

Hybridization expansion and non-crossing/one-crossing approximations

Lei Zhang^{1,*}

¹*Department of Physics, University of Michigan,
Ann Arbor, Michigan 48109, United States of America*

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I. INTRODUCTION

This is an introduction to hybridization expansion and its approximation schemes, especially for non-crossing and one-crossing approximations. Detailed derivation are given in this note. In addition, several simple rules to determine tricky signs in any configurations and in any self-energy expressions are presented. Notations in this note follow from Ref. [1] and Ref. [2]. Details of hybridization expansion and approximation schemes are given in Sec. II and Sec. III, respectively. But before moving on, it would be beneficial to first get familiar with the notations and the general form of the Hamiltonian.

For a general quantum impurity model, the Hamiltonian H_{QI} consists of three terms: H_{loc} , which describes the “impurity”, H_{bath} , which describes the “bath”, and H_{hyb} which describes the coupling between the impurity and the bath. Thus,

$$H_{\text{QI}} = H_{\text{loc}} + H_{\text{bath}} + H_{\text{hyb}}. \quad (1)$$

Usually, H_{loc} consists of two terms: hopping term H_{loc}^0 and interacting term H_{loc}^1 , both of which can be expressed in terms of fermionic operators d/d^\dagger . Explicit expressions for these terms are as follows:

$$H_{\text{loc}} = H_{\text{loc}}^0 + H_{\text{loc}}^1, \quad H_{\text{loc}}^0 = \sum_{ab} E^{ab} d_a^\dagger d_b, \quad H_{\text{loc}}^1 = \sum_{ijkl} I^{ijkl} d_i^\dagger d_j^\dagger d_k d_l + \dots, \quad (2)$$

where states are labeled by flavor indices a (including both orbital and spin degrees of freedom). As for H_{bath} , the general form is

$$H_{\text{bath}} = \sum_p \varepsilon_p c_p^\dagger c_p, \quad (3)$$

in which flavor p is the combination of momentum, orbital and spin indices. Finally, the coupling between the impurity and the bath can be written as

$$H_{\text{hyb}} = \sum_{pj} (V_p^j c_p^\dagger d_j + V_p^{j*} d_j^\dagger c_p). \quad (4)$$

II. HYBRIDIZATION EXPANSION

Hybridization expansion is a perturbative expansion regarding to H_{hyb} . Denote $H_{\text{loc}} + H_{\text{bath}}$ and H_{hyb} by H_a and H_b , respectively. Then the partition function of the impurity model can be expressed as

$$Z = \text{Tr}[e^{-\beta(H_a + H_b)}] = \text{Tr}[e^{-\beta H_a} T_\tau \exp(-\int_0^\beta d\tau H_b(\tau))] , \quad (5)$$

where $H_b(\tau) = e^{H_a \tau} H_b e^{-H_a \tau}$ and T_τ is the time-ordering operator. After applying the Taylor expansion to the exponential, the partition function can be reexpressed as

$$Z = \sum_{k=0}^{+\infty} (-1)^k \frac{1}{k!} \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_k \text{Tr}[T_\tau e^{-\beta H_a} H_b(\tau_k) \dots H_b(\tau_1)] . \quad (6)$$

Since H_b , which can be separated as $H_b = \sum_{pj} (V_p^j c_p^\dagger d_j + V_p^{j*} d_j^\dagger c_p) = \tilde{H}_{\text{hyb}} + \tilde{H}_{\text{hyb}}^\dagger$, contains only one operator in each term which creates or annihilates an electron on the impurity, only even numbers of H_b with equal numbers of \tilde{H}_{hyb} and $\tilde{H}_{\text{hyb}}^\dagger$ can make non-zero contribution. The partition function therefore becomes

$$\begin{aligned}
Z &= \sum_{k=0}^{+\infty} \frac{1}{(2k)!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_{2k} \text{Tr}[T_\tau e^{-\beta H_a} H_b(\tau_{2k}) \cdots H_b(\tau_1)] \\
&= \sum_{k=0}^{+\infty} \frac{1}{(2k)!} C_{2k}^k (k!)^2 \iiint_{\substack{\tau_1 < \dots < \tau_k \\ \tau'_1 < \dots < \tau'_k}} d\tau_1 \cdots d\tau'_k \text{Tr}[T_\tau e^{-\beta H_a} \tilde{H}_{\text{hyb}}(\tau_k) \tilde{H}_{\text{hyb}}^\dagger(\tau'_k) \cdots \tilde{H}_{\text{hyb}}(\tau_1) \tilde{H}_{\text{hyb}}^\dagger(\tau'_1)] \\
&= \sum_{k=0}^{+\infty} \iiint_{\substack{\tau_1 < \dots < \tau_k \\ \tau'_1 < \dots < \tau'_k}} d\tau_1 \cdots d\tau'_k \text{Tr}[T_\tau e^{-\beta H_a} \tilde{H}_{\text{hyb}}(\tau_k) \tilde{H}_{\text{hyb}}^\dagger(\tau'_k) \cdots \tilde{H}_{\text{hyb}}(\tau_1) \tilde{H}_{\text{hyb}}^\dagger(\tau'_1)], \tag{7}
\end{aligned}$$

where C_{2k}^k is the number of choices to select k \tilde{H}_{hyb} 's from $2k$ candidates and $(k!)^2$ comes from the time ordering of τ and τ' (i.e., let $\tau_1 < \tau_2 < \dots < \tau_k$ and $\tau'_1 < \tau'_2 < \dots < \tau'_k$).

Inserting the explicit expressions of \tilde{H}_{hyb} and $\tilde{H}_{\text{hyb}}^\dagger$ yields

$$\begin{aligned}
Z &= \sum_{k=0}^{+\infty} \iiint_{\substack{\tau_1 < \dots < \tau_k \\ \tau'_1 < \dots < \tau'_k}} d\tau_1 \cdots d\tau'_k \sum_{\substack{j_1, \dots, j_k, p_1, \dots, p_k \\ j'_1, \dots, j'_k, p'_1, \dots, p'_k}} V_{p'_k}^{j'_k*} V_{p_k}^{j_k} \cdots V_{p'_1}^{j'_1*} V_{p_1}^{j_1} \\
&\quad \times \text{Tr}[T_\tau e^{-\beta H_a} d_{j_k}(\tau_k) c_{p_k}^\dagger(\tau_k) c_{p'_k}(\tau'_k) d_{j'_k}^\dagger(\tau'_k) \cdots d_{j_1}(\tau_1) c_{p_1}^\dagger(\tau_1) c_{p'_1}(\tau'_1) d_{j'_1}^\dagger(\tau'_1)] \\
&= \sum_{k=0}^{+\infty} \iiint_{\substack{\tau_1 < \dots < \tau_k \\ \tau'_1 < \dots < \tau'_k}} d\tau_1 \cdots d\tau'_k \sum_{\substack{j_1, \dots, j_k, p_1, \dots, p_k \\ j'_1, \dots, j'_k, p'_1, \dots, p'_k}} V_{p'_k}^{j'_k*} V_{p_k}^{j_k} \cdots V_{p'_1}^{j'_1*} V_{p_1}^{j_1} \\
&\quad \times \text{Tr}_d[T_\tau e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j'_k}^\dagger(\tau'_k) \cdots d_{j_1}(\tau_1) d_{j'_1}^\dagger(\tau'_1)] \times \text{Tr}_c[T_\tau e^{-\beta H_{\text{bath}}} c_{p_k}^\dagger(\tau_k) c_{p'_k}(\tau'_k) \cdots c_{p_1}^\dagger(\tau_1) c_{p'_1}(\tau'_1)], \tag{8}
\end{aligned}$$

in which the second line is based on the fact that impurity and bath in the trace are decoupled from each other ($[H_{\text{loc}}, H_{\text{bath}}] = 0$, $d/d^\dagger(\tau) = e^{H_{\text{loc}}\tau} d/d^\dagger e^{-H_{\text{loc}}\tau}$ and $c/c^\dagger(\tau) = e^{H_{\text{bath}}\tau} c/c^\dagger e^{-H_{\text{bath}}\tau}$).

Since H_{bath} is bilinear in creation and annihilation operators, Wick's theorem is valid and therefore can be utilized to simplify the trace over the bath. Thus, we have

$$\begin{aligned}
&\frac{1}{Z_{\text{bath}}} \sum_{\substack{p_1, \dots, p_k \\ p'_1, \dots, p'_k}} V_{p'_k}^{j'_k*} V_{p_k}^{j_k} \cdots V_{p'_1}^{j'_1*} V_{p_1}^{j_1} \text{Tr}_c[T_\tau e^{-\beta H_{\text{bath}}} c_{p_k}^\dagger(\tau_k) c_{p'_k}(\tau'_k) \cdots c_{p_1}^\dagger(\tau_1) c_{p'_1}(\tau'_1)] \\
&= \sum_{\substack{p_1, \dots, p_k \\ p'_1, \dots, p'_k}} V_{p'_k}^{j'_k*} V_{p_k}^{j_k} \cdots V_{p'_1}^{j'_1*} V_{p_1}^{j_1} \langle T_\tau c_{p_k}^\dagger(\tau_k) c_{p'_k}(\tau'_k) \cdots c_{p_1}^\dagger(\tau_1) c_{p'_1}(\tau'_1) \rangle \\
&= \sum_s \sum_{\substack{p_1, \dots, p_k \\ p'_1, \dots, p'_k}} V_{p'_k}^{j'_k*} V_{p_k}^{j_k} \cdots V_{p'_1}^{j'_1*} V_{p_1}^{j_1} \text{sgn}(s) \langle T_\tau c_{p_k}^\dagger(\tau_k) c_{p'_{s(k)}}(\tau'_{s(k)}) \rangle \cdots \langle T_\tau c_{p_1}^\dagger(\tau_1) c_{p'_{s(1)}}(\tau'_{s(1)}) \rangle \\
&= \sum_s \sum_{\substack{p_1, \dots, p_k \\ p'_1, \dots, p'_k}} V_{p'_k}^{j'_k*} V_{p_k}^{j_k} \cdots V_{p'_1}^{j'_1*} V_{p_1}^{j_1} \text{sgn}(s) \langle T_\tau c_{p_k}^\dagger(\tau_k) c_{p'_k}(\tau'_{s(k)}) \rangle \cdots \langle T_\tau c_{p_1}^\dagger(\tau_1) c_{p'_1}(\tau'_{s(1)}) \rangle, \tag{9}
\end{aligned}$$

where s is a permutation of $(1, 2, \dots, k)$, $Z_{\text{bath}} = \text{Tr}[e^{-\beta H_{\text{bath}}}] = \prod_p \prod_\sigma (1 + e^{-\beta \varepsilon_p})$ and relation $\langle T_\tau c_{p_i}^\dagger(\tau) c_{p_j}(\tau') \rangle = \delta_{p_i=p'_j} \langle T_\tau c_{p_i}^\dagger(\tau) c_{p_i}(\tau') \rangle$ has been used. Define the hybridization function as

$$\Delta_{lm}(\tau'_l - \tau_m) = - \sum_p V_p^{j'_l*} V_p^{j_m} \langle T_\tau c_p(\tau'_l) c_p^\dagger(\tau_m) \rangle = \sum_p \frac{V_p^{j'_l*} V_p^{j_m}}{e^{\varepsilon_p \beta} + 1} \begin{cases} -e^{-\varepsilon_p(\tau - \beta)}, & 0 < \tau < \beta, \\ e^{-\varepsilon_p \tau}, & -\beta < \tau < 0, \end{cases} \tag{10}$$

where $\tau = \tau'_l - \tau_m$ is the time difference. Then equ (9) can be simplified as $\sum_s \text{sgn}(s) \Delta_{s(1)1} \Delta_{s(2)2} \cdots \Delta_{s(k)k} = \det \Delta$, where $\text{sgn}(s) = (-1)^n$ and n is the number of exchanges to obtain $(1, \dots, k)$ from $(s(1), \dots, s(k))$.

Unfortunately, since the interaction term makes H_{loc} not bilinear, the trace over impurity cannot be simplified in this way. As a result, the final form of the partition function is

$$Z = Z_{\text{bath}} \sum_{k=0}^{+\infty} \iiint_{\substack{\tau_1 < \dots < \tau_k \\ \tau'_1 < \dots < \tau'_k}} d\tau_1 \cdots d\tau'_k \sum_{\substack{j_1, \dots, j_k \\ j'_1, \dots, j'_k}} \text{Tr}_d[T_\tau e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j'_k}^\dagger(\tau'_k) \cdots d_{j_1}(\tau_1) d_{j'_1}^\dagger(\tau'_1)] \det \Delta. \tag{11}$$

In some specific cases, this expression can be simplified further, e.g., some models can be expressed in the so-called segment representation. But this is beyond the scope of this note.

One way to do simulations is to sample configurations stochastically by using continuous-time Monte Carlo method, called CT-HYB in this representation. According to equ (11), the configuration space is described by $\mathbf{x} = (k, \boldsymbol{\tau}, \mathbf{j})$, where $\boldsymbol{\tau} = (\tau_1, \dots, \tau_k, \tau'_1, \dots, \tau'_k)$ and $\mathbf{j} = (j_1, \dots, j_k, j'_1, \dots, j'_k)$. Denote the trace in equ (11) by w_{loc} . CT-HYB samples each configuration \mathbf{x} according to its weight $w_{\text{loc}}(\mathbf{x})\det\Delta(\mathbf{x})$. Note that the expression of hybridization expansion is exact as long as $H_b(\tau)$ is not infinite large (this will never happen in real simulations), so CT-HYB is always numerically accurate. In general, however, $w_{\text{loc}}(\mathbf{x})\det\Delta(\mathbf{x})$ is not always non-negative. So this method may suffer from severe sign problem.

III. APPROXIMATION SCHEMES

A. Expanding the configuration space

Another way to do simulations is to use self-consistent resummations of diagrams, which are popular approximations of the hybridization expansion. Generally speaking, we construct the Dyson equation of the dressed propagator, which will be defined later, and find the relation between this propagator and the self-energy based on some self-similar structures of the configurations. Then we just iterate these self-consistent equations to obtain convergent results. To achieve this goal, it is beneficial to expand the configuration space from \mathbf{x} to $\mathbf{x}' = (\mathbf{x}, s)$. In other words, in each fixed \mathbf{x} , there are $k!$ distinct configurations resulting from different pairings between (τ_1, \dots, τ_k) and $(\tau'_1, \dots, \tau'_k)$, which can be represented by some curves, called hybridization lines, connecting the corresponding pairs. Then it is easy to figure out the corresponding weight is $\text{sgn}(s)w_{\text{loc}}(\mathbf{x})\Delta_{s(1)1}\Delta_{s(2)2}\dots\Delta_{s(k)k}$. Define the bare propagator $R_0(\tau) = e^{-H_{\text{loc}}\tau}$ and the dress propagator

$$R(\tau) = \sum_{\mathbf{x}'} \text{sgn}(s)\Delta_{s(1)1}\Delta_{s(2)2}\dots\Delta_{s(k)k} T_{\tau} e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j'_k}^{\dagger}(\tau'_k) \dots d_{j_1}(\tau_1) d_{j'_1}^{\dagger}(\tau'_1). \quad (12)$$

Then it is easy to verify that

$$Z/Z_{\text{bath}} = \text{Tr}[R(\beta)]. \quad (13)$$

And the expectation value of an arbitrary local operator O can be computed easily:

$$\langle O \rangle = \text{Tr}[R(\beta)O]/\text{Tr}[R(\beta)]. \quad (14)$$

After some exploration, it is found that any configuration of $R(\tau)$ can be constructed by the following steps:

1. Choose an order $k \in \mathbb{N}$;
2. Specify values of $\boldsymbol{\tau}$ fulfilling the restrictions $0 < \tau_1 < \dots < \tau_k < \tau$ and $0 < \tau'_1 < \dots < \tau'_k < \tau$;
3. Pair (τ_1, \dots, τ_k) and $(\tau'_1, \dots, \tau'_k)$, represented by hybridization lines connecting the corresponding pairs.

A typical configuration is shown in Fig. 1. The contribution of each configuration can be written down by the overall sign “sgn” times the contribution calculated from the rules shown in Fig. 2. The overall sign comes from two places: (i) the time-ordering of d/d^{\dagger} operators and (ii) the pairing between (τ_1, \dots, τ_k) and $(\tau'_1, \dots, \tau'_k)$. For fig. 1, the former is +1 and the later is -1, so that $\text{sgn} = -1$ and the contribution is

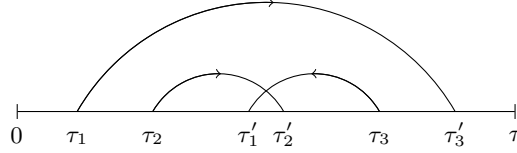
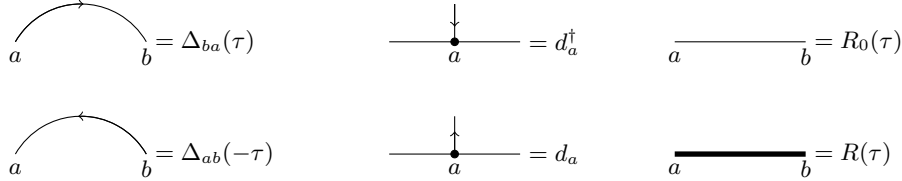
$$-R_0(\tau - \tau'_3) d_{j'_3}^{\dagger} R_0(\tau'_3 - \tau_3) d_{j_3} R_0(\tau_3 - \tau'_2) d_{j'_2}^{\dagger} R_0(\tau'_2 - \tau'_1) d_{j'_1}^{\dagger} R_0(\tau'_1 - \tau_2) d_{j_2} R_0(\tau_2 - \tau_1) d_{j_1} R_0(\tau_1).$$

(Note: in diagrams, right direction corresponds to time increasing while in the expression of $R(\tau)$, right direction corresponds to time decreasing because of the convention of the time-ordering operator.)

B. Dyson equation

By analyzing the structure of all diagrams, it is easy to formulate the Dyson equation:

$$R(\tau) = R_0(\tau) + \int_0^{\tau} d\tau_2 \int_0^{\tau_2} d\tau_1 R(\tau - \tau_2) S(\tau_2 - \tau_1) R_0(\tau_1), \quad (15)$$

FIG. 1: A typical configuration of $R(\tau)$.FIG. 2: Contribution for each segment of the diagram. Right direction corresponds to the increasing of the imaginary time and $\tau = \tau_b - \tau_a$ is the corresponding time increment.

which can be expressed graphically as

$$\overline{0 \tau} = \overline{0 \tau} + \overline{0 \tau_1} \circlearrowleft S \circlearrowright \overline{\tau_2 \tau} . \quad (16)$$

$S(\tau)$ is the set of all one-particle irreducible diagrams, corresponding to the “self-energy” of $R(\tau)$. However, because the structure of $S(\tau)$ is still complicated, we need do some approximations to get a relatively simple expression.

C. Non-crossing approximation

One popular approximation is the so-called non-crossing approximation (NCA), which neglects any configurations in which any two hybridization lines have a crossover point (the hybridization line is required to be “regular” so that it cannot have more than one crossover point with another line). In this situation, the self-similar structure of $S(\tau) = S_0(\tau)$ gives another relation with R :

$$\begin{aligned} S_0(\tau) &= \overline{0 \tau} + \overline{0 \tau} \\ &= \sum_{ab} \left[\text{sgn}_1 d_b^\dagger R(\tau) d_a \Delta_{ba}(\tau) + \text{sgn}_2 d_b R(\tau) d_a^\dagger \Delta_{ab}(-\tau) \right] . \end{aligned} \quad (17)$$

sgn_1 and sgn_2 are signs of corresponding diagrams, which will be analyzed later.

D. One-crossing approximation

One improvement to NCA is the so-called one-crossing approximation (OCA), which neglects any configurations in which any one hybridization line has more than one crossover points in total with all other lines. OCA can be considered as a more accurate approximation compared to NCA, because it includes more diagrams. For example, Fig. 1 is included in OCA but not in NCA. By similar analysis, a self-similar structure can be found: $S(\tau) = S_0(\tau) + S_1(\tau)$ and

$$\begin{aligned}
S_1(\tau) &= \begin{array}{c} \text{Diagram 1} \\ \text{Diagram 2} \\ \text{Diagram 3} \\ \text{Diagram 4} \end{array} + \begin{array}{c} \text{Diagram 5} \\ \text{Diagram 6} \\ \text{Diagram 7} \\ \text{Diagram 8} \end{array} \\
&= \sum_{abcd} \int_0^\tau d\tau_2 \int_0^{\tau_2} d\tau_1 \left[\text{sgn}_1 d_d^\dagger R(\tau - \tau_2) d_c^\dagger R(\tau_2 - \tau_1) d_b R(\tau_1) d_a \Delta_{db}(\tau - \tau_1) \Delta_{ca}(\tau_2) \right. \\
&\quad + \text{sgn}_2 d_d R(\tau - \tau_2) d_c^\dagger R(\tau_2 - \tau_1) d_b^\dagger R(\tau_1) d_a \Delta_{bd}(\tau_1 - \tau) \Delta_{ca}(\tau_2) \\
&\quad + \text{sgn}_3 d_d^\dagger R(\tau - \tau_2) d_c R(\tau_2 - \tau_1) d_b R(\tau_1) d_a^\dagger \Delta_{db}(\tau - \tau_1) \Delta_{ac}(-\tau_2) \\
&\quad \left. + \text{sgn}_4 d_d R(\tau - \tau_2) d_c R(\tau_2 - \tau_1) d_b^\dagger R(\tau_1) d_a^\dagger \Delta_{bd}(\tau_1 - \tau) \Delta_{ac}(-\tau_2) \right]. \tag{18}
\end{aligned}$$

E. Determining the overall sign

In this subsection, two useful theorems are presented to determine the overall signs in any configurations and in any self-energy expressions. As a result, one can determine signs by just observing the diagrams.

Theorem 1 *Moving a hybridization line across an arbitrary complete diagram D (any hybridization lines starting within D will also end within D) will not change its sign. It has the following graphical expressions:*

$$\begin{aligned}
\text{sgn}\left(\begin{array}{c} \downarrow \\ \text{---} \textcircled{D} \text{---} \end{array}\right) &= \text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \downarrow \end{array}\right) \\
\text{sgn}\left(\begin{array}{c} \uparrow \\ \text{---} \textcircled{D} \text{---} \end{array}\right) &= \text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \uparrow \end{array}\right)
\end{aligned}$$

As an exercise, sgn_1 in NCA can be obtained conveniently:

$$\text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) = \text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) = \text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) \times \text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right). \tag{19}$$

Because $\text{sgn}(-\textcircled{-})$ has been incorporated into R , we have $\text{sgn}_1 = \text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) = -1$. Using similar procedure, we get $\text{sgn}_2 = +1$. So the final form of NCA self-energy is

$$S_0(\tau) = - \sum_{ab} \left[d_b^\dagger R(\tau) d_a \Delta_{ba}(\tau) + d_b R(\tau) d_a^\dagger \Delta_{ab}(\beta - \tau) \right]. \tag{20}$$

Because in the configurations of $R_1(\tau)$, hybridization lines may have a crossover point. To deal with this situation, it is beneficial to introduce another theorem:

Theorem 2 *Switching two adjacent crossing lines will contribute a minus sign. It has the following graphical expressions:*

$$\begin{aligned}
\text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) &= -\text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) & \text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) &= -\text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) \\
\text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) &= -\text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) & \text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right) &= -\text{sgn}\left(\begin{array}{c} \text{---} \textcircled{D} \text{---} \\ \text{---} \end{array}\right)
\end{aligned}$$

As another exercise, we calculate sgn_1 in OCA.

$$\begin{aligned}
\text{sgn}\left(\begin{array}{c} \curvearrowright \\ \textcircled{D_1} \textcircled{D_2} \textcircled{D_3} \\ \curvearrowleft \end{array}\right) &= \text{sgn}\left(\begin{array}{c} \curvearrowright \\ \textcircled{D_1} \textcircled{D_2} \textcircled{D_3} \\ \curvearrowleft \end{array}\right) \times \text{sgn}\left(\begin{array}{c} \textcircled{D_1} \textcircled{D_2} \textcircled{D_3} \\ \text{---} \end{array}\right) \\
&= -\text{sgn}\left(\begin{array}{c} \curvearrowright \\ \textcircled{D_1} \textcircled{D_2} \textcircled{D_3} \\ \curvearrowleft \end{array}\right) \times \text{sgn}\left(\begin{array}{c} \textcircled{D_1} \textcircled{D_2} \textcircled{D_3} \\ \text{---} \end{array}\right). \tag{21}
\end{aligned}$$

So $\text{sgn}_1 = -\text{sgn}(\curvearrowright) = -1$. Similarly, we get $\text{sgn}_2 = \text{sgn}_3 = -\text{sgn}_4 = +1$. So the final form of $S_1(\tau)$ in OCA is

$$\begin{aligned}
S_1(\tau) &= - \sum_{abcd} \int_0^\tau d\tau_2 \int_0^{\tau_2} d\tau_1 \left[d_d^\dagger R(\tau - \tau_2) d_c^\dagger R(\tau_2 - \tau_1) d_b R(\tau_1) d_a \Delta_{db}(\tau - \tau_1) \Delta_{ca}(\tau_2) \right. \\
&\quad + d_d R(\tau - \tau_2) d_c^\dagger R(\tau_2 - \tau_1) d_b^\dagger R(\tau_1) d_a \Delta_{bd}(\beta - \tau + \tau_1) \Delta_{ca}(\tau_2) \\
&\quad + d_d^\dagger R(\tau - \tau_2) d_c R(\tau_2 - \tau_1) d_b R(\tau_1) d_a^\dagger \Delta_{db}(\tau - \tau_1) \Delta_{ac}(\beta - \tau_2) \\
&\quad \left. + d_d R(\tau - \tau_2) d_c R(\tau_2 - \tau_1) d_b^\dagger R(\tau_1) d_a^\dagger \Delta_{bd}(\beta - \tau + \tau_1) \Delta_{ac}(\beta - \tau_2) \right]. \tag{22}
\end{aligned}$$

Using theorem 1 and theorem 2, it is now straightforward to obtain two corollaries:

Corollary 1 $S(\tau)$ can be obtained by: i) replace R by R_0 in the self-energy expression; ii) write down its contribution, including sgn ; iii) replace R_0 by R .

Corollary 2 For any configuration, its sign equals $(-1)^n$, where n equals the total number of hybridization lines flowing rightward plus the total number of crossover points. In other words,

$$n = \# \text{ of } (\curvearrowright) + \# \text{ of } (\curvearrowleft).$$

It is straightforward to verify these corollaries are consistent with the results we obtained before. Using these corollaries, we can easily write a computer program to calculate the analytic expressions for higher-order approximations, which might be beneficial in the future.

* Electronic address: lzphy@umich.edu

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