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Approximate Treatments and Cluster Extensions I & II

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1 Introduction and Motivation

In this lecture I would like to introduce to you an unconventional perturbation theory for the single impurity Anderson model (SIAM) which can be used as "quick-and-dirty" method to study correlated models in the DMFT. During the past week you will already have heard about other "impurity solvers" such as Quantum Monte Carlo (QMC), perturbation theory in the Coulomb repulsion U or Wilson's numerical renormalization group (NRG). The obvious question thus is: Why do we yet need another technique to treat this model? Of course, QMC is numerically exact; however, for large Coulomb repulsion and small temperatures it becomes, even with modern computers, computationally very expensive. In addition, in order to obtain dynamical quantities one has to go through the numerically ill-defined process of analytic continuation. Perturbation theory in U (non self-consistent) is straightforward and numerically easy to implement; by its very nature it is in principle restricted to the weak coupling regime and can of course never produce exponentially small energy scales like the Kondo temperature, for example. Moreover, strictly speaking it leads to reasonable results only in the particle-hole symmetric case[1] and systematic improvements (self-consistency, additional diagram classes etc.) up to now always seem to severely worsen the result, and the reliability of an extension to orbitally degenerate models is also highly unclear. Last but not least NRG is designed to treat low-energy features correctly and becomes extremly expensive for multi-band models, especially when applied to DMFT (typically 16GB of memory, 5 hours or more using 8 – 16 processors on modern SMP machines).

Thus, especially in the strong coupling regime, a different approach might be desirable and helpful. Such an approach is the resolvent perturbation theory. In order to keep things simple, I will not attempt to present you the most general version of this theory together with the most general version of the SIAM. For the actual application to real materials, be it magnetic ions in metals, quantum dots or within the DMFT, this would of course be desirable; however, in the short time given such a program is impossible to carry through. Nevertheless I will try to convey the basic ideas and enable you to read the more advanced publications on this subject. As a very nice introductory reading, not only to the resolvent perturbation theory but to the subject of the physics of the SIAM and different methods to solve it in general, I can recommend the book by Alex Hewson "The Kondo problem to heavy fermions" and the article by Bickers, Cox and Wilkins, Phys. Rev. B**36**, 2036(1987). A comprehensive introduction how to extend the method to general multi-band Hamiltonians can be found in M.B. Zölfl et al., Phys. Rev. B**61**, 12810(2000).

[1] The interpolation scheme introduced to you last week is *not* systematic in the sense of perturbation theory, but rather a "recipe" to cure the problems away from particle-hole symmetry by hand.

2 The SIAM and the resolvents

Let me start by writing down the SIAM for a non-degenerate system consisting of a broad, non-interacting conduction band coupled to a localized state. In standard notation it reads

$$\begin{aligned} H &= \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \sum_\sigma (\epsilon_d + \frac{U}{2} d^\dagger_{-\sigma} d_{-\sigma}) d^\dagger_\sigma d_\sigma + \frac{1}{\sqrt{N}} \sum_{\vec{k}\sigma} (V_{\vec{k}} c^\dagger_{\vec{k}\sigma} d_\sigma + \text{h.c.}) \\ &= H_c + H_d + H_{dc} \end{aligned} \tag{1}$$

$c^{(\dagger)}_{\vec{k}\sigma}$ annihilates (creates) a conduction state with momentum $\vec{k}$ and spin σ, $\epsilon_{\vec{k}}$ is the dispersion relation for the band states; the $d^{(\dagger)}_\sigma$ annihilates (creates) a impurity state with spin σ and energy ϵ_d and U is the Coulomb energy one has to pay for doubly occupying the d state. Finally $V_{\vec{k}}$ describes the hybridization between the two subsystems. If W is the bandwidth of the conduction band, the relevant energies of the model are ϵ_d/W, U/W and $\Gamma_0/W = \Gamma(0)/W$, where

$$\Gamma(\omega) = -\Im m \frac{1}{N} \sum_{\vec{k}} \frac{|V_{\vec{k}}|^2}{\omega + i\delta - \epsilon_{\vec{k}}} = \frac{\pi}{N} \sum_{\vec{k}} |V_{\vec{k}}|^2 \delta(\omega - \epsilon_{\vec{k}}) \tag{2}$$

is the hybridization function.

For the typical strong coupling situation, the so-called Kondo limit, we have $|\epsilon_d/W|$,$(\epsilon_d + U)/W \gg \Gamma_0/W$. It thus seems reasonable to develop a perturbation expansion in the hybridization $V_{\vec{k}}$ or more precisely $\Gamma(\omega)$ rather than in U. It is however evident that such a perturbation theory will not lead to the conventional diagrammatic expansion with Feynman diagrams. The latter relies on the existence of Wick's theorem; since the unperturbed part of our problem will contain a two-particle interaction, namely the Coulomb repulsion in H_d, it is not bilinear in fermionic operators and therefore Wick's theorem does not apply for calculating expectation values of products of d operators. H_c on the other hand is bilinear in fermionic operators, so Wick's theorem may be used for this case. Thus, we will eventually be lead to something that may be called a mixed Feynman-Goldstone perturbation theory.

The first step now is to diagonalize H_d, i.e. find states $|M\rangle$ with $H_d|M\rangle = E_M|M\rangle$. For the current problem this step is rather trivial, but it becomes important in the case of a multi-band Hamiltonian. With these states we can write

$$H_d = \sum_M E_M |M\rangle\langle M|$$

and

$$H_{dc} = \frac{1}{\sqrt{N}} \sum_{\vec{k}\sigma MM'} (F^{MM'}_\sigma V_{\vec{k}} c^\dagger_{\vec{k}\sigma} |M'\rangle\langle M| + \text{h.c.})$$

with $F_\sigma^{MM'} = \langle M'|d_\sigma|M\rangle$ the transition matrix element. For the simple Hamiltonian H_d in (1) the result are the set of states $\{|0\rangle, |\sigma\rangle = d_\sigma^\dagger|0\rangle, |2\rangle = d_\uparrow^\dagger d_\downarrow^\dagger|0\rangle$ with energies $\{0, \epsilon_d, 2\epsilon_d + U\}$. The matrix elements are $F_\sigma^{\sigma 0} = 1$ and $F_\sigma^{2,-\sigma} = \sigma$.

As a second step we have to calculate the partition function of this system. Quite generally, we have $Z = \mathrm{Tr} e^{-\beta H}$, where $\beta = 1/k_\mathrm{B}T$ is the inverse temperature. The following idea is rather subtle, because it uses the fact that even for a macroscopically large system one still has a presumably very fine but nevertheless discrete spectrum for H. With this assertion one can write using the theorem on residues

$$Z = \oint\limits_{\mathcal{C}} \frac{dz}{2\pi i} e^{-\beta z} \mathrm{Tr} \frac{1}{z - H}$$

where the contour $\mathcal{C}$ surrounds all singularities of the integrand counterclockwise. Let us now perform a partial trace over the band states, i.e.

$$Z = Z_c^{(0)} \oint\limits_{\mathcal{C}} \frac{dz}{2\pi i} e^{-\beta z} \sum_M \frac{1}{Z_c^{(0)}} \sum_c \langle M|\langle c| \frac{1}{z - H} |c\rangle |M\rangle$$

where $|c\rangle$ is an eigenstate of H_c with $H_c|c\rangle = E_c|c\rangle$. Finally, we shift the integration by E_c for each summand in the trace over c and obtain

$$Z = Z_c^{(0)} \oint\limits_{\mathcal{C}} \frac{dz}{2\pi i} e^{-\beta z} \sum_M \langle M| \underbrace{\frac{1}{Z_c^{(0)}} \sum_c e^{-\beta E_c} \langle c| \frac{1}{z - H + E_c} |c\rangle}_{=:\, R(z)} |M\rangle \tag{3}$$

The quantity $R(z)$ is called *ionic resolvent operator*, its matrix elements $R_{MM'}(z)$ correspondingly *ionic resolvents* or *ionic propagators* and

$$Z_d := \oint\limits_{\mathcal{C}} \frac{dz}{2\pi i} e^{-\beta z} \sum_M \langle M|R(z)|M\rangle = \int\limits_{-\infty}^{\infty} d\omega e^{-\beta\omega} \sum_M \varrho_M(\omega) \tag{4}$$

is the partition function of the d-level. From the definition of $R(z)$ it is obvious that it is analytical everywhere except on the real axis. This property was used in the last step, where I deformed the contour in the standard fashion to obtain a spectral integral and introduced the spectral function $\varrho_M(\omega) = -\frac{1}{\pi}\Im m R_M(\omega + i\delta)$.

Up to now we have been exact and gained nothing except for a fancy way of writing the partition function. Before we continue to set up a perturbation expansion in H_{dc} for $R(z)$ let us try to get an idea about the behaviour of $R(z)$. Obviously, for $H_{dc} = 0$, we have $R(z) = 1/(z - H_d)$ and hence $\varrho_M(\omega) = \delta(\omega - E_M)$, i.e. $Z_d = \sum\limits_M e^{-\beta E_M}$. The situation is visualized in Fig. 1a. Since $\frac{1}{\beta} \ln Z_d$ is the contribution of the local system to the free energy, which should be finite, we further know that

- $\varrho_M(\omega) \sim e^{\beta\omega}$ as $\omega \to -\infty$ to ensure a finite integral in (4) and

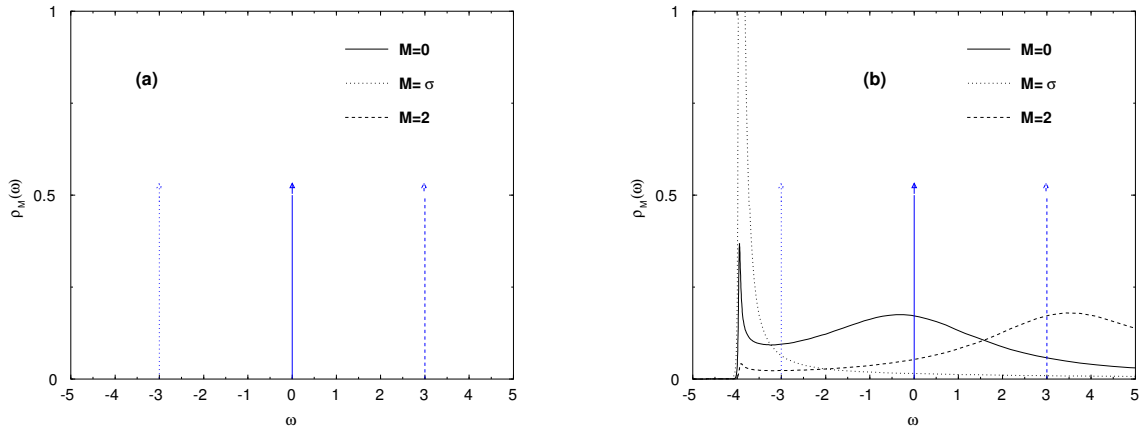


Figure 1: Typical behaviour of the spectral functions $\varrho_M(\omega)$ for the ionic resolvents for $H_{dc} = 0$ (a) and $H_{dc} \neq 0$ (b) for $\epsilon_d/W = -0.3$, $U/W = 0.9$ and $\Gamma_0/W = 0.1$

- there must exist a lower threshold E_s common to all resolvents below which this exponential decay of $\varrho_M(\omega)$ has to set in.

As $T \to 0$, this energy E_s becomes the ground state energy of the local system. This anticipated behaviour becomes apparent in Fig. 1b. Apart from a broadening (and slight shift) of the peaks at $E_0 = 0$, $E_\sigma = \epsilon_d$ and $E_2 = 2\epsilon_d + U$, all propagators show a lower threshold at $E_s \approx -0.39W$ with a very sharp peak in the spectra for the states $|0\rangle$ and $|\sigma\rangle$. While a peak in the spectrum of the state $|\sigma\rangle$ is expected, the aditional strong peak at the threshold in the spectrum of the state $|0\rangle$ is a signature of the Kondo effect in the SIAM, as will become clear later.

3 Resolvent perturbation theory and NCA

In the following let us denote $H_0 = H_c + H_d$. The desired perturbation theory is easily constructed from the observation that (proof left as an exercise)

$$\begin{aligned} \frac{1}{z - H + E_c} &= \frac{1}{z - H_0 + E_c} + \frac{1}{z - H_0 + E_c} H_{dc} \frac{1}{z - H + E_c} \\ &= \frac{1}{z - H_0 + E_c} + \\ &\quad \frac{1}{z - H_0 + E_c} H_{dc} \frac{1}{z - H_0 + E_c} + \\ &\quad \frac{1}{z - H_0 + E_c} H_{dc} \frac{1}{z - H_0 + E_c} H_{dc} \frac{1}{z - H_0 + E_c} + \dots \end{aligned} \tag{5}$$

Since we have to perform a trace over the band states to obtain $R(z)$, it is obvious that only terms with an even number in H_{dc} will contribute. For the simple SIAM (1) it is furthermore easy to show (exercise) that $R_{MM'}(z) = R_M(z)\delta_{MM'}$. This need not be the case for more complicated models, especially if H_{dc} mixes states with different quantum numbers; such a situation can e.g. occur in multi-band systems with hybridization processes between different orbital quantum numbers. In order to motivate the further evaluation of the perturbation series let us inspect the second order contribution to $R_0(z)$ in detail:

$$R_0^{(2)}(z) = \frac{1}{Z_c^{(0)}} \sum_c \langle c|e^{-\beta H_c} \frac{1}{z - H_c + E_c} \langle 0|H_{dc} \frac{1}{z - H_0 + E_c} H_{dc}|0\rangle \frac{1}{z - H_c + E_c}|c\rangle \tag{6}$$

Obviously, $\langle 0|H_{dc} = \frac{1}{\sqrt{N}} \sum_{\vec{k}\sigma} V_{\vec{k}} c^\dagger_{\vec{k}\sigma} \langle \sigma|$, and $H_{dc}|0\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{k}\sigma} V_{\vec{k}} c_{\vec{k}\sigma}|\sigma\rangle$. Noting furthermore (exercise) that

$$\begin{aligned} \frac{1}{z - H_0 + E_c} c_{\vec{k}\sigma} &= c_{\vec{k}\sigma} \frac{1}{z + \epsilon_{\vec{k}} - H_0 + E_c} \\ \frac{1}{z - H_0 + E_c} c^\dagger_{\vec{k}\sigma} &= c^\dagger_{\vec{k}\sigma} \frac{1}{z - \epsilon_{\vec{k}} - H_0 + E_c} \end{aligned} \tag{7}$$

it follows

$$R_0^{(2)}(z) = \frac{1}{z}\frac{1}{N} \sum_{\vec{k}\vec{k}'} \sum_\sigma V_{\vec{k}} V_{\vec{k}'} \frac{1}{Z_c^{(0)}} \sum_c \langle c|e^{-\beta H_c} c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma}|c\rangle \frac{1}{z + \epsilon_{\vec{k}'} - E_\sigma} \frac{1}{z} \tag{8}$$

Since

$$\frac{1}{Z_c^{(0)}} \sum_c \langle c|e^{-\beta H_c} c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma}|c\rangle = f(\epsilon_{\vec{k}}) \delta_{\vec{k}\vec{k}'}$$

where $f(x) = 1/(1 + e^x)$ is Fermi's function, we have

$$R_0^{(2)}(z) = \frac{1}{z}\frac{1}{N} \sum_{\vec{k}\sigma} \frac{|V_{\vec{k}}|^2 f(\epsilon_{\vec{k}})}{z + \epsilon_{\vec{k}} - E_\sigma} \frac{1}{z} \tag{9}$$

Using the relation (2), the $\vec{k}$-sum can be written as

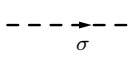
$$\frac{1}{N} \sum_{\vec{k}} |V_{\vec{k}}|^2 \ldots \to \int \frac{d\epsilon}{\pi} \Gamma(\epsilon) \ldots$$

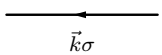
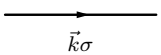
and we finally arrive at

$$R_0^{(2)}(z) = \frac{1}{z} \sum_\sigma \int \frac{d\epsilon}{\pi} \frac{\Gamma(\epsilon) f(\epsilon)}{z + \epsilon - E_\sigma} \frac{1}{z} \tag{10}$$

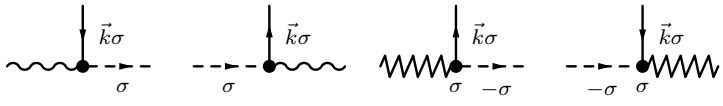
For a general contribution to (5) one follows the same scheme, i.e. first one moves all band operators to the left, each commutation with $1/(z - H_0 + E_c)$ leaving a

corresponding $\pm\epsilon_{\vec{k}}$ in the denominator. Finally, one has to calculate the thermal expectation value with respect to H_c of a product of band operators, which, due to Wick's theorem, breaks up into a sum over products of corresponding factors $f(\pm\epsilon_{\vec{k}})$. The transfer operators $|M\rangle\langle M'|$ together with the initial local state lead to a sequence of intermediate bare ionic propagators. The practical evaluation of such a contribution can most conveniently be done by means of diagrams. To this end we define symbols for the ionic propagators and the Fermi function:

$R_0^{(0)}(z) =$, $R_\sigma^{(0)}(z) =$  , $R_2^{(0)}(z) =$ 

$f(\epsilon_{\vec{k}}) =$  , $f(-\epsilon_{\vec{k}}) =$ 

In addition, we have the four basic vertices



A $2n$-th order diagram is then obtained as follows:

1. Draw on a straight horizontal line $2n$ dots and to the right of the rightmost and to the left of the leftmost dot a horizontal line denoting the propagator of the initial ionic state.

2. Fill the spaces between the dots with a sequence of intermediate ionic propagators as allowed by H_{dc}.

3. At each vertex, draw an incoming vertical band electron line, if the state to the left of the vertex has one electron less than the one to the right. Otherwise draw an outgoing vertical band electron line. Label the band electron lines such that at each vertex the spin is conserved.

4. Connect the band electron lines.

By building all possible sequences of intermediate states and all possible connections of band electron lines one generates all contributions to order $2n$. The translation of a diagram to an analytic expression proceeds as follows:

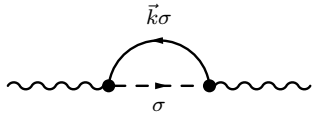
1. From right to left, assign to each ionic propagator of state $|M\rangle$ the quantity $R_M(z + \sum(\pm\epsilon_{\vec{k}_i}))$, where $\sum(\pm\epsilon_{\vec{k}_i})$ is the sum of the energies of all incoming $(-)$ and outgoing $(+)$ band electron lines to the right of this propagator.

2. Assign each band electron line pointing to the left (right) a factor $\frac{1}{N}|V_{\vec{k}}|^2 f(\epsilon_{\vec{k}})$ $(\frac{1}{N}|V_{\vec{k}}|^2 f(-\epsilon_{\vec{k}}))$.

3. Sum over all free internal spins and momenta $\vec{k}$.

4. Assign to each diagram a factor $(-1)^c$, where c is the number of crossing of band electron lines (each crossing means that one has to commutate two band operators to achieve the desired order for the Wick decomposition).

Within this diagrammatic language, the second order contribution $R_0^{(2)}(z)$ becomes

$R_0^{(2)}(z) =$ 

The translation of this diagram into an analytic expression and comparison to (10) is left as an exercise.

Just like in ordinary diagrammatic perturbation theory one can now define reducible diagrams

that can be separated into two diagrams by cutting one ionic line only, "self-energy" insertions

and vertex corrections

The concept of reducibility and self-energy insertions allows to reformulate the perturbation theory in terms of skeletons, i.e. diagrams that are irreducible in the above sense and do not contain self-energy insertions. In addition, one has to replace the bare ionic propagators by renormalized ones, i.e.

$$R_M^{(0)}(z) = \frac{1}{z - E_M} \rightarrow R_M(z) = \frac{1}{z - E_M - \Sigma_M(z)}$$

where the ionic self-energies $\Sigma_M(z)$ have been introduced. In the diagrams, renormalized ionic propagators are symbolized by double lines. The perturbation expansion for the self-energies $\Sigma_M(z)$ follows the same rules as for the propagators, with the exception that the external ionic legs, i.e. the left- and rightmost propagators, have to be cut off and that only skeletons must be considered. For example, to second order in H_{dc}, the self energies for the states $|0\rangle$, $|\sigma\rangle$ and $|2\rangle$ read

$$\Sigma_0^{(2)}(z) = \quad = \frac{1}{N} \sum_{\vec{k}\sigma} \frac{|V_{\vec{k}}|^2 f(\epsilon_{\vec{k}})}{z - E_\sigma + \epsilon_{\vec{k}} - \Sigma_\sigma(z + \epsilon_{\vec{k}})} \tag{11}$$

$\vec{k}\sigma$ (above), σ (below)

$$\Sigma_\sigma^{(2)}(z) = \quad + \quad = \frac{1}{N} \sum_{\vec{k}} \frac{|V_{\vec{k}}|^2 f(-\epsilon_{\vec{k}})}{z - E_\sigma - \epsilon_{\vec{k}} - \Sigma_0(z - \epsilon_{\vec{k}})} + \frac{1}{N} \sum_{\vec{k}\sigma} \frac{|V_{\vec{k}}|^2 f(\epsilon_{\vec{k}})}{z - E_\sigma + \epsilon_{\vec{k}} - \Sigma_2(z + \epsilon_{\vec{k}})} \tag{12}$$

$\vec{k}\sigma$ (left), $\vec{k}\sigma$ (right)

$$\Sigma_2^{(2)}(z) = \quad = \frac{1}{N} \sum_{\vec{k}\sigma} \frac{|V_{\vec{k}}|^2 f(-\epsilon_{\vec{k}})}{z - E_\sigma - \epsilon_{\vec{k}} - \Sigma_\sigma(z - \epsilon_{\vec{k}})} \tag{13}$$

$\vec{k}\sigma$ (above), $-\sigma$ (below)

The diagrams in equations (11)-(12) have a particular property, viz they contain no diagrams with crossing band electron lines. This feature has been used to coin the name **N**on-**C**rossing **A**pproximation (NCA) for this second order approximation of the ionic self-energies. They constitute a set of coupled nonlinear integral equations for the ionic self energies. It is interesting to note that the band states and the hybridization enter only in the combination

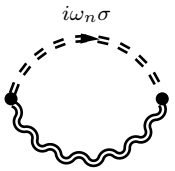
$$\frac{1}{N}\sum_{\vec{k}}|V_{\vec{k}}|^2 F(\epsilon_{\vec{k}}) = \int \frac{d\epsilon}{\pi}\Gamma(\epsilon)F(\epsilon)$$

This feature, which remains true in all orders, is particularly important for the application to the DMFT since the quantity $\Gamma(\epsilon)$ simply is the imaginary part of the Weiss field and thus can readily be calculated from the site excluded Green function.

Up to now this whole effort has been made in order to calculate the ionic propagators for the SIAM, i.e. the partition function only! Can one also extract dynamical quantities? The answer is, of course, yes. Let me outline the procedure for the one-particle Green function $G_\sigma(z) = \langle\langle d_\sigma; d_\sigma^\dagger\rangle\rangle_z$. Other dynamic correlation functions can be calculated accordingly. With the help of the Hubbard transfer operators $X_{MM'} = |M\rangle\langle M'|$ we can write

$$G_\sigma^d(z) = \langle\langle X_{0\sigma}; X_{\sigma 0}\rangle\rangle_z + \langle\langle X_{-\sigma,2}; X_{2,-\sigma}\rangle\rangle_z \tag{14}$$

If we formally identify $R_M(z) = \langle\langle X_{MM}\rangle\rangle_z$ with the "single-particle" propagator, then the expressions in (14) can be interpreted as "two-particle" Green functions. Stressing this analogy to standard perturbation theory a little bit further, the perturbation expansion of these "two-particle" propagators should consist of bubbles built from the $R_M(z)$. Although this reasoning is far from constituting a proof, it can serve as guideline. It actually turns out that the diagrammatic expression for the first term is

$\langle\langle X_{0\sigma}; X_{\sigma 0}\rangle\rangle_{i\omega_n} =$ 

$+\ldots$ (15)

and we have to add to the diagram rules

5) For a closed loop of ionic propagators let the integral operator

$$\frac{1}{Z_d}\oint_{\mathcal{C}}\frac{dz}{2\pi i}e^{-\beta z}$$

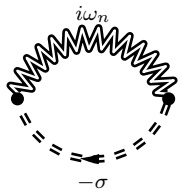
act on the result, where the contour $\mathcal{C}$ surrounds all singularities of the integrand counterclockwise.

For our expression (15) this leads to

$$\langle\langle X_{0\sigma}; X_{\sigma 0}\rangle\rangle_{i\omega_n} = \frac{1}{Z_d} \oint\limits_{\mathcal{C}} \frac{dz}{2\pi i} e^{-\beta z} R_0(z) R_\sigma(z + i\omega_n) \quad + \ldots \tag{16}$$

The ... represent higher order diagrams. However, if we use the NCA as approximation for the ionic self-energies, these diagrams can be neglected. Similarly, the second term in (14) yields

$$\langle\langle X_{-\sigma,2}; X_{2,-\sigma}\rangle\rangle_{i\omega_n} =$$



$$+ \ldots \tag{17}$$

$$= \frac{1}{Z_d} \oint\limits_{\mathcal{C}} \frac{dz}{2\pi i} e^{-\beta z} R_2(z + i\omega_n) R_{-\sigma}(z) \quad + \ldots$$

Again, within the NCA the higher order terms may be neglected.

Since the ionic resolvents are, just like ordinary Green functions, analytic everywhere except on the real axis, the contour integrals can be transformed into spectral integrals with the result

$$\langle\langle X_{0\sigma}; X_{\sigma 0}\rangle\rangle_{i\omega_n} = \frac{1}{Z_d} \int\limits_{-\infty}^{\infty} d\epsilon \; e^{-\beta\epsilon} \left(\varrho_0(\epsilon) R_\sigma(\epsilon + i\omega_n) - R_0(\epsilon - i\omega_n)\varrho_\sigma(\epsilon)\right) \tag{18}$$

and

$$\langle\langle X_{-\sigma,2}; X_{2,-\sigma}\rangle\rangle_{i\omega_n} = \frac{1}{Z_d} \int\limits_{-\infty}^{\infty} d\epsilon \; e^{-\beta\epsilon} \left(R_2(\epsilon + i\omega_n)\varrho_{-\sigma}(\epsilon) - \varrho_2(\epsilon) R_{-\sigma}(\epsilon - i\omega_n)\right) \tag{19}$$

It is quite instructive to think about these relations in connection with the ionic spectra of Fig. 1. Taking for instance the imaginary part of (18), after analytic continuation $i\omega_n \to \omega + i\delta$, yields

$$\frac{1}{\pi} \Im m \langle\langle X_{0\sigma}; X_{\sigma 0}\rangle\rangle_{\omega + i\delta} = \frac{1}{Z_d} \int\limits_{-\infty}^{\infty} d\epsilon \; e^{-\beta\epsilon} \left(\varrho_0(\epsilon)\varrho_\sigma(\epsilon + \omega) + \varrho_0(\epsilon - \omega)\varrho_\sigma(\epsilon)\right)$$

This is a convolution of the ionic spectra $\varrho_0(\omega)$ and $\varrho_\sigma(\omega)$ in Fig. 1 and in particular the existence of rather sharp structures at the common threshold will lead to a sharp resonance at $\omega \to 0$ – the well-known Abrikosov-Suhl resonance of the Kondo effect. Thus, the appearance of these sharp structures at the threshold in the ionic propagators is an extremely important physical aspect.

4 Some concluding remarks

In the previous sections I have introduced to you the concept of the resolvent perturbation theory and the NCA as an approximation within this formalism. The equations (11)-(13) and (18), (19) are in principle all one needs to calculate the thermodynamics and one-particle Green function for the SIAM (1). Actually coding (11)-(13) is not very complicated, as long as one takes care of the peculiar properties of the $\varrho_M(\omega)$, namely the existence of a common threshold with possibly rather sharp structures there (cf. Fig. 1), which are directly responsible for the physics of the model. More cumbersome is the expected exponential decay as $\omega \to -\infty$. While formally quantities like $e^{-\beta\epsilon}\varrho_M(\epsilon)$ are well defined in the limit as $\omega \to -\infty$, the numerical evaluation is ill defined, since one multiplies something exponentially small with something exponentially large; the result would of course be meaningless. To overcome this problem and do calculations for low temperatures, one introduces a new set of quantities, the so-called *defect propagators* or *negative energy propagators* defined as

$$\xi_M(\omega) = \frac{1}{Z_d} e^{-\beta\omega} \varrho_M(\omega) \tag{20}$$

With equations (11)-(13) one can then set up an additional set of self-consistency equations for those $\xi_M(\omega)$ and use them to evaluate the Green function etc. reliably even for low temperatures.

Since the NCA is an approximation it has, like any approximation, some deficiencies. The most spectacular deficiency is known under the name NCA-pathology and occurs for very low temperatures or very low energies, typically for $\omega,\ T < T_{\mathrm{K}}/10$, where T_{K} is the Kondo temperature or more generally the lowest energy scale in the problem. It leads to a violation of Fermi liquid properties. This means for example, that, while the imaginary part of the Green function itself has of course always a definite sign, the proper one-particle self-energy

$$\Sigma^d(z) = z - \epsilon_d - \frac{1}{N}\sum_{\vec{k}} \frac{|V_{\vec{k}}|^2}{z - \epsilon_{\vec{k}}} - G^d(z)^{-1}$$

may become acausal, i.e. $\Im m\Sigma(\omega + i\delta) > 0$ for some frequency range. This breakdown of course limits the applicability of the NCA to the DMFT, especially for "low temperatures". What "low" precisely means has to be clarified for each model and each paramter set independently. For example in the one-band Hubbard model at half filling and large U "low" actually means $T = 0$, since here an insulating state is realized and the effective low-energy scale is zero. On the other hand, for large U but a doping of say 30% "low" means something of the order of the band width W, since here the effective energy scale is of the order of W. Between these two extremes the breakdown occurs at lower and lower temperatures as one approaches half filling.