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Anderson impurity model: Vertex corrections within the finite U non-crossing approximation

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ABSTRACT

We revise the simplest possible approximations to solve numerically the vertex equations for the single impurity Anderson model (SIAM) within the finite U non-crossing approximation (UNCA), considering the self-energies at lowest order in the $1/N$ diagrammatic expansion. We introduce an approximation to the vertex corrections that includes the double energy dependence and compare it with an approximation (NCAf^{2}v) that neglects a second energy argument. Finally, we analyse the influence of the different approximations on the estimated Kondo scale for simple electronic models.

1. Introduction

One of the most studied models for strongly correlated electron systems is the single Anderson impurity model (SIAM), which can account for the Kondo regime, where conduction electrons scatter off a localized magnetic impurity and form a local singlet. Among the several methods proposed to solve the SIAM, the so-called non-crossing approximation (NCA) occupies a special place due to its computational simplicity. NCA can be thought of as a perturbative expansion with respect to $1/N$, where N is the degeneracy of the impurity levels. In particular, the NCA has been widely used to solve the SIAM in the infinite U limit, in which the double occupancy of the impurity site is prohibited. This scheme was successfully applied to theoretical models [1] and real materials [2], in order to analyse different physical properties, like magnetic susceptibilities, crystal-field splittings and spectral properties.

For $U \to \infty$ and large N degeneracy of the local states, NCA captures the Kondo temperature (T_K) scale and provides a qualitative description of the formation of the Kondo resonance when the temperature approaches the Kondo regime ($T \to T_K$) from above [1]. However, this is not the case for temperatures much lower than T_K ($T \ll T_K$), where NCA yields unphysical results. Furthermore, the T_K's are often underestimated in the infinite U limit.

The deficiencies that restrict the usefulness of NCA are greatly reduced if a finite on-site Coulomb repulsion U is considered together with the inclusion of vertex corrections [3]. While NCA in the infinite U limit contains all non-crossing diagrams up to the order $(1/N)^1$, with a finite U there appear crossing diagrams of order $(1/N)^0$ which have to be included at least through vertex corrections.

An extension of the NCA technique has been introduced by Haule et al. [5]. This extension, known as the symmetrized finite-U NCA (SUNCA), treats the fluctuation processes into the empty and into the doubly occupied intermediate states on an equal footing, by means of a proper symmetrization of the vertex corrections. Although SUNCA provides the correct energy scale, its practical computation is not easy due to the double energy dependence of the vertex functions, even considering a very simple function for the conduction electron band. Recently, Sakai et al. [4] have introduced the NCAf^{2}v approximation, that simplifies the vertex functions by neglecting its second energy argument.

In this contribution we apply an approximation to the vertex functions that includes the double energy dependence in two different ways within U non-crossing approximation (UNCA), working at lowest order in $1/N$ and study the influence of this treatment on T_K.

2. Auxiliary particle representation and the large-N limit

The Anderson impurity model with finite U is described by the Hamiltonian

$$\hat{H} = \sum_{km} \varepsilon_{km} \hat{c}^{\dagger}_{km} \hat{c}_{km} + \sum_{m} \varepsilon_m \hat{f}^{\dagger}_m \hat{f}_m + U \sum_{m<n} \hat{N}_m \hat{N}_n + \sum_{km} (V_{km} \hat{f}^{\dagger}_m \hat{c}_{km} + V^{*}_{km} \hat{c}^{\dagger}_{km} \hat{f}_m), \quad (1)$$

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where the indices m, n label the quantum numbers of the impurity levels. The operators $\hat{c}^{\dagger}_{km}$, $\hat{f}^{\dagger}_{m}$ create a conduction and a localized electron state, respectively, and $\hat{N}_m = \hat{f}^{\dagger}_{m}\hat{f}_m$ is the f-number operator. The last term represents the hybridization between conduction and localized electrons, and V_{km} are the hybridization matrix elements. In the auxiliary particle representation the Hamiltonian becomes

$$\begin{aligned}\hat{H} = &\sum_{km} \varepsilon_{km}\hat{c}^{\dagger}_{km}\hat{c}_{km} + \sum_{m} \varepsilon_m \hat{s}^{\dagger}_{m}\hat{s}_m + \sum_{m<n} (\varepsilon_m + \varepsilon_n + U)\hat{d}^{\dagger}_{mn}\hat{d}_{mn} \\ &+ \sum_{km} (V_{km}\hat{s}^{\dagger}_{m}\hat{b}\hat{c}_{km} + \text{h.c.}) \\ &+ \sum_{kmm'(m'\neq m)} (V_{km}\hat{d}^{\dagger}_{mm'}\hat{s}_{m'}\hat{c}_{km} + \text{h.c.}),\end{aligned} \tag{2}$$

where the operators $\hat{b}$, $\hat{s}_m$ and $\hat{d}_{mn}$ represent the vacuum, single and double occupied states, respectively.

In the context of the NCA, the simplest picture that contains the two elementary spin-flip scattering processes, involving empty and doubly occupied intermediate states, respectively, is obtained with the inclusion of vertex corrections in a large-N expansion, retaining only the lowest order diagrams in $(1/N)$, that is, $(1/N)^0$ [6], see Figs. 1 and 2. The order of the diagrams is clarified in Ref. [7]. In this approximation, called from now on UNCA$^{(0)}$, the self-energy of the heavy boson propagator vanishes. Consequently, Green's function of the doubly occupied states can be written in the simple form $\mathcal{G}^{-1}_{mn}(z) = z - \varepsilon_m + \varepsilon_n + U$. On the other hand, the self-energy for the pseudo-fermion propagators contains only the contribution coming from the heavy boson while the self-energy of the light boson propagator contains vertex corrections.

The final result is the following set of non-coupled equations for the self-energies, $\Sigma_m(\omega)$ and $\Sigma_b(\omega)$ and for the vertex correction $\Lambda_m(\omega, \varepsilon)$:

$$\Sigma_m(\omega) = \sum_{m'\neq m} \int \frac{d\varepsilon}{\pi} f(\varepsilon)\Gamma_{m'}(\varepsilon)\mathcal{G}_{mm'}(\omega + \varepsilon), \tag{3}$$

$$\begin{aligned}\Lambda_m(\omega, \varepsilon) = 1 + \sum_{m'\neq m} \int \frac{d\varepsilon'}{\pi} &\Lambda_{m'}(\omega, \varepsilon')f(\varepsilon')\Gamma_{m'}(\varepsilon') \\ &\times \mathcal{G}_{m'}(\omega + \varepsilon')\mathcal{G}_{mm'}(\omega + \varepsilon' + \varepsilon),\end{aligned} \tag{4}$$

$$\Sigma_b(\omega) = \sum_{m} \int \frac{d\varepsilon}{\pi} f(\varepsilon)\Gamma_m(\varepsilon)\Lambda_m(\omega, \varepsilon)\mathcal{G}_m(\omega + \varepsilon). \tag{5}$$

Here, $f(\varepsilon)$ is the Fermi function and $\Gamma_m(\varepsilon) = \pi\sum_k V_{km}V^{*}_{km}\delta(\varepsilon - \varepsilon_{km})$ are the hybridization functions between the conduction electron band and the impurity states, m. It is easy to see that, using the self-energies for the pseudo-fermions computed from (3), one can obtain the vertex functions through (4). Finally, the self-energy for the light boson propagator is obtained directly from (5). The crucial advantage of this scheme is that the system of equations does not need to be solved in a self-consistent way after having performed some approximation to vertex equation.

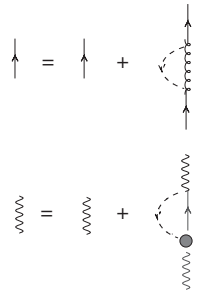

Fig. 1. Dyson's equation for the pseudo-fermion and light boson propagators within the non-crossing approximation up to $(1/N)^0$ order. The full, wiggly, dashed, and curly lines stand for pseudo-fermion, light boson, conduction electron, and heavy boson propagators, respectively. The bold (light) lines represent the full (free) propagators. The big dot represents the vertex function.

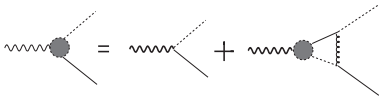

Fig. 2. Diagrammatic representation of the integral equation for the vertex function in the ladder approximation.

3. Approximations to the vertex functions

A complete solution of the set of integral equations (4) implies a lot of computational effort, hence, some simplification could be useful in view of future extensions of these impurity solvers within Dynamical Mean Field Theory (DMFT). In this section we compare the simplest possible approximations to solve numerically the vertex equations and analyse their influence on the calculated Kondo temperature for different values of the on-site Coulomb repulsion U. Recently, Sakai et al. [4] have pointed out that the exchange coupling due to virtual transitions to the doubly occupied state can be obtained even when the ε energy dependence of the vertex function $\Lambda_m(\omega, \varepsilon)$ is neglected,

$$\Lambda_m(\omega, \varepsilon) \to \Lambda^{(a)}_m(\omega). \tag{6}$$

In this way, (4) and (5) are simplified as follows:

$$\Lambda^{(a)}_m(\omega) + \sum_{m'\neq m} \frac{\Lambda^{(a)}_{m'}(\omega)}{\varepsilon_m + U} F_{m'}(\omega) = 1, \tag{7}$$

$$F_m(\omega) = \int \frac{d\varepsilon}{\pi} f(\varepsilon)\Gamma_m(\varepsilon)\mathcal{G}_m(\omega + \varepsilon), \tag{8}$$

$$\Sigma^{(a)}_b(\omega) = \sum_{m} \Lambda^{(a)}_m(\omega)F_m(\omega). \tag{9}$$

The second energy dependence, ε, can be recovered in the vertex functions, avoiding at the same time to solve the integral equations, if we interchange energy variables in the integrand of (4) as follows:

$$\Lambda_{m'}(\omega, \varepsilon') \to \Lambda^{(b)}_{m'}(\omega, \varepsilon). \tag{10}$$

This procedure is justified under the assumption that the ε dependence of the vertex functions is relatively weak [6]. Under this approximation, the vertex equations (4) become a set of linear algebraic equations for given values of ω and ε,

$$\begin{aligned}\Lambda^{(b)}_m(\omega, \varepsilon) = 1 + \sum_{m'\neq m} &\Lambda^{(b)}_{m'}(\omega, \varepsilon) \int \frac{d\varepsilon'}{\pi} f(\varepsilon') \\ &\times \Gamma_{m'}(\varepsilon')\mathcal{G}_{m'}(\omega + \varepsilon')\mathcal{G}_{mm'}(\omega + \varepsilon' + \varepsilon).\end{aligned} \tag{11}$$

To further simplify the integral, we can evaluate the doubly occupied Green's functions at some specific value of ω, as before. The energy dependence on ε of the doubly occupied Green's functions could be kept if we set $\omega + \varepsilon' = \varepsilon_{m'}$,

$$\mathcal{G}_{mm'}(\omega + \varepsilon' + \varepsilon)|_{\omega+\varepsilon'=\varepsilon_{m'}} = \frac{-1}{\varepsilon_m + U - \varepsilon - i\eta}.$$

The final form of the vertex function is again obtained from a set of linear algebraic equations. This and the corresponding self-energy of the boson propagator are given, respectively, by

$$\Lambda^{(b)}_m(\omega, \varepsilon) + \sum_{m'\neq m} \frac{F_{m'}(\omega)\Lambda^{(b)}_{m'}(\omega, \varepsilon)}{\varepsilon_m + U - \varepsilon - i\eta} = 1, \tag{12}$$

$$\Sigma_b^{(b)}(\omega) = \sum_m \int \frac{d\varepsilon}{\pi} f(\varepsilon)\Gamma_m(\varepsilon)\Lambda_m^{(b)}(\omega,\varepsilon)\mathcal{G}_m(\omega+\varepsilon). \quad (13)$$

The vertex function can be further improved by evaluating the doubly occupied Green's functions (11) at the value of $\omega+\varepsilon'$ that most likely maximizes the rest of the integrand, that is, $\omega+\varepsilon' \sim \tilde{\varepsilon}_{m'}$, where $\tilde{\varepsilon}_{m'}$ are the renormalized poles of the pseudo-fermion Green's functions. From (3), we compute directly the spectral functions $\rho_m(\omega) = -(1/\pi)\mathrm{Im}\,\mathcal{G}_m(\omega)$. The poles of $\rho_m(\omega)$ are the energies $\tilde{\varepsilon}_m$ that satisfy $\tilde{\varepsilon}_m - \varepsilon_m - \Sigma_m(\tilde{\varepsilon}_m) = 0$.

If we set $\omega+\varepsilon' = \tilde{\varepsilon}_{m'}$ in the argument of the doubly occupied Green's functions in (11), the vertex functions and the boson self-energy are then given, respectively, by

$$\Lambda_m^{(c)}(\omega,\varepsilon) + \sum_{m'\neq m} \frac{F_{m'}(\omega)\Lambda_{m'}^{(c)}(\omega,\varepsilon)}{\tilde{\varepsilon}_m + U - \varepsilon - i\eta} = 1, \quad (14)$$

$$\Sigma_b^{(c)}(\omega) = \sum_m \int \frac{d\varepsilon}{\pi} f(\varepsilon)\Gamma_m(\varepsilon)\Lambda_m^{(c)}(\omega,\varepsilon)\mathcal{G}_m(\omega+\varepsilon). \quad (15)$$

In the following section we analyse the effect of the different approximations for the vertex functions (a, b and c) described above on the Kondo temperature, within a simple model. We use a constant and degenerate hybridization intensity $\Gamma_m(\varepsilon) = 0.15$ eV for $-B<\varepsilon<B$ and 0 otherwise. Here B is the half bandwidth and we set $B = 3$ eV. The degeneracy N in this section is taken to be equal to 6 and we set $\varepsilon_m = -2$ eV for all m. With these parameters we solve the UNCA$^{(0)}$ set of equations within different vertex approximations and obtain the spectral functions for the boson ($\rho_b(\omega,T)$) and pseudo-fermions ($\rho_m(\omega,T)$), in the $T\to 0$ limit, in order to calculate the T_K. This temperature is obtained from the difference between the lowest pole of $\rho_b(\omega)$ and the corresponding one for $\rho_m(\omega)$ [1]. We obtain T_K for different values of the Coulomb interaction U and within the different approaches to the vertex corrections previously introduced, taking $U = 5$, 10 and 100 eV. We consider that $U = 100$ eV already gives the $U\to\infty$ limit. The $U\to\infty$ limit is characterized by $\Lambda_m = 1$ (to leading order in the large-N expansion) and this limit is recovered perfectly with $U = 100$ eV. The results are shown in Table 1.

In Fig. 3 we compare the real parts of the vertex functions for approximations (a) and (c) as a function of ω. To plot the function $\mathrm{Re}\,\Lambda_m^{(c)}(\omega,\varepsilon)$, we set its second argument equal to the value of the lowest pole of the boson spectral function, E_0. From this figure it can be seen that the different approximations to the vertex corrections agree qualitatively among themselves. As it can be drawn from Table 1, for a given U all the approximations give the same order of magnitude for the Kondo scale. However, there is a quantitative difference in the calculated T_K's that can go up to 30%.

On the other hand, in Fig. 4 we plot $\Lambda_m^{(b)}(E_0,\varepsilon)$ and $\Lambda_m^{(c)}(E_0,\varepsilon)$ as functions of their second arguments. For ω we have chosen, just as an example, the value of the boson propagator pole. Both curves seem to have been rigidly shifted one with respect to the other, as a consequence of the different argument values in which Green's functions of the heavy bosons are evaluated in the vertex corrections. These differences show up in the values obtained for T_K.

Comparing Figs. 3 and 4, it can be observed that, as a function of ω, there is an important variation of the functions in a wide energy range while, as a function of ε, the energy window of variation is narrower. However, in this last case the amplitude of the variation is up to five times greater than in the first one. From this fact, it is clear that the second dependence in energy cannot be neglected for $U = 5$ eV, if precise values of T_K are desired.

Table 1
Results for the Kondo temperature, in Kelvin, obtained from different approximations to the vertex functions.

U (eV)	$T_K^{(a)}$	$T_K^{(b)}$	$T_K^{(c)}$
5	260	208	183
10	85	81	77
100	33	34	31

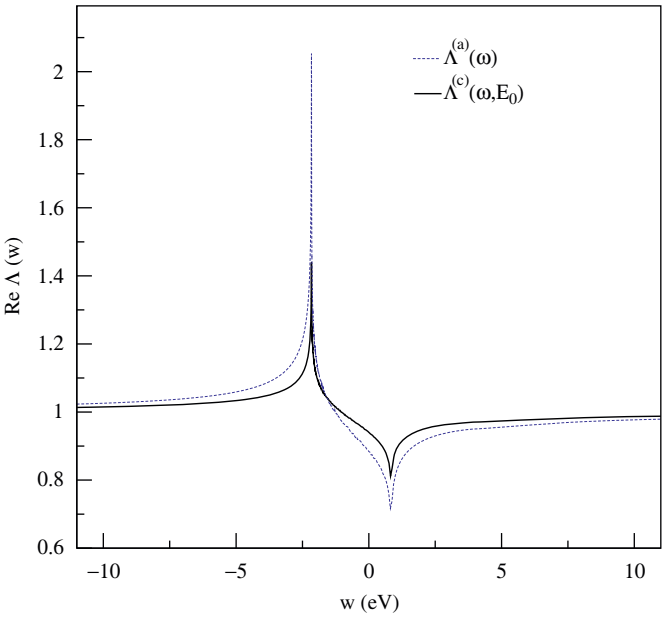

Fig. 3. Real part of the vertex functions as a function of ω for $U = 5$ eV. The second argument of $\Lambda_m^{(c)}(\omega,\varepsilon)$ is evaluated at the pole of the boson spectral function, E_0.

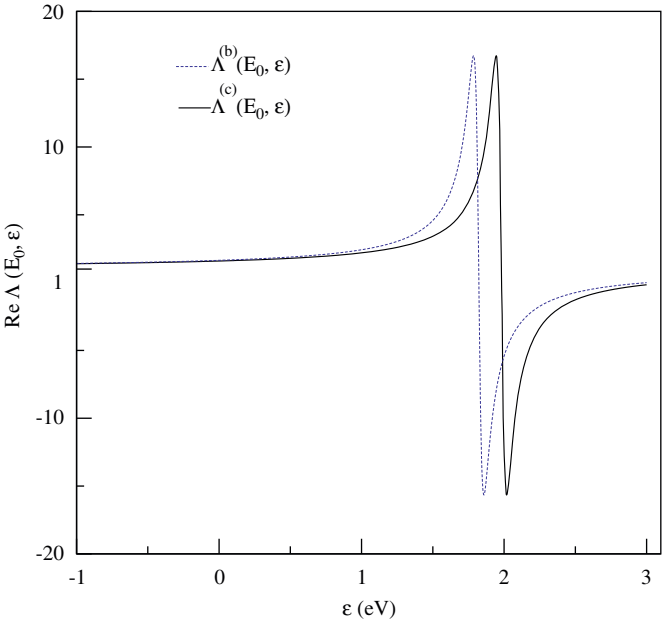

Fig. 4. Real part of the vertex functions in the (b) and (c) approximations as a function of ε for $U = 5$ eV. The first argument of both functions is evaluated at the pole of the boson spectral function, E_0.

4. Discussion and conclusions

In this work, we have extended the $\Lambda_m^{(a)}(\omega)$ approximation to the vertex functions introduced by Sakai et al. [4], including the second energy variable in two different ways $\Lambda_m^{(b)}(\omega,\varepsilon)$ and $\Lambda_m^{(c)}(\omega,\varepsilon)$. We have calculated and compared the T_K obtained using these three different approximations. Our results confirm that, even when the $\Lambda_m^{(a)}$ approximation gives the correct Kondo energy scale, the double dependence in energy cannot be disregarded for small U values.

Summarizing, this work presents an analysis of the different corrections that can be made on the vertex functions within the finite U NCA showing, quantitatively, the importance of its double energy dependence on the Kondo temperature.

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[7] The fermion self-energy coming from vacuum state is given by $\Sigma_m(\omega) = \int(d\varepsilon/\pi)f(-\varepsilon)\Gamma_m(\varepsilon)\mathcal{G}_b(\omega-\varepsilon)$ and there is no sum over any flavor m'. Therefore this contribution results to be the order $1/N$ with respect to the one given in Eq. (3).