mathcal{D}[\bar{c}, c]e^{-S_{eff}[\bar{c},c]}(-\delta S_{eff}\bar{c}(\tau) + \delta\bar{c}(\tau)) \tag{36}$$

If we set $\delta c = 0$ and notice that $D^0(\tau_1 - \tau_2) = D^0(\tau_2 - \tau_1)$, then the variation for the action is

$$\delta S_{eff} = \int_0^\beta d\tau \delta\bar{c}(\partial_\tau + \epsilon)c + g^2 \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \delta\bar{c}(\tau_1)c(\tau_1)D^0(\tau_1 - \tau_2)\bar{c}(\tau_2)c(\tau_2) \tag{37}$$

Thus we have

$$\begin{aligned} & \delta\bar{c}(\tau) - \delta S_{eff}\bar{c}(\tau) \qquad (38) \\ = & \int_0^\beta d\tau' \delta\bar{c}(\tau')\left[\delta(\tau - \tau') - (\partial_{\tau'} + \epsilon)c(\tau')\bar{c}(\tau) - g^2 c(\tau')\bar{c}(\tau)\int_0^\beta d\tau_2 D^0(\tau' - \tau_2)\bar{c}(\tau_2)c(\tau_2)\right] \end{aligned}$$

It is required that Equation [36] should hold for any variation $\delta\bar{c}$, thus we have the equation of motion for Green function as

$$\begin{aligned} & (\partial_{\tau'} + \epsilon)G(\tau', \tau) \qquad (39) \\ - & g^2\frac{1}{Z}\int \mathcal{D}[\bar{c}, c]e^{-S_{eff}}\left[c(\tau')\bar{c}(\tau)\int_0^\beta d\tau_2 D^0(\tau' - \tau_2)\bar{c}(\tau_2)c(\tau_2)\right] = -\delta(\tau' - \tau) \end{aligned}$$

For the above equation of motion, if we set $\tau = 0, \tau' = 0^-$, then we have the expectation value of the interaction energy as

$$\begin{aligned} & g^2\frac{1}{Z}\int \mathcal{D}[\bar{c}, c]e^{-S_{eff}}\left[\bar{c}(0)c(0)\int_0^\beta d\tau_2 D^0(\tau_2)\bar{c}(\tau_2)c(\tau_2)\right] \qquad (40) \\ = & -(\partial_{\tau'} + \epsilon)G(\tau')\Big|_{\tau'=0^-} - \delta(0^-) \\ = & \frac{1}{\beta}\sum_{i\omega_n}\Sigma(i\omega_n)G(i\omega_n)e^{i\omega_n 0^+} \end{aligned}$$

1.3 Schwinger-Dyson method for derivation of equation of motion for periodic Anderson model with electron-phonon interactions

The model that we are studying, the periodic Anderson model with electron-phonon interactions, with the phonons being integrated out, is represented by this effective action

$$
\begin{aligned}
S &= \int_0^\beta d\tau \sum_{\boldsymbol{k},\sigma} \begin{pmatrix} \bar{c}_{\boldsymbol{k}\sigma} & \bar{f}_{\boldsymbol{k}\sigma} \end{pmatrix} \cdot \begin{pmatrix} \partial_\tau + \epsilon_{\boldsymbol{k}} & V \\ V & \partial_\tau + \epsilon_f \end{pmatrix} \cdot \begin{pmatrix} c_{\boldsymbol{k}\sigma} \\ f_{\boldsymbol{k}\sigma} \end{pmatrix} \\
&+ \frac{1}{2} g^2 \sum_{\boldsymbol{q}} \sum_{\boldsymbol{k},\sigma} \sum_{\boldsymbol{p},s} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \bar{c}_{\boldsymbol{k},\sigma}(\tau_1) c_{\boldsymbol{k}-\boldsymbol{q},\sigma}(\tau_1) D^0(\tau_1 - \tau_2) \bar{c}_{\boldsymbol{p}-\boldsymbol{q},s}(\tau_2) c_{\boldsymbol{p},s}(\tau_2) \\
&- U \int_0^\beta d\tau \sum_{\boldsymbol{kpq}} \bar{f}_{\boldsymbol{p}\uparrow} \bar{f}_{\boldsymbol{q}\downarrow} f_{\boldsymbol{k}\uparrow} f_{\boldsymbol{p}+\boldsymbol{q}-\boldsymbol{k},\downarrow}
\end{aligned}
\tag{41}
$$

Consider the transformation of the variables,

$$
\begin{aligned}
c_{k,\sigma}(\tau) &\to c'_{k,\sigma}(\tau) = c_{k,\sigma}(\tau) + \delta c_{k,\sigma}(\tau) \\
\bar{c}_{k,\sigma}(\tau) &\to \bar{c}'_{k,\sigma}(\tau) = \bar{c}_{k,\sigma}(\tau) + \delta \bar{c}_{k,\sigma}(\tau) \\
f_{k,\sigma}(\tau) &\to f'_{k,\sigma}(\tau) = f_{k,\sigma}(\tau) + \delta f_{k,\sigma}(\tau) \\
\bar{f}_{k,\sigma}(\tau) &\to \bar{f}'_{k,\sigma}(\tau) = \bar{f}_{k,\sigma}(\tau) + \delta \bar{f}_{k,\sigma}(\tau)
\end{aligned}
\tag{42}
$$

With this transformation, the action becomes $S[\bar{c}, c; \bar{f}, f] \to S[\bar{c}', c'; \bar{f}', f'] = S[\bar{c}, c; \bar{f}, f] + \delta S$. Define a quantity that is invariant under this transformation,

$$
\begin{aligned}
& \int \mathcal{D}[\bar{c}, c] \mathcal{D}[\bar{f}, f] e^{-S[\bar{c}, c; \bar{f}, f]} \Big(\bar{c}_{k,\sigma}(\tau), \bar{f}_{k,\sigma}(\tau) \Big) \\
= & \int \mathcal{D}[\bar{c}', c'] \mathcal{D}[\bar{f}', f'] e^{-S[\bar{c}', c'; \bar{f}', f']} \Big(\bar{c}'_{k,\sigma}(\tau), \bar{f}'_{k,\sigma}(\tau) \Big) \\
= & \int \mathcal{D}[\bar{c}, c] \mathcal{D}[\bar{f}, f] e^{-S[\bar{c}, c; \bar{f}, f] - \delta S} \Big(\bar{c}_{k,\sigma}(\tau) + \delta \bar{c}_{k,\sigma}(\tau), \bar{f}_{k,\sigma}(\tau) + \delta \bar{f}_{k,\sigma}(\tau) \Big)
\end{aligned}
\tag{43}
$$

After expanding to first order, we have

$$
0 = \int \mathcal{D}[\bar{c}, c] \mathcal{D}[\bar{f}, f] e^{-S} \Big(\delta \bar{c}_{k,\sigma}(\tau) - \delta S \bar{c}_{k,\sigma}(\tau), \delta \bar{f}_{k,\sigma}(\tau) - \delta S \bar{f}_{k,\sigma}(\tau) \Big) \tag{44}
$$

Here, the variation of action is

$$
\begin{aligned}
\delta S &= \int_0^\beta d\tau \sum_{\boldsymbol{k},\sigma} \begin{pmatrix} \delta\bar{c}_{\boldsymbol{k}\sigma} & \delta\bar{f}_{\boldsymbol{k}\sigma} \end{pmatrix} \cdot \begin{pmatrix} \partial_\tau + \epsilon_{\boldsymbol{k}} & V \\ V & \partial_\tau + \epsilon_f \end{pmatrix} \cdot \begin{pmatrix} c_{\boldsymbol{k}\sigma} \\ f_{\boldsymbol{k}\sigma} \end{pmatrix} \\
&+ \int_0^\beta d\tau \sum_{\boldsymbol{k},\sigma} \begin{pmatrix} \bar{c}_{\boldsymbol{k}\sigma} & \bar{f}_{\boldsymbol{k}\sigma} \end{pmatrix} \cdot \begin{pmatrix} \partial_\tau + \epsilon_{\boldsymbol{k}} & V \\ V & \partial_\tau + \epsilon_f \end{pmatrix} \cdot \begin{pmatrix} \delta c_{\boldsymbol{k}\sigma} \\ \delta f_{\boldsymbol{k}\sigma} \end{pmatrix} \\
&+ \frac{g^2}{2} \sum_q \sum_{k,\sigma} \sum_{p,s} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \Big[\bar{c}_{k,\sigma}(\tau_1) \delta c_{k-q,\sigma}(\tau_1) D^0(\tau_1 - \tau_2) \bar{c}_{p-q,s}(\tau_2) c_{p,s}(\tau_2) \\
&+ \delta\bar{c}_{k,\sigma}(\tau_1) c_{k-q,\sigma}(\tau_1) D^0(\tau_1 - \tau_2) \bar{c}_{p-q,s}(\tau_2) c_{p,s}(\tau_2) \\
&+ \bar{c}_{k,\sigma}(\tau_1) c_{k-q,\sigma}(\tau_1) D^0(\tau_1 - \tau_2) \bar{c}_{p-q,s}(\tau_2) \delta c_{p,s}(\tau_2) \\
&+ \bar{c}_{k,\sigma}(\tau_1) c_{k-q,\sigma}(\tau_1) D^0(\tau_1 - \tau_2) \delta\bar{c}_{p-q,s}(\tau_2) c_{p,s}(\tau_2) \Big] \\
&- U \sum_{pqk} \int_0^\beta d\tau \Big[\delta\bar{f}_{p,\uparrow} \bar{f}_{q,\downarrow} f_{k,\uparrow} f_{p+q-k,\downarrow} + \bar{f}_{p,\uparrow} \delta\bar{f}_{q,\downarrow} f_{k,\uparrow} f_{p+q-k,\downarrow} \\
&+ \bar{f}_{p,\uparrow} \bar{f}_{q,\downarrow} f_{k,\uparrow} \delta f_{p+q-k,\downarrow} + \bar{f}_{p,\uparrow} \bar{f}_{q,\downarrow} \delta f_{k,\uparrow} f_{p+q-k,\downarrow} \Big]
\end{aligned} \tag{45}
$$

We have two independent equations, which are

$$
\begin{aligned}
\int \mathcal{D}[\bar{c}, c] \mathcal{D}[\bar{f}, f] e^{-S} \Big[\delta\bar{c}_{k,\sigma}(\tau) - \delta S \bar{c}_{k,\sigma}(\tau) \Big] = 0 \\
\int \mathcal{D}[\bar{c}, c] \mathcal{D}[\bar{f}, f] e^{-S} \Big[\delta\bar{f}_{k,\sigma}(\tau) - \delta S \bar{f}_{k,\sigma}(\tau) \Big] = 0
\end{aligned} \tag{46}
$$

For the first equation, we can set $\delta c = 0, \delta f = 0, \delta \bar{f} = 0$, and then we have

$$
\begin{aligned}
& \delta\bar{c}_{k,\sigma}(\tau) - \delta S \bar{c}_{k,\sigma}(\tau) \qquad (47) \\
= \; & \delta\bar{c}_{k,\sigma}(\tau) - \int_0^\beta d\tau' \sum_{k',\sigma'} \begin{pmatrix} \delta\bar{c}_{k',\sigma'}(\tau') & 0 \end{pmatrix} \begin{pmatrix} \partial_{\tau'} + \epsilon_{k'} & V \\ V & \partial_{\tau'} + \epsilon_f \end{pmatrix} \begin{pmatrix} c_{k',\sigma'}(\tau')\bar{c}_{k,\sigma}(\tau) \\ f_{k',\sigma'}(\tau')\bar{c}_{k,\sigma}(\tau) \end{pmatrix} \\
- \; & \frac{g^2}{2} \sum_q \sum_{k',\sigma'} \sum_{p,s} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \Big[\delta\bar{c}_{k',\sigma'}(\tau_1) c_{k'-q,\sigma'}(\tau_1) D^0(\tau_1 - \tau_2) \bar{c}_{p-q,s}(\tau_2) c_{p,s}(\tau_2) \bar{c}_{k,\sigma}(\tau) \\
+ \; & \bar{c}_{k',\sigma'}(\tau_1) c_{k'-q,\sigma'}(\tau_1) D^0(\tau_1 - \tau_2) \delta\bar{c}_{p-q,s}(\tau_2) c_{p,s}(\tau_2) \bar{c}_{k,\sigma}(\tau) \Big] \\
= \; & \delta\bar{c}_{k,\sigma}(\tau) - \int_0^\beta d\tau' \sum_{k',\sigma'} \left[\delta\bar{c}_{k',\sigma'}(\tau') \Big((\partial_{\tau'} + \epsilon_{k'}) c_{k',\sigma'}(\tau') \bar{c}_{k,\sigma}(\tau) + V f_{k',\sigma'}(\tau') \bar{c}_{k,\sigma}(\tau) \Big) \right] \\
- \; & \frac{g^2}{2} \sum_q \sum_{k',\sigma'} \sum_{p,s} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \Big[\delta\bar{c}_{k',\sigma'}(\tau_1) c_{k'-q,\sigma'}(\tau_1) D^0(\tau_1 - \tau_2) \bar{c}_{p-q,s}(\tau_2) c_{p,s}(\tau_2) \bar{c}_{k,\sigma}(\tau) \\
+ \; & \delta\bar{c}_{k',\sigma'}(\tau_1) c_{k'+q,\sigma'}(\tau_1) D^0(\tau_1 - \tau_2) \bar{c}_{p,s}(\tau_2) c_{p-q,s}(\tau_2) \bar{c}_{k,\sigma}(\tau) \Big] \\
= \; & \int_0^\beta d\tau' \sum_{k',\sigma'} \delta\bar{c}_{k',\sigma'}(\tau') \Bigg[\delta_{k,k'} \delta_{\sigma,\sigma'} \delta(\tau - \tau') - \Big((\partial_{\tau'} + \epsilon_{k'}) c_{k',\sigma'}(\tau') \bar{c}_{k,\sigma}(\tau) + V f_{k',\sigma'}(\tau') \bar{c}_{k,\sigma}(\tau) \Big) \\
+ \; & \frac{g^2}{2} \sum_q \sum_{p,s} \int_0^\beta d\tau_2 \Big[\bar{c}_{k,\sigma}(\tau) c_{k'-q,\sigma'}(\tau') D^0(\tau' - \tau_2) \bar{c}_{p,s}(\tau_2) c_{p+q,s}(\tau_2) \\
+ \; & \bar{c}_{k,\sigma}(\tau) c_{k'+q,\sigma'}(\tau') D^0(\tau' - \tau_2) \bar{c}_{p,s}(\tau_2) c_{p-q,s}(\tau_2) \Big] \Bigg] \\
= \; & \int_0^\beta d\tau' \sum_{k',\sigma'} \delta\bar{c}_{k',\sigma'}(\tau') \Bigg[\delta_{k,k'} \delta_{\sigma,\sigma'} \delta(\tau - \tau') - \Big((\partial_{\tau'} + \epsilon_{k'}) c_{k',\sigma'}(\tau') \bar{c}_{k,\sigma}(\tau) + V f_{k',\sigma'}(\tau') \bar{c}_{k,\sigma}(\tau) \Big) \\
- \; & g^2 \sum_q \sum_{p,s} \int_0^\beta d\tau_2 \Big[c_{k'-q,\sigma'}(\tau') \bar{c}_{k,\sigma}(\tau) D^0(\tau' - \tau_2) \bar{c}_{p,s}(\tau_2) c_{p+q,s}(\tau_2) \Big] \Bigg]
\end{aligned}
$$

Plug this into the path integral, we have the equation

$$
\begin{aligned}
& -\Big\langle g^2 \sum_q \sum_{p,s} \int_0^\beta d\tau_2 \Big[c_{k'-q,\sigma'}(\tau') \bar{c}_{k,\sigma}(\tau) D^0(\tau' - \tau_2) \bar{c}_{p,s}(\tau_2) c_{p+q,s}(\tau_2) \Big] \Big\rangle \qquad (48) \\
= \; & -\delta_{k,k'} \delta_{\sigma,\sigma'} \delta(\tau' - \tau) - \Big[(\partial_{\tau'} + \epsilon_{k'}) G^{cc}_{k,\sigma;k',\sigma'}(\tau' - \tau) + V G^{fc}_{k,\sigma;k',\sigma'}(\tau' - \tau) \Big]
\end{aligned}
$$

For the second equation, we can set $\delta f = 0, \delta c = 0, \delta \bar{c} = 0$, and then we have

$$\begin{aligned}
& \delta \bar{f}_{k,\sigma}(\tau) - \delta S \bar{f}_{k,\sigma}(\tau) \qquad (49)\\
= \; & \delta \bar{f}_{k,\sigma}(\tau) - \int_0^\beta d\tau' \sum_{k',\sigma'} \begin{pmatrix} 0 & \delta \bar{f}_{k',\sigma'}(\tau') \end{pmatrix} \begin{pmatrix} \partial_{\tau'} + \epsilon_{k'} & V \\ V & \partial_{\tau'} + \epsilon_f \end{pmatrix} \begin{pmatrix} c_{k',\sigma'}(\tau') \bar{f}_{k,\sigma}(\tau) \\ f_{k',\sigma'}(\tau') \bar{f}_{k,\sigma}(\tau) \end{pmatrix} \\
- \; & U \sum_{pqk'} \int_0^\beta d\tau' \Big[\delta \bar{f}_{p,\uparrow} \bar{f}_{q,\downarrow} f_{k',\uparrow} f_{p+q-k',\downarrow} \bar{f}_{k,\sigma}(\tau) + \bar{f}_{p,\uparrow} \delta \bar{f}_{q,\downarrow} f_{k',\uparrow} f_{p+q-k',\downarrow} \bar{f}_{k,\sigma}(\tau) \Big] \\
= \; & \delta \bar{f}_{k,\sigma}(\tau) - \sum_{k',\sigma'} \int_0^\beta d\tau' \delta \bar{f}_{k',\sigma'}(\tau') \Big[V c_{k',\sigma'}(\tau') \bar{f}_{k,\sigma}(\tau) + (\partial_{\tau'} + \epsilon_f) f_{k',\sigma'}(\tau') \bar{f}_{k,\sigma}(\tau) \Big] \\
- \; & U \sum_{k'qp} \int_0^\beta d\tau' \Big[\delta \bar{f}_{k',\uparrow} \bar{f}_{q,\downarrow} f_{p,\uparrow} f_{k'+q-p,\downarrow} \bar{f}_{k,\sigma}(\tau) - \delta \bar{f}_{k',\downarrow} \bar{f}_{p,\uparrow} f_{q,\uparrow} f_{p+k'-q,\downarrow} \bar{f}_{k,\sigma}(\tau) \Big] \\
= \; & \sum_{k',\sigma'} \int_0^\beta d\tau' \delta \bar{f}_{k',\sigma'}(\tau') \Bigg[\delta_{k,k'} \delta_{\sigma,\sigma'} \delta(\tau - \tau') - \Big(V c_{k',\sigma'}(\tau') \bar{f}_{k,\sigma}(\tau) + (\partial_{\tau'} + \epsilon_f) f_{k',\sigma'}(\tau') \bar{f}_{k,\sigma}(\tau) \Big) \\
+ \; & U \sum_{pq} \Big(\delta_{\sigma',\uparrow} \bar{f}_{k,\sigma}(\tau) \bar{f}_{q,\downarrow} f_{p,\uparrow} f_{k'+q-p,\downarrow} + \delta_{\sigma',\downarrow} \bar{f}_{p,\uparrow} \bar{f}_{k,\sigma}(\tau) f_{q,\uparrow} f_{p+k'-q,\downarrow} \Big) \Bigg]
\end{aligned}$$

Plug this into the path integral, we have

$$\begin{aligned}
& \Big\langle U \sum_{pq} \Big(\delta_{\sigma',\uparrow} \bar{f}_{k,\sigma}(\tau) \bar{f}_{q,\downarrow} f_{p,\uparrow} f_{k'+q-p,\downarrow} + \delta_{\sigma',\downarrow} \bar{f}_{p,\uparrow} \bar{f}_{k,\sigma}(\tau) f_{q,\uparrow} f_{p+k'-q,\downarrow} \Big) \Big\rangle \qquad (50)\\
= \; & -\delta_{k,k'} \delta_{\sigma,\sigma'} \delta(\tau' - \tau) - \Big[V G^{cf}_{k,\sigma;k',\sigma'}(\tau' - \tau) + (\partial_{\tau'} + \epsilon_f) G^{ff}_{k,\sigma;k',\sigma'}(\tau' - \tau) \Big]
\end{aligned}$$

Combining the above two equations together, we have the matrix equation

$$\begin{aligned}
& \begin{pmatrix} E^g_{k,\sigma;k',\sigma'}(\tau',\tau) & \phi \\ \tilde{\phi} & E^U_{k,\sigma;k',\sigma'}(\tau',\tau) \end{pmatrix} \qquad (51)\\
= \; & \begin{pmatrix} -\delta_{k,k'} \delta_{\sigma,\sigma'} \delta(\tau' - \tau) & 0 \\ 0 & -\delta_{k,k'} \delta_{\sigma,\sigma'} \delta(\tau' - \tau) \end{pmatrix} \\
- \; & \begin{pmatrix} \partial_{\tau'} + \epsilon_{k'} & V \\ V & \partial_{\tau'} + \epsilon_f \end{pmatrix} \begin{pmatrix} G^{cc}_{k,\sigma;k',\sigma'}(\tau' - \tau) & G^{cf}_{k,\sigma;k',\sigma'}(\tau' - \tau) \\ G^{fc}_{k,\sigma;k',\sigma'}(\tau' - \tau) & G^{ff}_{k,\sigma;k',\sigma'}(\tau' - \tau) \end{pmatrix}
\end{aligned}$$

Here, in the above equation, we have defined two quantities

$$\begin{aligned}
E^g_{k,\sigma;k',\sigma'}(\tau',\tau) &= -\Big\langle g^2 \sum_q \sum_{p,s} \int_0^\beta d\tau_2 \Big[c_{k'-q,\sigma'}(\tau') \bar{c}_{k,\sigma}(\tau) D^0(\tau' - \tau_2) \bar{c}_{p,s}(\tau_2) c_{p+q,s}(\tau_2) \Big] \Big\rangle \\
E^U_{k,\sigma;k',\sigma'}(\tau',\tau) &= \Big\langle U \sum_{pq} \Big(\delta_{\sigma',\uparrow} \bar{f}_{k,\sigma}(\tau) \bar{f}_{q,\downarrow} f_{p,\uparrow} f_{k'+q-p,\downarrow} + \delta_{\sigma',\downarrow} \bar{f}_{p,\uparrow} \bar{f}_{k,\sigma}(\tau) f_{q,\uparrow} f_{p+k'-q,\downarrow} \Big) \Big\rangle
\end{aligned}$$

If we set $k=k', \sigma=\sigma', \tau=0, \tau'=0^-$ in Equation [51], then we have

$$
\begin{aligned}
&\begin{pmatrix} E^g_{k,\sigma} & \phi \\ \tilde{\phi} & E^U_{k,\sigma} \end{pmatrix} \\
=& \begin{pmatrix} -\delta(0^-) & 0 \\ 0 & -\delta(0^-) \end{pmatrix} \\
-& \begin{pmatrix} \partial_{\tau'}+\epsilon_k & V \\ V & \partial_{\tau'}+\epsilon_f \end{pmatrix} \begin{pmatrix} G^{cc}_{k,\sigma}(0^-) & G^{cf}_{k,\sigma}(0^-) \\ G^{fc}_{k,\sigma}(0^-) & G^{ff}_{k,\sigma}(0^-) \end{pmatrix} \\
=& \begin{pmatrix} -\delta(0^-) & 0 \\ 0 & -\delta(0^-) \end{pmatrix} \\
-& \frac{1}{\beta}\sum_{i\omega_n} \begin{pmatrix} \partial_{\tau'}+\epsilon_k & V \\ V & \partial_{\tau'}+\epsilon_f \end{pmatrix} \begin{pmatrix} G^{cc}_{k,\sigma}(i\omega_n) & G^{cf}_{k,\sigma}(i\omega_n) \\ G^{fc}_{k,\sigma}(i\omega_n) & G^{ff}_{k,\sigma}(i\omega_n) \end{pmatrix} e^{-i\omega_n\tau'}\Big|_{\tau'=0^-} \\
=& \begin{pmatrix} -\delta(0^-) & 0 \\ 0 & -\delta(0^-) \end{pmatrix} \\
-& \frac{1}{\beta}\sum_{i\omega_n} \begin{pmatrix} -i\omega_n+\epsilon_k & V \\ V & -i\omega_n+\epsilon_f \end{pmatrix} \begin{pmatrix} G^{cc}_{k,\sigma}(i\omega_n) & G^{cf}_{k,\sigma}(i\omega_n) \\ G^{fc}_{k,\sigma}(i\omega_n) & G^{ff}_{k,\sigma}(i\omega_n) \end{pmatrix} e^{i\omega_n 0^+} \\
=& \begin{pmatrix} -\delta(0^-) & 0 \\ 0 & -\delta(0^-) \end{pmatrix} + \frac{1}{\beta}\sum_{i\omega_n} \Big(G^0_k(i\omega_n)\Big)^{-1} G_{k,\sigma}(i\omega_n) e^{i\omega_n 0^+} \\
=& \begin{pmatrix} -\delta(0^-) & 0 \\ 0 & -\delta(0^-) \end{pmatrix} + \frac{1}{\beta}\sum_{i\omega_n} \Big(G^{-1}_{k,\sigma}(i\omega_n)+\Sigma_{k,\sigma}(i\omega_n)\Big) G_{k,\sigma}(i\omega_n) e^{i\omega_n 0^+} \\
=& -\delta(0^-)\mathbb{I}_{2\times 2} + \frac{1}{\beta}\sum_{i\omega_n}\mathbb{I}_{2\times 2} e^{i\omega_n 0^+} + \frac{1}{\beta}\sum_{i\omega_n}\Sigma_{k,\sigma}(i\omega_n) G_{k,\sigma}(i\omega_n) e^{i\omega_n 0^+} \\
=& \frac{1}{\beta}\sum_{i\omega_n}\Sigma_{k,\sigma}(i\omega_n) G_{k,\sigma}(i\omega_n) e^{i\omega_n 0^+}
\end{aligned} \tag{52}
$$

Therefore, the total potential energy is

$$
\begin{aligned}
E_V &= \frac{1}{2}\sum_{k,\sigma} \mathrm{Tr} \begin{pmatrix} E^g_{k,\sigma} & \phi \\ \tilde{\phi} & E^U_{k,\sigma} \end{pmatrix} \\
&= \frac{1}{2}\frac{1}{\beta}\sum_{i\omega_n}\sum_{k,\sigma} \mathrm{Tr}\Big(\Sigma_{k,\sigma}(i\omega_n) G_{k,\sigma}(i\omega_n)\Big) e^{i\omega_n 0^+}
\end{aligned} \tag{53}
$$

1.4 Total energy for periodic Anderson model with electron-phonon interactions

In the previous section, we have shown how to calculate the potential energy in periodic Anderson model (PAM) with electron-phonon interactions. In order to obtain the total energy of the system, it is also necessary to calculate the kinetic energy. The calculation of kinetic energy is pretty straightforward. The only thing that calls for special attention is that high-frequency conditioning is indispensable while summing over all the Matsubara frequencies.

1.4.1 Numerical calculation of kinetic energy

First define some variables that are useful for expressing the Green function.

$$\begin{aligned}\alpha_n &= i\omega_n - (\epsilon_f - \mu) - \Sigma^{ff} \\ \beta_n &= i\omega_n + \mu - \Sigma^{cc} \\ \gamma_n &= \beta_n - \frac{(V+\Sigma^{cf})(V+\Sigma^{fc})}{\alpha_n}\end{aligned} \tag{54}$$

The kinetic energy is

$$\begin{aligned}E_{kinetic} &= \frac{1}{\beta}\mathrm{Tr}\sum_{\boldsymbol{k},\sigma,i\omega_n}\begin{pmatrix}\epsilon_{\boldsymbol{k}} & V \\ V & \epsilon_f\end{pmatrix}\begin{pmatrix}G^{cc}_{\boldsymbol{k},\sigma}(i\omega_n) & G^{cf}_{\boldsymbol{k},\sigma}(i\omega_n) \\ G^{fc}_{\boldsymbol{k},\sigma}(i\omega_n) & G^{ff}_{\boldsymbol{k},\sigma}(i\omega_n)\end{pmatrix} \\ &= \frac{2}{\beta}\mathrm{Tr}\sum_{\boldsymbol{k},i\omega_n}\begin{pmatrix}\epsilon_{\boldsymbol{k}} & V \\ V & \epsilon_f\end{pmatrix}\begin{pmatrix}G^{cc}_{\boldsymbol{k}}(i\omega_n) & G^{cf}_{\boldsymbol{k}}(i\omega_n) \\ G^{fc}_{\boldsymbol{k}}(i\omega_n) & G^{ff}_{\boldsymbol{k}}(i\omega_n)\end{pmatrix} \\ &= \frac{2}{\beta}\mathrm{Tr}\sum_{\boldsymbol{k},i\omega_n}\begin{pmatrix}\epsilon_{\boldsymbol{k}} & V \\ V & \epsilon_f\end{pmatrix}\begin{pmatrix}\frac{1}{\gamma_n-\epsilon_{\boldsymbol{k}}} & \frac{V+\Sigma^{cf}}{\alpha_n}\frac{1}{\gamma_n-\epsilon_{\boldsymbol{k}}} \\ \frac{V+\Sigma^{fc}}{\alpha_n}\frac{1}{\gamma_n-\epsilon_{\boldsymbol{k}}} & \frac{1}{\alpha_n}\frac{\beta_n-\epsilon_{\boldsymbol{k}}}{\gamma_n-\epsilon_{\boldsymbol{k}}}\end{pmatrix} \\ &= \frac{2}{\beta}\sum_{\boldsymbol{k},i\omega_n}\left(\frac{\epsilon_{\boldsymbol{k}}}{\gamma_n-\epsilon_{\boldsymbol{k}}} + \frac{V+\Sigma^{fc}}{\alpha_n}\frac{V}{\gamma_n-\epsilon_{\boldsymbol{k}}} + \frac{V+\Sigma^{cf}}{\alpha_n}\frac{V}{\gamma_n-\epsilon_{\boldsymbol{k}}} + \frac{\epsilon_f}{\alpha_n}\frac{\beta_n-\epsilon_{\boldsymbol{k}}}{\gamma_n-\epsilon_{\boldsymbol{k}}}\right) \\ &= \frac{2}{\beta}\sum_{\boldsymbol{k},i\omega_n}\frac{\epsilon_{\boldsymbol{k}}}{\gamma_n-\epsilon_{\boldsymbol{k}}} + \frac{2}{\beta}\sum_{i\omega_n}\left(V\overline{G}^{fc}(i\omega_n) + V\overline{G}^{cf}(i\omega_n) + \epsilon_f\overline{G}^{ff}(i\omega_n)\right)\end{aligned} \tag{55}$$

The first term in the kinetic energy is

$$\sum_{\boldsymbol{k}}\frac{\epsilon_{\boldsymbol{k}}}{\gamma_n-\epsilon_{\boldsymbol{k}}} = \int_{-\infty}^{\infty} d\epsilon \frac{\epsilon}{\gamma_n-\epsilon}\rho(\epsilon), \tag{56}$$

and $\rho(\epsilon)$ is the one-particle density of states which, for infinite dimensional hyper-cubic lattice, is

$$\rho(\epsilon) = \frac{1}{\sqrt{2\pi}t}e^{-\frac{\epsilon^2}{2t^2}}. \tag{57}$$

In order to have the best possible result, we need to apply the high-frequency conditioning to the summation in the calculation of kinetic energy. We are to evaluate the summations analytically with the assumptions that the self-energy is zero. Thus, we have a summation like this:

$$\frac{1}{\beta}\sum_{i\omega_n}\frac{1}{\gamma_n-\epsilon}, \gamma_n = i\omega_n + \mu - \frac{V^2}{i\omega_n+\mu-\epsilon_f} \tag{58}$$

In order to get a physically meaningful result, we need to introduce a convergence factor in the summation. That is,

$$\begin{aligned} & \frac{1}{\beta}\sum_{i\omega_n}\frac{e^{i\omega_n 0^+}}{\gamma_n-\epsilon} \\ = & \frac{1}{\beta}\sum_{i\omega_n}\frac{i\omega_n+\mu-\epsilon_f}{(i\omega_n+\mu-\epsilon)(i\omega_n+\mu-\epsilon_f)-V^2}e^{i\omega_n 0^+} \end{aligned} \tag{59}$$

Consider this contour integral.

$$\oint_{z=Re^{i\theta}}\frac{(z+\mu-\epsilon_f)e^{z0^+}}{(z+\mu-\epsilon)(z+\mu-\epsilon_f)-V^2}\frac{1}{e^{\beta z}+1}dz \tag{60}$$

It can be shown that the integral on the outer circle $z=Re^{i\theta}$ is zero, as $R\to\infty$. From Cauchy's theorem, we have

$$\begin{aligned} & \oint_{z=Re^{i\theta}}=0=\oint_{z=z_+ +\delta e^{i\theta}}+\oint_{z=z_- +\delta e^{i\theta}}+\sum_{i\omega_n}\oint_{z=i\omega_n+\delta e^{i\theta}}, \\ & z_\pm=-\mu+\frac{1}{2}(\epsilon+\epsilon_f\pm\sqrt{\Delta}),\Delta=(\epsilon-\epsilon_f)^2+4V^2 \end{aligned} \tag{61}$$

$$\begin{aligned} \oint_{z=z_+ +\delta e^{i\theta}} &= 2\pi i\frac{\frac{1}{2}(\epsilon-\epsilon_f+\sqrt{\Delta})}{\sqrt{\Delta}}\frac{1}{e^{\beta z_+}+1} \\ \oint_{z=z_- +\delta e^{i\theta}} &= 2\pi i\frac{\frac{1}{2}(\epsilon-\epsilon_f-\sqrt{\Delta})}{-\sqrt{\Delta}}\frac{1}{e^{\beta z_-}+1} \\ \oint_{z=i\omega_n+\delta e^{i\theta}} &= -\frac{2\pi i}{\beta}\frac{1}{\gamma_n-\epsilon} \end{aligned} \tag{62}$$

Therefore, we have

$$\begin{aligned} & \frac{1}{\beta}\sum_{i\omega_n}\frac{e^{i\omega_n 0^+}}{\gamma_n-\epsilon}=\frac{\frac{1}{2}(\epsilon-\epsilon_f+\sqrt{\Delta})}{\sqrt{\Delta}}\frac{1}{e^{\beta z_+}+1}+\frac{\frac{1}{2}(\epsilon-\epsilon_f-\sqrt{\Delta})}{-\sqrt{\Delta}}\frac{1}{e^{\beta z_-}+1}, \\ & z_\pm=-\mu+\frac{1}{2}(\epsilon+\epsilon_f\pm\sqrt{\Delta}),\Delta=(\epsilon-\epsilon_f)^2+4V^2, \\ & \gamma_n=i\omega_n+\mu-\frac{V^2}{i\omega_n+\mu-\epsilon_f} \end{aligned} \tag{63}$$

Another term that requires high-frequency conditioning is the summation over $G^{ff}(i\omega_n)$. Here, we have

$$\frac{1}{\beta}\sum_{i\omega_n}G_0^{ff}(i\omega_n)e^{i\omega_n 0^+}=\frac{1}{\beta}\sum_{i\omega_n}\frac{i\omega_n+\mu-\epsilon}{(i\omega_n+\mu-\epsilon_f)(i\omega_n+\mu-\epsilon)-V^2}e^{i\omega_n 0^+} \tag{64}$$

Consider this contour integral.

$$\oint_{z=Re^{i\theta}} \frac{(z+\mu-\epsilon)e^{z0^+}}{(z+\mu-\epsilon_f)(z+\mu-\epsilon)-V^2}\frac{1}{e^{\beta z}+1}dz \tag{65}$$

Similarly, we have

$$\oint_{z=Re^{i\theta}} = 0 = \oint_{z=z_+ +\delta e^{i\theta}} + \oint_{z=z_- +\delta e^{i\theta}} + \sum_{i\omega_n}\oint_{z=i\omega_n+\delta e^{i\theta}}, \tag{66}$$

$$z_\pm = -\mu + \frac{1}{2}(\epsilon+\epsilon_f \pm \sqrt{\Delta}), \Delta = (\epsilon-\epsilon_f)^2 + 4V^2$$

$$\begin{aligned}
\oint_{z=z_+ +\delta e^{i\theta}} &= 2\pi i \frac{\frac{1}{2}(-\epsilon+\epsilon_f+\sqrt{\Delta})}{\sqrt{\Delta}}\frac{1}{e^{\beta z_+}+1} \\
\oint_{z=z_- +\delta e^{i\theta}} &= 2\pi i \frac{\frac{1}{2}(-\epsilon+\epsilon_f-\sqrt{\Delta})}{-\sqrt{\Delta}}\frac{1}{e^{\beta z_-}+1} \\
\oint_{z=i\omega_n+\delta e^{i\theta}} &= \frac{2\pi i}{-\beta}\frac{i\omega_n+\mu-\epsilon}{(i\omega_n+\mu-\epsilon_f)(i\omega_n+\mu-\epsilon)-V^2}
\end{aligned} \tag{67}$$

Therefore, we have the summation formula

$$\begin{aligned}
& \frac{1}{\beta}\sum_{i\omega_n} G_0^{ff} e^{i\omega_n 0^+} \\
= & \frac{1}{\beta}\sum_{i\omega_n} \frac{i\omega_n+\mu-\epsilon}{(i\omega_n+\mu-\epsilon_f)(i\omega_n+\mu-\epsilon)-V^2} e^{i\omega_n 0^+} \\
= & \frac{\frac{1}{2}(-\epsilon+\epsilon_f+\sqrt{\Delta})}{\sqrt{\Delta}}\frac{1}{e^{\beta z_+}+1} + \frac{\frac{1}{2}(-\epsilon+\epsilon_f-\sqrt{\Delta})}{-\sqrt{\Delta}}\frac{1}{e^{\beta z_-}+1}
\end{aligned} \tag{68}$$

With the introduction of high-frequency conditioning, the formula for the calculation of kinetic energy needs to be modified. We are going to use the fully interacting Green function and here the self energy dependence of the variables $\alpha_n, \beta_n, \gamma_n$ is restored. That is,

$$\begin{aligned}
\alpha_n &= i\omega_n - (\epsilon_f - \mu) - \Sigma^{ff} \\
\beta_n &= i\omega_n + \mu - \Sigma^{cc} \\
\gamma_n &= \beta_n - \frac{(V+\Sigma^{cf})(V+\Sigma^{fc})}{\alpha_n}
\end{aligned} \tag{69}$$

With these notations, the kinetic energy is

$$\begin{aligned}
E_{kinetic} &= \frac{2}{\beta}\sum_{\boldsymbol{k},i\omega_n}\left(\frac{\epsilon_{\boldsymbol{k}}}{\gamma_n-\epsilon_{\boldsymbol{k}}} + \frac{V+\Sigma^{fc}}{\alpha_n}\frac{V}{\gamma_n-\epsilon_{\boldsymbol{k}}} + \frac{V+\Sigma^{cf}}{\alpha_n}\frac{V}{\gamma_n-\epsilon_{\boldsymbol{k}}} + \frac{\epsilon_f}{\alpha_n}\frac{\beta_n-\epsilon_{\boldsymbol{k}}}{\gamma_n-\epsilon_{\boldsymbol{k}}}\right) \\
&= \frac{2}{\beta}\sum_{\boldsymbol{k},i\omega_n}\frac{\epsilon_{\boldsymbol{k}}}{\gamma_n-\epsilon_{\boldsymbol{k}}} + \frac{2}{\beta}\sum_{\boldsymbol{k},i\omega_n}\frac{\epsilon_f}{\alpha_n}\frac{\beta_n-\epsilon_{\boldsymbol{k}}}{\gamma_n-\epsilon_{\boldsymbol{k}}} + \frac{2V}{\beta}\sum_{i\omega_n}\left(\overline{G}^{fc}(i\omega_n) + \overline{G}^{cf}(i\omega_n)\right) \\
&= \int_{-\infty}^{\infty} d\epsilon\rho(\epsilon)\frac{2}{\beta}\sum_{i\omega_n}\frac{\epsilon}{\gamma_n-\epsilon} + \int_{-\infty}^{\infty} d\epsilon\rho(\epsilon)\frac{2}{\beta}\sum_{i\omega_n}\frac{\epsilon_f}{\alpha_n}\frac{\beta_n-\epsilon}{\gamma_n-\epsilon} + \frac{2V}{\beta}\sum_{i\omega_n}\left(\overline{G}^{fc}(i\omega_n) + \overline{G}^{cf}(i\omega_n)\right)
\end{aligned} \tag{70}$$

To apply high-frequency conditioning, we are to make the following replacements:

$$\begin{aligned}
\frac{1}{\beta}\sum_{i\omega_n}\frac{1}{\gamma_n-\epsilon} &\rightarrow \frac{1}{\beta}\sum_{i\omega_n}\frac{1}{\gamma_n-\epsilon} \\
&+ \left(\frac{\frac{1}{2}(\epsilon-\epsilon_f+\sqrt{\Delta})}{\sqrt{\Delta}}\frac{1}{e^{\beta z_+}+1}+\frac{\frac{1}{2}(\epsilon-\epsilon_f-\sqrt{\Delta})}{-\sqrt{\Delta}}\frac{1}{e^{\beta z_-}+1}-\frac{1}{\beta}\sum_{i\omega_n}G_0^{cc}(i\omega_n)\right) \\
\frac{1}{\beta}\sum_{i\omega_n}\frac{1}{\alpha_n}\frac{\beta_n-\epsilon}{\gamma_n-\epsilon} &\rightarrow \frac{1}{\beta}\sum_{i\omega_n}\frac{1}{\alpha_n}\frac{\beta_n-\epsilon}{\gamma_n-\epsilon} \\
&+ \left(\frac{\frac{1}{2}(-\epsilon+\epsilon_f+\sqrt{\Delta})}{\sqrt{\Delta}}\frac{1}{e^{\beta z_+}+1}+\frac{\frac{1}{2}(-\epsilon+\epsilon_f-\sqrt{\Delta})}{-\sqrt{\Delta}}\frac{1}{e^{\beta z_-}+1}-\frac{1}{\beta}\sum_{i\omega_n}G_0^{ff}(i\omega_n)\right)
\end{aligned} \tag{71}$$

Here, we have made the following definitions:

$$\begin{aligned}
z_\pm &= -\mu+\frac{1}{2}(\epsilon+\epsilon_f\pm\sqrt{\Delta}), \\
\Delta &= (\epsilon-\epsilon_f)^2+4V^2.
\end{aligned} \tag{72}$$

1.4.2 Numerical calculation of potential energy

Now with both kinetic energy and potential energy, we can calculate the total energy of the system. The total energy of the system can be written compactly as

$$\begin{aligned}
E &= E_{kinetic}+E_V \\
&= \frac{1}{\beta}\sum_{k,\sigma,i\omega_n}\mathrm{Tr}\left[\left(\tilde{\epsilon}_k+\frac{1}{2}\tilde{\Sigma}_{k,\sigma}(i\omega_n)\right)\tilde{G}_{k,\sigma}(i\omega_n)\right]e^{i\omega_n 0^+}
\end{aligned} \tag{73}$$

Here, $\tilde{\epsilon}_k, \tilde{\Sigma}_{k,\sigma}(i\omega_n), \tilde{G}_{k,\sigma}(i\omega_n)$ are all 2×2 matrices, which are defined as

$$\begin{aligned}
\tilde{\epsilon}_k &= \begin{pmatrix} \epsilon_{\boldsymbol{k}} & V \\ V & \epsilon_f \end{pmatrix} \\
\tilde{\Sigma}_{k,\sigma}(i\omega_n) &= \begin{pmatrix} \Sigma_{k,\sigma}^{cc}(i\omega_n) & \Sigma_{k,\sigma}^{cf}(i\omega_n) \\ \Sigma_{k,\sigma}^{fc}(i\omega_n) & \Sigma_{k,\sigma}^{ff}(i\omega_n) \end{pmatrix} \\
\tilde{G}_{k,\sigma}(i\omega_n) &= \begin{pmatrix} G_{k,\sigma}^{cc}(i\omega_n) & G_{k,\sigma}^{cf}(i\omega_n) \\ G_{k,\sigma}^{fc}(i\omega_n) & G_{k,\sigma}^{ff}(i\omega_n) \end{pmatrix}
\end{aligned} \tag{74}$$

To calculate the numerical value of the potential energy, we also need high frequency conditioning. The high frequency behavior of self-energy in DMFT is known to be

$$\begin{pmatrix} \Sigma_{k,\sigma}^{cc}(i\omega_n) & \Sigma_{k,\sigma}^{cf}(i\omega_n) \\ \Sigma_{k,\sigma}^{fc}(i\omega_n) & \Sigma_{k,\sigma}^{ff}(i\omega_n) \end{pmatrix} \rightarrow \begin{pmatrix} a+\frac{b}{\omega_n^2}+\frac{ic}{\omega_n} & 0 \\ 0 & a'+\frac{b'}{\omega_n}+\frac{ic'}{\omega_n} \end{pmatrix} \tag{75}$$

It is already shown that the potential energy is

$$E_V = \frac{1}{2\beta}\sum_{k,\sigma,i\omega_n} \mathrm{Tr}\Big[\tilde{\Sigma}_{k,\sigma}(i\omega_n)\tilde{G}_{k,\sigma}(i\omega_n)\Big]e^{i\omega_n 0^+} = \frac{1}{\beta}\sum_{k}\sum_{n=-\infty}^{\infty} \mathrm{Tr}\Big[\tilde{\Sigma}_{k}(i\omega_n)\tilde{G}_{k}(i\omega_n)\Big]e^{i\omega_n 0^+} \tag{76}$$

Next we will only focus on the summation over frequencies. The frequency summation is

$$\begin{aligned}
S_k &= \frac{1}{\beta}\sum_{n=-\infty}^{\infty} \mathrm{Tr}\Big[\tilde{\Sigma}_{k}(i\omega_n)\tilde{G}_{k}(i\omega_n)\Big]e^{i\omega_n 0^+} \qquad (77)\\
&= \frac{1}{\beta}\sum_{n=-N}^{N} \mathrm{Tr}\Big[\tilde{\Sigma}_{k}(i\omega_n)\tilde{G}_{k}(i\omega_n)\Big]e^{i\omega_n 0^+}\\
&+ \frac{1}{\beta}\sum_{n=-\infty}^{-N-1} \mathrm{Tr}\Big[\tilde{\Sigma}_{k}(i\omega_n)\tilde{G}_{k}(i\omega_n)\Big]e^{i\omega_n 0^+} + \frac{1}{\beta}\sum_{n=N+1}^{\infty} \mathrm{Tr}\Big[\tilde{\Sigma}_{k}(i\omega_n)\tilde{G}_{k}(i\omega_n)\Big]e^{i\omega_n 0^+}\\
&\approx \frac{1}{\beta}\sum_{n=-N}^{N} \mathrm{Tr}\Big[\tilde{\Sigma}_{k}(i\omega_n)\tilde{G}_{k}(i\omega_n)\Big]e^{i\omega_n 0^+}\\
&+ \frac{1}{\beta}\sum_{n=-\infty}^{-N-1} \mathrm{Tr}\left[\begin{pmatrix} a & 0\\ 0 & a'\end{pmatrix}\begin{pmatrix} G_k^{cc(0)}(i\omega_n) & G_k^{cf(0)}(i\omega_n)\\ G_k^{fc(0)}(i\omega_n) & G_k^{ff(0)}(i\omega_n)\end{pmatrix}\right]e^{i\omega_n 0^+}\\
&+ \frac{1}{\beta}\sum_{n=N+1}^{\infty} \mathrm{Tr}\left[\begin{pmatrix} a & 0\\ 0 & a'\end{pmatrix}\begin{pmatrix} G_k^{cc(0)}(i\omega_n) & G_k^{cf(0)}(i\omega_n)\\ G_k^{fc(0)}(i\omega_n) & G_k^{ff(0)}(i\omega_n)\end{pmatrix}\right]e^{i\omega_n 0^+}\\
&= \frac{1}{\beta}\sum_{n=-N}^{N} \mathrm{Tr}\Big[\tilde{\Sigma}_{k}(i\omega_n)\tilde{G}_{k}(i\omega_n)\Big]e^{i\omega_n 0^+}\\
&+ \frac{1}{\beta}\sum_{n=-\infty}^{\infty} \mathrm{Tr}\left[\begin{pmatrix} a & 0\\ 0 & a'\end{pmatrix}\begin{pmatrix} G_k^{cc(0)}(i\omega_n) & G_k^{cf(0)}(i\omega_n)\\ G_k^{fc(0)}(i\omega_n) & G_k^{ff(0)}(i\omega_n)\end{pmatrix}\right]e^{i\omega_n 0^+}\\
&- \frac{1}{\beta}\sum_{n=-N}^{N} \mathrm{Tr}\left[\begin{pmatrix} a & 0\\ 0 & a'\end{pmatrix}\begin{pmatrix} G_k^{cc(0)}(i\omega_n) & G_k^{cf(0)}(i\omega_n)\\ G_k^{fc(0)}(i\omega_n) & G_k^{ff(0)}(i\omega_n)\end{pmatrix}\right]e^{i\omega_n 0^+}\\
&= \frac{1}{\beta}\sum_{n=-N}^{N} \mathrm{Tr}\Big[\tilde{\Sigma}_{k}(i\omega_n)\tilde{G}_{k}(i\omega_n)\Big]e^{i\omega_n 0^+}\\
&+ \frac{1}{\beta}\sum_{n=-\infty}^{\infty}\Big(aG_k^{cc(0)}(i\omega_n) + a'G_k^{ff(0)}(i\omega_n)\Big)e^{i\omega_n 0^+} - \frac{1}{\beta}\sum_{n=-N}^{N}\Big(aG_k^{cc(0)}(i\omega_n) + a'G_k^{ff(0)}(i\omega_n)\Big)e^{i\omega_n 0^+}
\end{aligned}$$

The potential energy is thus

$$
\begin{aligned}
E_V &= \sum_k S_k \qquad (78)\\
&= \frac{1}{\beta}\sum_{n=-N}^{N} \mathrm{Tr}\Big[\tilde{\Sigma}(i\omega_n)\tilde{G}(i\omega_n)\Big]\\
&+ a\int_{-\infty}^{\infty} d\epsilon\rho(\epsilon)\left(\frac{\frac{1}{2}(\epsilon-\epsilon_f+\sqrt{\Delta})}{\sqrt{\Delta}}\frac{1}{e^{\beta z_+}+1}+\frac{\frac{1}{2}(\epsilon-\epsilon_f-\sqrt{\Delta})}{-\sqrt{\Delta}}\frac{1}{e^{\beta z_-}+1}\right)\\
&+ a'\int_{-\infty}^{\infty} d\epsilon\rho(\epsilon)\left(\frac{\frac{1}{2}(-\epsilon+\epsilon_f+\sqrt{\Delta})}{\sqrt{\Delta}}\frac{1}{e^{\beta z_+}+1}+\frac{\frac{1}{2}(-\epsilon+\epsilon_f-\sqrt{\Delta})}{-\sqrt{\Delta}}\frac{1}{e^{\beta z_-}+1}\right)\\
&- \frac{1}{\beta}\sum_{n=-N}^{N}\Big(aG^{cc(0)}(i\omega_n)+a'G^{ff(0)}(i\omega_n)\Big)
\end{aligned}
$$

Here, we have made the following definitions:

$$
\begin{aligned}
z_\pm &= -\mu+\frac{1}{2}(\epsilon+\epsilon_f\pm\sqrt{\Delta}), \qquad (79)\\
\Delta &= (\epsilon-\epsilon_f)^2+4V^2.
\end{aligned}
$$

References

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