Magnetic Impurity in a Metal with Correlated Conduction Electrons: 
An Infinite Dimensions Approach

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We consider the Hubbard model with a magnetic Anderson impurity coupled to a lattice site. In the case of infinite dimensions, one-particle correlations of the impurity electron are described by the effective Hamiltonian of the two-impurity system. One of the impurities interacts with a bath of free electrons and represents the Hubbard lattice, and the other is coupled to the first impurity by the bare hybridization interaction. A study of the effective two-impurity Hamiltonian in the frame of the 1/N expansion and for the case of a weak conduction-electron interaction (small $U$) reveals an enhancement of the usual exponential Kondo scale. However, an intermediate interaction ($U/D = 1 - 3$), treated by the variational principle, leads to the loss of the exponential scale. The Kondo temperature $T_K$ of the effective two-impurity system is calculated as a function of the hybridization parameter and it is shown that $T_K$ decreases with an increase of $U$. The non-Fermi-liquid character of the Kondo effect in the intermediate regime at the half filling is discussed.

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I. INTRODUCTION

The physics of a magnetic impurity embedded in a metal with non-interacting conduction electrons is well now understood and documented [1,2]. Its characteristic feature is the many-body non-perturbative renormalization of the impurity-host interaction which turns to be strong at temperatures lower than the Kondo temperature $T_K$. This $T_K$ is an exponential in the inverse impurity-host coupling parameter. Recently both the Kondo-spin model [3,4,5] and the Anderson impurity model were studied [6,7,8] in one-dimensional systems with interacting conduction electrons. It turns out that the influence of the conduction-electron interaction (CEI) on the Kondo effect in a Luttinger liquid is not trivial: the Kondo screening of the impurity spin may also be possible for a ferromagnetic exchange coupling $J$ [9]; for a sufficiently large CEI, a power-law dependence of $T_K$ upon $J$ replaces the usual exponential law [10]; in the case of the Anderson model a small CEI enhances $T_K$ (just because more conduction electrons effectively participate in the interaction with an impurity) but this trend changes for a large enough CEI and $T_K$ falls due to the suppression of the charge transfer between the impurity and the lattice [11]. A generalized Anderson impurity model for a Luttinger liquid which was introduced in [12] and studied there by the renormalization-group techniques shows a rich phase diagram in the parameter space.

The interest in the Kondo effect in the interacting host for 2d and 3d was sparked by the discovery of heavy-fermions in $Nd_{2−x}Ce_xCuO_4$ [13,14]. The Schrieffer-Wolff transformation for the magnetic impurity coupled to the Hubbard host was discussed in [15] and the Kondo-spin model in the above host was investigated in [16]. The Anderson impurity model for interacting conduction electrons was considered too. Its ground state energy was calculated in the frame of the 1/N expansion [17] and the Non-Crossing-Approximation (NCA) theory was generalized to the interacting case [18]. As was shown first in [19], two-particle Green’s functions of host eletrons (vertex corrections) are an essential ingredient of the correct theory of the Kondo effect in the interacting host. Actual calculations were carried out in the lowest order in the Hubbard $U$ approximation and an enhancement of $T_K$ was obtained both for the Kondo-spin model [20] and the Anderson [21,22]. However, contrary to the 1d case, the theory of the Anderson impurity in 2d and 3d is not developed sufficiently beyond the case of the weak host interaction.

It is much easier to treat strongly interacting systems in the limit of infinite dimensions, $d → ∞$ [23]. We use here the Local Impurity Self Consistent Approximation (LISA) [24] to map the Hubbard host with an Anderson impurity to a simpler model. As we show, this system is a two-impurity system in which one of the impurities represents the Hubbard host and the other
is the original (bare) impurity coupled solely to the first impurity by the bare hybridization interaction. In the LISA approach the effective two-impurity Hamiltonian preserves all the features of the one particle Green’s function of the impurity electron. Using for simplicity the Bethe lattice in its large connectivity limit, we show by employing the NCA for a weak CEI that the effective two-impurity Hamiltonian leads to an enhanced Kondo scale $T_K$ in full agreement with [17,18]. For an intermediate CEI we solve the effective two-impurity Hamiltonian by using the variational principle, and calculate numerically the singlet and the triplet ground state energies. Their difference is no longer exponential in the inverse coupling parameter. For a small hybridization interaction it is linear in this parameter (i.e., in the Anderson width) and eventually exhibits a maximum. The latter appears at values of the Anderson width which are less than the impurity energy level. Moreover, in the intermediate range of CEI this difference decreases with the increase of $U$. This dependence of $T_K$ upon the strength of CEI indicates that for intermediate values of $U$ the suppression of the charge transfer between the impurity and host starts to be a dominant factor in the CEI influence on the singlet formation.

The paper is organized as follows: in section II the two-impurity effective Hamiltonian is derived, section III deals with a weak CEI and section IV is devoted to the intermediate one. Discussions and Conclusions are in section V.

II. THE EFFECTIVE TWO-IMPURITY HAMILTONIAN

We consider the Hubbard model with a magnetic impurity coupled to a lattice site. The Hamiltonian is

$$ H = H_h + H_{imp} + H_{int} $$  \hspace{1cm} (1)

The first term is the Hubbard Hamiltonian for the host lattice, the second is the impurity Hamiltonian and the third is the hybridization interaction between the impurity and the host. Figure [3] illustrates the system for the case of a Bethe lattice but the mapping discussed in this section is not limited to the Bethe type of lattice only. The Hubbard Hamiltonian for the host is

$$ H_h = - \sum_{ij\sigma}(t_{ij} + \mu)c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2} \sum_{i\sigma \neq \sigma'} n_{i\sigma} n_{i\sigma'} $$  \hspace{1cm} (2)

The operators $c_{i\sigma}^\dagger$ ( $c_{i\sigma}$) create (annihilate) conduction electrons in spin states $\sigma$ at site $i$ and the corresponding density operators are $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. The hopping between different sites $i$ and $j$ is given by $t_{ij}$, $\mu$ is the chemical potential while $U$ is the Coulomb repulsion between two conduction electrons at the same site $i$. The impurity Hamiltonian is given by

$$ H_{imp} = \sum_{\sigma} \epsilon_f n_{f\sigma} + \frac{U_f}{2} \sum_{\sigma \neq \sigma'} n_{f\sigma} n_{f\sigma'} $$  \hspace{1cm} (3)

Here $n_{f\sigma} = f_{\sigma}^\dagger f_{\sigma}$ is the density operator for the impurity electron and $f_{\sigma}^\dagger$ its creation (annihilation) operators. The impurity level $\epsilon_f$ is taken here relative to the chemical potential and the Coulomb repulsion between two f-electrons at the impurity site is $U_f$. The hybridization interaction is chosen in the simple form:

$$ H_{int} = V \sum_{\sigma} (f_{\sigma}^\dagger c_{0\sigma} + h.c.) $$  \hspace{1cm} (4)

and 0 denotes the lattice site to which the impurity is coupled. We will assume a half-filled case, $<n_{i\uparrow}>=<n_{i\downarrow}>=1/2$. Our treatment of the Hamiltonian of Eq. (3) is based on the results of the LISA approach to the Hubbard model in infinite dimensions. Below we formulate some of the results which we use for the Anderson impurity in the Hubbard host.

A. A short overview of the LISA approach to the Hubbard model, $d \to \infty$

Following [22] we recall briefly the dynamical mean-field theory of the Hubbard model. In the limit of infinite dimensions the one-particle Green’s function for the Hubbard Hamiltonian, Eq. (2), is local [20]:

$$ G_{i\sigma}(i\omega_n) = \delta_{ij} G_{i\sigma}(i\omega_n) $$  \hspace{1cm} (5)

and the usual definition

$$ G_{i\sigma}(i\omega_n) = -\int_0^\beta d\tau <T_{c_{i\sigma}(\tau)} c_{i\sigma}^\dagger(\tau')> e^{i\omega_n(\tau-\tau')} $$

with $\omega_n = (2n+1)\pi \beta^{-1}$ is used everywhere. For the paramagnetic phase which is assumed in further discussions and in the absence of the f-impurity we may omit indices in the local Green’s function of the Hubbard model, Eq. (3). The latter may be calculated by the means of the effective action $S_{eff}$:

$$ S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\sigma} \epsilon_{0\sigma}(\tau) G_{0\sigma}^{-1}(\tau-\tau') c_{0\sigma}(\tau') + \frac{U}{2} \int_0^\beta d\tau n_{0\uparrow}(\tau) n_{0\downarrow}(\tau) $$  \hspace{1cm} (6)

Here Grassmann variables are used and the effective action is obtained by tracing out all fermions except for a site labeled by 0 in the partition function:

$$ e^{-S_{eff}} = \int \prod_{\beta \neq 0} Dc_{i\sigma}^\dagger Dc_{i\sigma} e^{-S} $$  \hspace{1cm} (7)

where $S$ is the action of the Hubbard model, Eq. (2). The dynamic mean-field Green’s function $G_0(\tau-\tau')$, Eq. (3),
is connected to the local Green’s function of the Hubbard model \[22\]. The latter may be calculated by the self-consistent iteration procedure via the use of the definition:

\[
G(\tau - \tau\prime) = \frac{\prod_{\sigma\tau} Dc_{\tau\sigma}^\dagger Dc_{\tau\sigma} e^{-S_{\text{eff}}} [-Tc_{\tau\sigma}(\tau)c_{\tau\sigma}(\tau\prime)]}{\prod_{\sigma\tau} Dc_{\tau\sigma}^\dagger Dc_{\tau\sigma} e^{-S_{\text{eff}}}}
\]

(8)

The dynamic mean-field Green’s function \(G_0\) may be viewed as the bare Green’s function of the impurity electron in the auxiliary Anderson impurity model \[22\]. In the latter the orbital \(c_{\tau\sigma}^0\) appears as the Anderson impurity and it possesses both the local energy level equal to \(-\mu\) and the on-site Coulomb interaction equal to the same interaction as in the original Hubbard model, Eq. \([4]\). This fictitious Anderson impurity (not to be confused with the original one in Eqs. \([4, 3]\)) is coupled to a free-electron bath and the appropriate Hamiltonian reads \[22\]:

\[
H_{AM} = \sum_{i\sigma} \tilde{\varepsilon}_i a_i^\dagger a_i + \sum_{i\sigma} V_i (a_i^\dagger c_{0\sigma} + h.c.) - \mu \sum_{\sigma} c_{0\sigma}^\dagger c_{0\sigma} + \bar{U}_{00} n_{0\downarrow}
\]

(9)

The action for the Hamiltonian \(H_{AM}\) is like \(S_{\text{eff}}\) in Eq. \([4]\) with the dynamic mean-field Green’s function \(G_0(\tau - \tau\prime)\) given in the explicit form as a function of the parameters \(\tilde{\varepsilon}_i\) and \(V_i\). Using the Fourier transform of \(G_0(\tau - \tau\prime)\) we have \[22\]:

\[
G_0(i\omega_n) = \frac{1}{i\omega_n + \mu - \int_{-\infty}^{\infty} d\epsilon \frac{\Delta(\epsilon)}{i\omega_n - \epsilon}};
\]

\[
\Delta(\epsilon) = \sum_{i\sigma} V_i^2 \delta(\epsilon - \tilde{\varepsilon}_i)
\]

(10)

Due to the structure of the Bethe lattice which disconnects itself into two separate parts by removing a lattice site, the dependence between \(G_0(\omega_n)\) and the local Green’s function for the original Hubbard model \(G(\omega_n)\) is simplest. It may be shown \[22\] that

\[
G(\omega_n) = \frac{1}{t^2} \int_{-\infty}^{\infty} d\epsilon \frac{\Delta(\epsilon)}{i\omega_n - \epsilon}
\]

(11)

Here the n.m. hopping is assumed in the Hamiltonian \(H_h\), Eq. \([2]\): \(t_{ij} = t/\sqrt{d}\) for nearest neighbors and zero otherwise. Eqs. \([10, 11]\) together with Eq. \([8]\) permit to find \(\Delta(\epsilon)\). For the non-interacting case, \(U = 0\), the function \(\Delta(\epsilon)/t^2\) is just the density of states of the Bethe lattice, \(\rho(\epsilon)\) \[22\]:

\[
\rho(\epsilon) = \frac{1}{\pi t} \sqrt{1 - \frac{\epsilon^2}{2t^2}}, \abs{\epsilon} \leq 2t
\]

(12)

For finite values of \(U\) calculations were done in \[25\] (see also \[22\]) and Figure 3 from \[25\] illustrates results of these calculations. We are interested in the paramagnetic phase and to avoid Néel order a quenched disorder may be introduced in the n. n. hopping. The details are presented in \[22\] and we only note that by this generalisation neither the Bethe lattice semicircular density of states, Eq. \([12]\), nor other local properties are changed.

B. The cavity method for the Anderson impurity in the Hubbard host

It is clear that the Anderson impurity being coupled to the site 0 destroys the equivalency between different sites of the Hubbard host. Let the index \(i_m, m = 1, 2, \ldots\) denotes one of equivalent neighbors of the site 0 on the Bethe lattice, \(m\) bonds away from it. Taking a site \(i_m\) as the “cavity place” for the dynamical mean-field treatment and tracing out all fermions but \(c_{i_m}\) the effective action \(S_{\text{eff}}[c_{i_m}^\dagger c_{i_m}]\) may be calculated in close analogy with the pure Hubbard model. This action defines all local properties of the \(i_m\)-site and its form exactly as in Eq. \([4]\) with the mean-field Green’s function \(G_0^{(i_m)}(\tau - \tau\prime)\) instead of the \(G_0(\tau - \tau\prime)\). By straightforward calculations \[27\] it may be shown that

\[
G_0^{(i_m)}(i\omega_n) = i\omega_n + \mu + \sum_{i\text{n.n. of } i_m \neq 0} \frac{t^2}{d} G_{ii}(i\omega_n) + \frac{t^2}{d} G_{00}(i\omega_n)
\]

(13)

It is obvious that for the case of infinite dimensions Eqs. \([13]\) are solved by the \(G_0(\omega_n)\) and \(G(\omega_n)\), Eqs. \([10, 11]\) of the pure Hubbard model. In fact an impurity can not break the equivalency between different sites \(i \neq 0\) of the Hubbard host and does not influence their local properties.

To calculate the correlation function of the impurity electron we trace out all fermions except two, \(c_{i_m}^\dagger c_{i_m}\) and \(f_{i_m}^\dagger f_{i_m}\), in the partition function and define the effective action \(S_{\text{eff}}[0, f]\):

\[
e^{-S_{\text{eff}}[0, f]} = \int \prod_{i\neq 0, \sigma} Dc_{i\sigma}^\dagger Dc_{i\sigma} e^{S}
\]

\[
S = \int_0^\beta d\tau \left( \sum_{i\sigma} c_{i\sigma}^\dagger(\tau) \partial_\tau c_{i\sigma}(\tau) + \sum_{\sigma} f_{i_m}^\dagger(\tau) \partial_\tau f_{i_m}(\tau) + H_h(\tau) + H_{\text{imp}}(\tau) + H_{\text{int}}(\tau) \right)
\]

(14)

Here \(H_h, H_{\text{imp}}, H_{\text{int}}\) are from Eqs. \([2, 3, 4]\) respectively. Repeating the same calculations which lead to \(S_{\text{eff}}\)
of Eq. (6) for the Hubbard model without impurity \[22\], we obtain for the Bethe lattice of infinite connectivity

\[
S_{\text{eff}}[0, f] = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma \epsilon_{\text{b},\sigma}(\tau)G_0^{-1}(\tau - \tau') + \int_0^\beta d\tau (Un_{0\uparrow}(\tau)n_{0\downarrow}(\tau) + \sum_\sigma f_{\text{f},\sigma}(\tau) \partial_\tau f_{\sigma}(\tau) + H_{\text{imp}}(\tau) + H_{\text{int}}(\tau))
\]

Note that here the dynamic mean-field Green’s function \(G_0(\tau - \tau')\) coincides with the Green’s function for the pure Hubbard model, Eq. (11).

To study the Kondo effect it is convenient to work with the effective Hamiltonian \(H_{\text{eff}}[0, f]\), which produces the same action as in Eq. (15). Because the Hubbard host is represented in Eq. (15) exactly like in the case of the Hubbard model without impurity it is easy to see that

\[
H_{\text{eff}}[0, f] = H_{\text{AM}} + H_{\text{imp}} + H_{\text{int}}
\]

Using Eqs. (3), (4), (9) we obtain finally

\[
H_{\text{eff}}[0, f] = \sum_{l\sigma} \epsilon_l a_{l\sigma}^\dagger a_{l\sigma} + \sum_{l\sigma} V_l (a_{l\sigma}^\dagger c_{0\sigma} + \text{h.c.}) - \mu \sum_\sigma c_{0\sigma}^\dagger c_{0\sigma} + U n_{0\uparrow} n_{0\downarrow} + \sum_\sigma \epsilon_{\text{f},n_{f\sigma}} + \frac{U}{2} \sum_{\sigma \neq \sigma'} n_{f\sigma} n_{f\sigma'} + V \sum_\sigma (f_{\sigma}^\dagger c_{0\sigma} + \text{h.c.})
\]

The above Hamiltonian describes the two-impurity system in which the first one, \(c_{0\sigma}^{\dagger}\), represents, together with the free-electron bath, the Hubbard host (see subsection A) and the second impurity is coupled to the first one only. It is still a non-trivial model but because the influence of the impurity on the fitting set of parameters \(\epsilon_l\) and \(V_l\) is negligible we may use the function \(\Delta(\epsilon)\), Eq. (10), as it is calculated for the Hubbard model.

The function \(\Delta(\epsilon)\) depends of course on the type of the lattice. In the following Section we consider the Kondo effect as it emerges from the Hamiltonian, Eq. (11), for the case of the Bethe lattice of infinite connectivity with the function \(\Delta(\epsilon)\) taken from [23]. We assume that the energy \(U_f\) is much larger than other energetical scales in the problem and will take it infinitely large to exclude the double occupation of the impurity site.

### III. WEAK CORRELATED HOST

To take into account the absence of double f-occupation we follow [28] and introduce the slave boson field \(b^\dagger, b\) with the restriction

\[
b^\dagger b + \sum_\sigma c_{0\sigma}^{\dagger} c_{0\sigma} = 1
\]

The two-impurity Hamiltonian has to be modified in the well known fashion [28,29] and its form now is

\[
H_{\text{eff}}[0, f, b] = \sum_{l\sigma} \epsilon_l a_{l\sigma}^\dagger a_{l\sigma} + \sum_{l\sigma} V_l (a_{l\sigma}^\dagger c_{0\sigma} + \text{h.c.}) - \mu \sum_\sigma c_{0\sigma}^\dagger c_{0\sigma} + U n_{0\uparrow} n_{0\downarrow} + \sum_\sigma \epsilon_{\text{f},n_{f\sigma}} + \lambda b^\dagger b + V \sum_\sigma (f_{\sigma}^\dagger b c_{0\sigma} + \text{h.c.})
\]

Here \(\lambda\) is the slave boson chemical potential which in the final stage of calculations has to be put to \(-\infty\) in order to satisfy the restriction of Eq. (17).

We begin with free electrons in the original Hamiltonian, Eq. (6), that is \(U = 0\). Using the NCA in the lowest 1/N approximation the boson and f-pseudofermion self-energies may be calculated by the use of the Hamiltonian \(H_{\text{eff}}[0, f, b]\) and compared with the well known results [28,29]. Figures 3 a, b depict these self-energies. The propagator of the first impurity electron in our two-impurity system (states \(c_{0\sigma}^{\dagger}\)) is labeled by \(G_{\text{AM}}(i\omega_n)\). For \(U = 0\) it is easy to calculate that

\[
G_{\text{AM}}(i\omega_n) = \frac{1}{i\omega_n + \mu + \sum_{l} \frac{\eta_l^2}{i\omega_n - \epsilon_l}}
\]

The self-consistent mapping of the original system with \(U = 0\) onto the two-impurity one means that the local Green’s function \(G(i\omega_n)\) coincides with \(G_{\text{AM}}(i\omega_n)\). So we obtain

\[
G_{\text{AM}}(i\omega_n) \equiv G(i\omega_n) = \int_{-\infty}^{\infty} d\epsilon \frac{\rho(\epsilon)}{i\omega_n - \epsilon + \mu}
\]

Here \(\rho(\epsilon)\) is the DOS of the host lattice, Eq. (2). Substituting in the expressions for the self-energies of Figures 3 a, b instead of the propagator \(G_{\text{AM}}(i\omega_n)\) the Green’s function \(G(i\omega_n)\) from Eq. (20) one can recover, as it is expected for the non-interacting case, self-energy expressions as they emerge by the direct application of the NCA to the original Hamiltonian Eq. (6) [28,29]. The Kondo temperature \(T_K\) changes exponentially as a function of the coupling and in the lowest iteration of the NCA it has the form

\[
T_K = 2 t \exp \frac{\pi \epsilon_f}{2 \Gamma}
\]

Here \(\Gamma = \pi V^2 \rho(0)\) is the Anderson width.

The interaction case, \(U \neq 0\), may also be considered in the frame of the NCA. In the lowest 1/N approximation the slave boson and f-pseudofermion self-energies acquire vertex corrections which take into account the CEI. These vertex corrections \(U^V(1, 2, 3, 4)\) were discussed in [17] and shown in Figures 3 c, d. Now neither the propagator \(G_{\text{AM}}\) has the simple form of Eq. (19), nor \(G\) is of the non-interacting nature of Eq. (20). However, for
weak correlations the self-energies, Figures 3, c, d, may be calculated [17]. In this case of small U one may neglect the mass renormalization of band electrons [15] and use for $G_{AM}$ Eq. (20), besides $\Gamma^U (1, 2; 3, 4) = U$. With these approximations the self-energies of Figures 3, c, d are exactly the same as calculated in [17] for the Hamiltonian, Eq. (4), in the usual three-dimensional case in the local approximation. According to [17] Eq. (21) is preserved (in the lowest iteration of the NCA) but the parameters $\epsilon_f$ and $\Gamma$ undergo the renormalization (both $|\epsilon_f|$ and $\Gamma$ increase linearly with $U$) leading to the enhancement of $T_K$. Details of this renormalization may be found in [17]. Note that in this section we did not use any specific properties of the Bethe lattice and its results are valid for any host lattice. It would be interesting to go in the NCA beyond the linear in the Hubbard approximation. According to [17] Eq. (21) is preserved (Eq. (1), in the usual three-dimensional case in the lattice which is considered throughout this section we take $U/2t \gtrsim 3$ somewhat loosely for the upper limit. The lower limit in our case is dictated by the variational function. The range of the ratio $U/2t$ for which the host is still in the metallic regime, i.e. much before the metal-insulator transition takes place. From Figure 2 for the Bethe lattice which is considered throughout this section we take $U/2t \sim 1$ (see subsection IV.B).

We construct here variational functions for the singlet and triplet states and find the ground singlet and lowest triplet energies. Essentially, we follow ideas of 1/N variational treatment of the Anderson impurity Hamiltonian developed in [11,12]. It is convenient to introduce a new representation for the bath states in Eq. (16):

$$\Psi_{\epsilon} = \mathcal{V}^{-1}(\epsilon) \sum_{\sigma} V_\sigma^\dagger \delta(\epsilon - \epsilon_i) a_{\sigma}^\dagger$$

$$\mathcal{V}(\epsilon) \equiv \sqrt{\Delta(\epsilon)}$$

(22)

Here $\Delta(\epsilon)$ is from Eq. (10). Using this definition the Hamiltonian $H_{eff}[0, f]$ may be rewritten as follows:

$$H_{eff}[0, f] = \sum_{\sigma} \int d\epsilon (\epsilon \Psi_{\epsilon}^\dagger \Psi_{\epsilon} + \mathcal{V}(\epsilon) (\Psi_{\epsilon}^\dagger c_{\epsilon \sigma} + h.c.)) - \sum_{\sigma} (\mu n_{0,\sigma} - \epsilon_f n_{f,\sigma}) + V \sum_{\sigma} (f_{\sigma}^0 c_{0,\sigma} + h.c.) + U n_{0\uparrow} n_{0\downarrow} + \frac{U_f}{2} \sum_{\sigma \neq \sigma'} n_{f,\sigma} n_{f,\sigma'}$$

(23)

Note that since $\mu = U/2$ the $c_{0}$-impurity is described by the symmetric Anderson model while the double occupancy of the $f$-level is forbidden ($U_f \rightarrow \infty$).

### A. Variational functions

Figure 3 schematically represents the singlet state variational function. We have two groups of states: one contains four states in which the $f$-level is unoccupied, the other is of six states in which the $f$-level is singly occupied. For vanishing hybridization coupling $V = 0$ two groups are decoupled and the first one is just the variational function of the symmetric Anderson impurity. We want to keep only the lowest contributions in $1/N$ which come from the states without electron-hole pairs [11,12]. For the symmetrical Anderson impurity the occupation of the empty state has to equal that of the doubly-occupied one which may be achieved only by including states with one electron-hole pair at least [12]. We included only one such state ($\phi_3$ in Figure 3) and we checked that the four-state variational function for the symmetric Anderson impurity produces the required equality between occupancies of the empty and doubly-occupied states. There are two additional states with one electron-hole pair [12]. Including them, however, would make calculations too cumbersome. Being interested in the qualitative influence of the Hubbard $U$ on the Kondo effect we limited ourself to the lowest possible combination of states which is expected to give correct qualitative results at least. The second group of states (states 4 - 9 in Figure 3) are chosen from the same considerations.

We denote states by $\phi_i$, $i = 0, 1, \ldots, 9$, so $\phi_0 = |0 \rangle >$ represents the vacuum (full Fermi sea and empty local states), $\phi_1(\epsilon) = 1/\sqrt{2} \sum_{\sigma} \Psi_{\epsilon,\sigma}^\dagger c_{0,\sigma} |0 \rangle >$, $\ldots$, $\phi_9(\epsilon_1, \epsilon_2, E) = 1/\sqrt{2} \sum_{\sigma} \Psi_{\epsilon_1,\sigma}^\dagger \Psi_{\epsilon_2,\sigma}^\dagger |0 \rangle >$. All $\phi$-functions are listed in the Appendix A. In this basis the singlet ground state of the Hamiltonian Eq. (23) has the following form:

$$\psi_s = \mathcal{N}[\phi_0 + \int_{-D}^{0} dc_1 \left( r_1(\epsilon_1) \phi_1 + \int_{-D}^{\epsilon_1} dc_2 d_2(\epsilon_1, \epsilon_2) \phi_2 + \int_{0}^{D} dE r_3(\epsilon_1, E) \phi_3 + \right)$$

$$+ \int_{-D}^{0} dc_4(\epsilon_1, \epsilon_2) \phi_4 + \int_{-D}^{\epsilon_1} dc_5(\epsilon_1, \epsilon_2) \phi_5 + \int_{-D}^{\epsilon_1} dc_2 d_2(\epsilon_1, \epsilon_2) \phi_6 + \int_{-D}^{\epsilon_1} dc_3 d_3(\epsilon_1, \epsilon_2, E) \phi_7 + \int_{-D}^{\epsilon_1} dc_4 d_4(\epsilon_1, \epsilon_2, E) \phi_8$$

$$+ \int_{-D}^{\epsilon_1} dc_5 d_5(\epsilon_1, \epsilon_2, E) \phi_9)$$

(24)

Here $\mathcal{N}$ is the normalization factor and $r_1$ are superposition functions which have to be determined by the energy minimization. For convenience, the energies of free electrons are denoted here by $\epsilon$ for a negative part of their spectrum and by $E$ for the positive part and $D \equiv 2t$. Because the replacement $\epsilon_1 \leftrightarrow \epsilon_2$ for $\phi_2(\epsilon_1, \epsilon_2)$, $\phi_6(\epsilon_1, \epsilon_2)$ and $\phi_9(\epsilon_1, \epsilon_2, E)$ does not give new independent functions the upper limit of appropriate inner integrals is equal to $\epsilon_1$. The first four out of ten integral equations connecting different $r_i$, $i = 0, 1, \ldots, 9$ are
where the rest of the integral equations may be found in Appendix B. Here \( \Delta E_{s} \) is the energy difference between the singlet ground state energy and the energy of the filled Fermi sea of the conduction band, Eq. (23), \( \tilde{r}_{2}(\epsilon, e_{1}) = r_{2}(\epsilon, e_{1}) \) if \( \epsilon \geq e_{1} \) and \( \tilde{r}_{2}(\epsilon, e_{1}) = r_{2}(\epsilon, e_{1}) \) if \( \epsilon \leq e_{1} \). Before we proceed with the numeric variational calculations let us discuss the variational functions for magnetic states.

We consider triplet, \( S = 1 \), states. Because of the rotational symmetry it is sufficient for our purposes to deal with the state of \( S_{z} = 1 \). The basis of this state may be generated from the singlet basis of Appendix A by applying to them the operator \( \Psi_{\epsilon_{i}e_{0}^{\uparrow}} \). The magnetic basis consists of functions \( \Phi_{i}, i = 1, \ldots, 12 \) and the first three are \( \Phi_{1}(\epsilon) = \Psi_{\epsilon_{i}e_{0}^{\uparrow}}|0\rangle \), \( \Phi_{2}(\epsilon, e_{1}) = \Psi_{\epsilon_{i}e_{0}^{\uparrow}}\Psi_{\epsilon_{2}e_{0}^{\uparrow}}|0\rangle \), and \( \Phi_{3}(\epsilon, E) = \Psi_{\epsilon_{i}e_{0}^{\uparrow}}|0\rangle \). These three states compose the \( S_{z} = 1 \) state of the symmetric Anderson impurity when it is decoupled from the rest of the system, Eq. (23). Other basis states are written in Appendix A. The triplet \( S_{z} = 1 \) variational function therefore reads:

\[
\psi_{t} = N[\int_{-D}^{0} d\epsilon_{1} (\\)
\]

\[
R_{1}(\epsilon_{1})\Phi_{1} + \int_{-D}^{\epsilon_{1}} d\epsilon_{2}R_{2}(\epsilon_{1}, \epsilon_{2})\Phi_{2} + \int_{0}^{D} d\epsilon R_{3}(\epsilon_{1}, E)\Phi_{3} + \\
R_{4}(\epsilon_{1})\Phi_{4} + \int_{-D}^{\epsilon_{1}} d\epsilon_{2}R_{5}(\epsilon_{1}, \epsilon_{2})\Phi_{5} + \int_{0}^{D} d\epsilon_{2}R_{6}(\epsilon_{1}, \epsilon_{2})\Phi_{6} + \\
\int_{-D}^{\epsilon_{1}} d\epsilon_{2}R_{7}(\epsilon_{1}, \epsilon_{2})\Phi_{7} + \int_{-D}^{\epsilon_{1}} d\epsilon_{2}R_{8}(\epsilon_{1}, \epsilon_{2}, \epsilon_{3})\Phi_{8} + \\
\int_{-D}^{\epsilon_{1}} d\epsilon_{2}R_{9}(\epsilon_{1}, \epsilon_{2}, \epsilon_{3})\Phi_{9} + \\
\int_{-D}^{\epsilon_{1}} d\epsilon_{2}R_{10}(\epsilon_{1}, \epsilon_{2}, E)\Phi_{10} + \\
\int_{-D}^{\epsilon_{1}} d\epsilon_{2}R_{11}(\epsilon_{1}, \epsilon_{2}, E)\Phi_{11} + \\
\int_{-D}^{\epsilon_{1}} d\epsilon_{2}R_{12}(\epsilon_{1}, \epsilon_{2}, E)\Phi_{12} )]
\]

(27)

Here upper limits of some integrals are chosen to avoid double counting of states and functions \( R_{i} \) must be obtained from the minimization of the triplet energy. As it is seen from the list of the functions in Appendix A the \( S_{z} = 1 \) basis is composed from three groups of states. The first group contains the above written symmetric Anderson impurity states, in the two others the real impurity level is occupied, the difference between the second and the third group being the origin of the triplet. In the second the triplet originates from the real impurity and a conduction electron and in the third group it is from the symmetric Anderson impurity and a conduction electron. Integral equations which connect different functions \( R_{i} \) are collected in Appendix B. In the next subsection we suggest an effective numerical iteration method which was implemented here for carrying out the energy minimization both for the singlet and for the triplet.

**B. An iteration method for the energy minimization and results**

The direct numerical diagonalization of the two systems of linear integral equations, Eqs. (25), (26) for the singlet state and (B1 - B6) for the magnetic state, would be a very time consuming task. To find the energy shift \( \Delta E_{s} \) together with the \( r_{i} \) functions we solve the integral equations system of Eqs. (25), (26), (31 - 36) numerically for an arbitrary given value of \( \Delta E_{s}, \) say \( iE \). This is done by the controlled iteration procedure which starts with a most resonable guess about the initial \( r_{i} \) functions. A fast convergence is usually obtained by choosing all but two initial \( r_{i} \) equal to zero and by selecting these two from states which are expected to contribute significaly to the superposition \( \psi_{s} \). Let \( r_{i}^{\Delta E} \) are functions calculated in the above procedure. Then we obtain by the use of Eq. (25) the following function \( f(\Delta E) \):

\[
f(\Delta E) = \frac{\int_{-D}^{0} d\epsilon r_{i}\Delta E^{i}(\epsilon)}{r_{0}^{\Delta E}}
\]

(28)

In view of the arbitrariness of \( \Delta E \), \( f(\Delta E) \) does not coincide with \( \Delta E_{s} \), the equality between them is realized by \( \Delta E_{s} \) (see Eq. (25)). So the latter may be seen as a minimal possible fixed point of the function \( f \), Eq. (28):

\[
f(\Delta E_{s}) = \Delta E_{s}.
\]

This fixed point may be found after a few trials. Note that this scheme does not require the normalization of the \( \psi_{s} \), Eq. (24), to be fulfilled in each stage of iterations. To find the energy shift \( \Delta E_{l} \) between the lowest magnetic state and the energy of the filled Fermi sea of the conduction band of Eq. (24) the anagolous iteration method is applied to the above magnetic state, Eq. (27). An illustration of the iteration procedure and some details of it are given in Appendix C.

It is clear from general considerations that values of \( U \) here have to be limited from below just because of the restricted basis which is used (see Figure 9). In addition,
in our case we are interested in the Kondo limit of almost filled states $\phi_5$ and $\phi_6$. Therefore the local energy $U/2$ of the Anderson impurity with states $e_{0,\sigma}^\dagger$ in the two-impurity Hamiltonian, Eq. (23), has to be much larger than the maximal coupling parameter $\Gamma_1 = \pi V^2(0)$. By the definition of $V(\epsilon)$, Eq. (22), this gives:

$$U/D \gg 1/4$$

The hybridization coupling parameter for the real impurity in the two-impurity Hamiltonian, Eq. (23), may be defined in the usual way from the original Hamiltonian, Eq. (1), as the Anderson width $\Gamma = \pi V^2(0)$ with $\rho(0) = 2/\pi D$ (see Figure 3). The Kondo limit for the real impurity is given then by the condition:

$$|\epsilon_f| > 2V^2/D.$$  

Two values of $\epsilon_f/D = -0.67$ and -0.3 were used in our calculations. Figure 4 presents the dependence of the energy difference $T_K = \Delta E_0 - \Delta E_s$ on $V^2$ for both values of $\epsilon_f$ and $U/D = 1$ as calculated by the described above iteration method.

Figure 5 compares $T_K$ as a function of $V^2$ for different values of $U$ and $\epsilon_f/D = -0.3$. Figure 6 illustrates the decrease of $T_K$ with the $U$ increase. Here for the comparison the standard Kondo temperature from Eq. (21) is also shown.

V. DISCUSSIONS AND CONCLUSIONS

Summarizing the above we note that i) weak coupling between conduction electrons does not destroy the usual exponential Kondo scale (for $\Gamma \ll \epsilon_f$) but renormalizes the parameters $\Gamma$ and $\epsilon_f$; ii) the exponential scale of $T_K$ is lost already for $U/D = 1$. Moreover, for small $\Gamma$ the Kondo temperature $T_K$ is proportional to $V^2$ (see Figures 4 and 5); iii) there is a pronounced maximum on Figure 5 for $U = 2$, 2.5 and an indication on a broad one in Figure 6 (or $U = 1$ and iv) in the range of $U \geq D$ the $T_K$ decreases with the increase of $U$.

The enhancement of $T_K$ in the Kondo regime by a weak coupling between conduction electrons is understood (see 13,14) and is caused by the reduced probability of finding doubly occupied and empty lattice sites in the correlated system. This leads to the increased number of uncompensated conduction electron spins and to increase of the effective hybridisation. Our two-impurity model for $d \rightarrow \infty$ gives just the same result. The loss of the exponential scale for intermediate $U/D = 2$ and 2.5 does not come as a surprise because for these values the DOS of Figure 4 has the typical three peak structure of the Anderson impurity and the Hubbard host excitations in this case are not of the Fermi-liquid character 22. However, for $U = 1$ there are no gaps in the DOS and $\epsilon_f$ lies within the metallic looking DOS. Nevertheless also this case is qualitatively different from the non-interacting one. This difference can be seen in the frame of our two-impurity model. Indeed when the real impurity is decoupled, $V = 0$, the rest of the system is just the symmetric Anderson impurity embedded in the bath. At $T = 0$ and provided that $U \gg \Gamma_1$ this system possesses the Kondo temperature which may be viewed as the energy difference between the ground singlet and lowest relevant magnetic states 23 of the symmetric Anderson model. This Kondo temperature for the symmetric Anderson impurity is referred to as $T_K^{AM}$ and it was calculated in Appendix C for several values of $U$ (see Appendix C). By coupling the real Anderson impurity to the system with a precursory non-zero energy difference between the ground singlet and the lowest relevant magnetic states we may expect for small coupling $2V^2/D \ll T_K^{AM}$ a perturbative linear dependence between $T_K$ and $V^2$. Using values of $T_K^{AM}$ from Appendix C we obtain regions of linear dependence which are in a fair agreement with Figures 4 and 5. For small enough $U < \Gamma_1$ the symmetric Anderson impurity enters in the non-magnetic regime of the resonance level (see 4). Using $\Gamma_1 = \pi V^2(0)$ and Eqs. (12) and (22) we see that this happens at $U/D \sim 1/2$ and we expect that the usual Fermi-liquid picture of the Kondo effect emerges below this value of $U/D$. Unfortunately, as was discussed in the subsection III B, we cannot treat this region of smaller $U$ in the frame of the above variational approach. So the physics of the crossover from the Fermi-liquid regime with the exponential Kondo scale to the new regime where the Kondo exponential scale is lost is waiting for further investigations, perhaps in the frame of the diagrammatic approach but beyond the weak coupling which was discussed in Section III.

In general a non-monotonic behaviour of $T_K$ as a function of $V^2$ may be expected at $\Gamma \sim |\epsilon_f|$ when the transition from the Kondo regime to the mixed valence regime occurs 23. The maximum of the upper curve with $|\epsilon_f| = 0.3$, Figure 5, occurs at $\Gamma = 2V^2/D \sim 0.2$, and is in accordance with this expectation. However the lower curve of this figure which corresponds to the same $U/D = 1$ and about twice larger $|\epsilon_f|$ seems to saturate in the same region as the upper curve. In view of the specific form of the DOS of Figure 4 one has to be cautious to directly use the criteria taken from the non-interacting case. It is especially true for the cases of larger $U = 2$, 2.5 and $\epsilon_f = -0.3$ on Figure 5. The maximum appears there at $\Gamma \sim 0.1$ and 0.04 correspondingly showing a strong dependence of $T_K$ upon $U$. In both last cases the local bare level $\epsilon_f$ is on the edge of the central portion of DOS, Figure 5, which narrows much with $U$. This narrowing of DOS determines the $U$-dependence of $T_K$.

The decrease of $T_K$ as $U$ increases is expected for sufficiently large $U$ because the charge transfer from the impurity to the lattice eventually will be inhibited by the energy cost of the double occupancy of the lattice sites. The most interesting region of $U$ values, where the crossover from the exponential Kondo scale to the perturbative one takes place, has yet to be explored. It
would be desirable to study the entire range of $U$ by one method of treatment. It would be interesting also to look into the experimental aspects of the Kondo effect as a tool for detecting non-Fermi-liquid properties of a strongly correlated metal.

In conclusion, we reduced the treatment of the Kondo effect in the Hubbard host of infinite dimensions to study of a simpler two-impurity Hamiltonian. The weakly correlated case was treated by the NCA and relations to previous studies of the Anderson impurity in a correlated host in 2d and 3d were shown. The variational treatment of the two-impurity Hamiltonian for intermediate interactions reveals a non-exponential behaviour of the Kondo scale and qualitative explanations for this behavior were proposed.

VI. ACKNOWLEDGEMENT

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APPENDIX A: TABLES OF FUNCTIONS

The basis of the singlet ground state, Eq. (24), follows:

\[
\phi_0 = |0> \quad (A1)
\]

\[
\phi_1(\epsilon) = \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\epsilon \sigma} c_{\sigma \downarrow}^\dagger |0> \quad (A2)
\]

\[
\phi_2(\epsilon_1, \epsilon_2) = \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\epsilon_1 \sigma} \Psi_{\epsilon_2 - \sigma} c_{\sigma 0 \downarrow}^\dagger c_{\sigma 0 \uparrow}^\dagger |0> \quad (A3)
\]

\[
\phi_3(\epsilon, E) = \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\epsilon \sigma} \Psi_{E \sigma}^\dagger |0> \quad (A4)
\]

\[
\phi_4(\epsilon) = \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\epsilon \sigma} f_{\sigma \downarrow}^\dagger |0> \quad (A5)
\]

\[
\phi_5(\epsilon_1, \epsilon_2) = \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\epsilon_1 \sigma} \Psi_{\epsilon_2 - \sigma} c_{\sigma 0 \downarrow}^\dagger f_{\sigma \uparrow}^\dagger |0> \quad (A6)
\]

\[
\phi_6(\epsilon_1, \epsilon_2) = \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\epsilon_1 \sigma} \Psi_{\epsilon_2 \sigma} c_{\sigma 0 \uparrow}^\dagger f_{\sigma \downarrow}^\dagger |0> \quad (A7)
\]

\[
\phi_7(\epsilon_1, \epsilon_2, \epsilon_3) = \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\epsilon_1 \sigma} \Psi_{\epsilon_2 - \sigma} \Psi_{\epsilon_3 - \sigma} c_{\sigma 0 \uparrow}^\dagger c_{\sigma 0 \downarrow}^\dagger f_{\sigma \downarrow}^\dagger |0> \quad (A8)
\]

\[
\phi_8(\epsilon_1, \epsilon_2, E) = \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\epsilon_1 \sigma} \Psi_{\epsilon_2 - \sigma} \Psi_{E \sigma}^\dagger f_{\sigma \uparrow}^\dagger |0> \quad (A9)
\]

\[
\phi_9(\epsilon_1, \epsilon_2, E) = \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\epsilon_1 \sigma} \Psi_{\epsilon_2 \sigma} \Psi_{E \sigma}^\dagger f_{\sigma \uparrow}^\dagger |0> \quad . \quad (A10)
\]

Beneath is the basis of the magnetic state, Eq. (27):

\[
\Phi_1(\epsilon) = \Psi_{\epsilon 0 \uparrow}^\dagger c_{0 \downarrow}^\dagger |0> \quad (A11)
\]

\[
\Phi_2(\epsilon_1, \epsilon_2) = \Psi_{\epsilon_1 \uparrow}^\dagger \Psi_{\epsilon_2 \uparrow}^\dagger c_{0 \uparrow}^\dagger c_{0 \downarrow}^\dagger |0> \quad (A12)
\]

\[
\Phi_3(\epsilon, E) = \Psi_{\epsilon \uparrow}^\dagger \Psi_{E \sigma}^\dagger |0> \quad (A13)
\]

\[
\Phi_4(\epsilon) = \Psi_{\epsilon \uparrow}^\dagger f_{\uparrow}^\dagger |0> \quad (A14)
\]

\[
\Phi_5(\epsilon_1, \epsilon_2) = \Psi_{\epsilon_1 \uparrow}^\dagger \Psi_{\epsilon_2 \downarrow}^\dagger c_{0 \uparrow}^\dagger f_{\uparrow}^\dagger |0> \quad (A15)
\]

\[
\Phi_6(\epsilon_1, \epsilon_2) = \Psi_{\epsilon_1 \downarrow}^\dagger \Psi_{\epsilon_2 \uparrow}^\dagger c_{0 \uparrow}^\dagger f_{\uparrow}^\dagger |0> \quad (A16)
\]

\[
\Phi_7(\epsilon_1, \epsilon_2) = \Psi_{\epsilon_1 \uparrow}^\dagger \Psi_{\epsilon_2 \downarrow}^\dagger c_{0 \uparrow}^\dagger f_{\uparrow}^\dagger |0> \quad (A17)
\]

\[
\Phi_8(\epsilon_1, \epsilon_2, \epsilon_3) = \Psi_{\epsilon_1 \uparrow}^\dagger \Psi_{\epsilon_2 \downarrow}^\dagger \Psi_{\epsilon_3 \uparrow}^\dagger c_{0 \uparrow}^\dagger f_{\uparrow}^\dagger |0> \quad (A18)
\]

\[
\Phi_9(\epsilon_1, \epsilon_2, \epsilon_3) = \Psi_{\epsilon_1 \uparrow}^\dagger \Psi_{\epsilon_2 \downarrow}^\dagger \Psi_{\epsilon_3 \uparrow}^\dagger c_{0 \uparrow}^\dagger f_{\uparrow}^\dagger |0> \quad (A19)
\]

\[
\Phi_{10}(\epsilon_1, \epsilon_2, E) = \Psi_{\epsilon_1 \uparrow}^\dagger \Psi_{\epsilon_2 \downarrow}^\dagger \Psi_{E \uparrow}^\dagger f_{\uparrow}^\dagger |0> \quad (A20)
\]

\[
\Phi_{11}(\epsilon_1, \epsilon_2, E) = \Psi_{\epsilon_1 \uparrow}^\dagger \Psi_{\epsilon_2 \uparrow}^\dagger \Psi_{E \uparrow}^\dagger f_{\uparrow}^\dagger |0> \quad (A21)
\]

\[
\Phi_{12}(\epsilon_1, \epsilon_2, E) = \Psi_{\epsilon_1 \uparrow}^\dagger \Psi_{\epsilon_2 \uparrow}^\dagger \Psi_{E \uparrow}^\dagger f_{\uparrow}^\dagger |0> \quad . \quad (A22)
\]

APPENDIX B: INTEGRAL EQUATIONS

The equations for the functions $r_4, \ldots, r_9$ are

\[
r_4(\epsilon) = [Vr_1(\epsilon) + \int_{-\Delta}^0 d\epsilon_1 \mathcal{V}(\epsilon_1) r_5(\epsilon, \epsilon_1) + \int_{-\Delta}^0 d\epsilon_1 \mathcal{V}(\epsilon_1) r_6(\epsilon_1, \epsilon_1, \epsilon_2)] / (\Delta E_s + \epsilon - \epsilon_f) \quad (B1)
\]

\[
r_5(\epsilon_1, \epsilon_2) = [V\tilde{r}_2(\epsilon_1, \epsilon_2) + \mathcal{V}(\epsilon_2) r_4(\epsilon_1) + \int_{-\Delta}^0 d\epsilon_1 \mathcal{V}(\epsilon_1) \tilde{r}_7(\epsilon_1, \epsilon_3, \epsilon_2) + \int_{-\Delta}^0 d\epsilon_1 \mathcal{V}(\epsilon_1) \tilde{r}_8(\epsilon_1, \epsilon_2, \epsilon_3)] / (\Delta E_s + \epsilon + \epsilon_2 + \mu - \epsilon_f) \quad (B2)
\]

\[
\tilde{r}_6(\epsilon_1, \epsilon_2) = [\mathcal{V}(\epsilon_1) r_4(\epsilon_2) + \mathcal{V}(\epsilon_2) r_4(\epsilon_1)] + \int_{-\Delta}^0 d\epsilon_1 \mathcal{V}(\epsilon_1) \tilde{r}_4(\epsilon_1, \epsilon_2, \epsilon_3) + \int_{-\Delta}^0 d\epsilon_1 \mathcal{V}(\epsilon_1) \tilde{r}_9(\epsilon_1, \epsilon_2, \epsilon_3)] / (\Delta E_s + \epsilon + \epsilon_2 + \mu - \epsilon_f) \quad (B3)
\]

\[
\tilde{r}_7(\epsilon_1, \epsilon_2, \epsilon_3) = [\mathcal{V}(\epsilon_1) r_5(\epsilon_1, \epsilon_2) + \mathcal{V}(\epsilon_2) r_5(\epsilon_1, \epsilon_3) + \mathcal{V}(\epsilon_3) r_5(\epsilon_1, \epsilon_2)] / (\Delta E_s + \epsilon_1 + \epsilon_2 + \epsilon_3 - \epsilon_f) \quad (B4)
\]

\[
r_8(\epsilon_1, \epsilon_2, E) = \mathcal{V}(\epsilon_1) r_5(\epsilon_1, \epsilon_2) \quad (B5)
\]
\[\tilde{r}_0(\epsilon_1, \epsilon_2, E) = V(E)\tilde{r}_0(\epsilon_1, \epsilon_2) \]

\[/ (\Delta E_\epsilon + \epsilon_1 + \epsilon_2 - E - \epsilon_f). \tag{B6}\]

where

\[\tilde{r}_2(\epsilon_1, \epsilon_2) = \Theta(\epsilon_1 - \epsilon_2)r_2(\epsilon_1, \epsilon_2) + \Theta(\epsilon_2 - \epsilon_1)r_2(\epsilon_2, \epsilon_1) \tag{B7}\]

\[\tilde{r}_6(\epsilon_1, \epsilon_2) = \Theta(\epsilon_1 - \epsilon_2)r_6(\epsilon_1, \epsilon_2) + \Theta(\epsilon_2 - \epsilon_1)r_6(\epsilon_2, \epsilon_1) \tag{B8}\]

\[\tilde{r}_7(\epsilon_1, \epsilon_2, \epsilon_3) = \Theta(\epsilon_1 - \epsilon_2)r_7(\epsilon_1, \epsilon_2, \epsilon_3) + \Theta(\epsilon_2 - \epsilon_1)r_7(\epsilon_2, \epsilon_1, \epsilon_3) \tag{B9}\]

\[\tilde{r}_9(\epsilon_1, \epsilon_2, E) = \Theta(\epsilon_1 - \epsilon_2)r_9(\epsilon_1, \epsilon_2, E) + \Theta(\epsilon_2 - \epsilon_1)r_9(\epsilon_2, \epsilon_1, E). \tag{B10}\]

The equations for the functions \(R_1, \ldots, R_{12}\) are

\[R_1(\epsilon) = [ VR_4(\epsilon) + \int_0^D d\epsilon_1 V(\epsilon_1)\tilde{R}_2(\epsilon, \epsilon_1) + \int_0^D dEV(\epsilon)d(\epsilon, E) ] / (\Delta E_\epsilon + \epsilon + \mu) \tag{B11}\]

\[\tilde{R}_2(\epsilon_1, \epsilon_2) = [V(\epsilon_1)R_1(\epsilon_2) + V(\epsilon_2)R_1(\epsilon_1) + V\left[\tilde{R}_5(\epsilon_1, \epsilon_2) + \tilde{R}_7(\epsilon_1, \epsilon_2)\right]] / (\Delta E_\epsilon + \epsilon_1 + \epsilon_2) \tag{B12}\]

\[R_3(\epsilon, E) = V(E)R_1(\epsilon) / (\Delta E_\epsilon + \epsilon - E) \tag{B13}\]

\[R_4(\epsilon) = [ VR_3(\epsilon) + \int_0^D d\epsilon_1 V(\epsilon_1) \left[\tilde{R}_5(\epsilon, \epsilon_1) + R_6(\epsilon, \epsilon_1)\right] ] / (\Delta E_\epsilon + \epsilon - \epsilon_f) \tag{B14}\]

\[\tilde{R}_5(\epsilon_1, \epsilon_2) = [ V\tilde{R}_2(\epsilon_1, \epsilon_2) + V(\epsilon_2)R_4(\epsilon_1) + V(\epsilon_1)R_4(\epsilon_2) + \int_0^D d\epsilon_3 V(\epsilon_3)\tilde{R}_8(\epsilon_1, \epsilon_3, \epsilon_2) \]

\[+ \int_0^D dEV(\epsilon)\tilde{R}_{10}(\epsilon_1, \epsilon_2, E) ] / (\Delta E_\epsilon + \epsilon_1 + \epsilon_2 - E - \epsilon_f) \tag{B15}\]

\[R_6(\epsilon_1, \epsilon_2) = [V(\epsilon_2)R_4(\epsilon_1) + \int_0^D d\epsilon_3 V(\epsilon_3)\tilde{R}_8(\epsilon_1, \epsilon_2, \epsilon_3) + \int_0^D dEV(\epsilon)\tilde{R}_{11}(\epsilon_1, \epsilon_2, E) ] / (\Delta E_\epsilon + \epsilon_1 + \epsilon_2 + \mu - \epsilon_f) \tag{B16}\]

\[\tilde{R}_7(\epsilon_1, \epsilon_2) = [ V\tilde{R}_2(\epsilon_1, \epsilon_2) + \int_0^D d\epsilon_3 V(\epsilon_3)\tilde{R}_9(\epsilon_1, \epsilon_2, \epsilon_3) + \int_0^D dEV(\epsilon)\tilde{R}_{12}(\epsilon_1, \epsilon_2, E) ] / (\Delta E_\epsilon + \epsilon_1 + \epsilon_2 + \mu - \epsilon_f) \tag{B17}\]

\[\tilde{R}_8(\epsilon_1, \epsilon_2, \epsilon_3) = [V(\epsilon_1)R_6(\epsilon_2, \epsilon_3) + V(\epsilon_2)R_6(\epsilon_1, \epsilon_3) + V(\epsilon_3)R_6(\epsilon_1, \epsilon_2) ] / (\Delta E_\epsilon + \epsilon_1 + \epsilon_2 + \epsilon_3 - \epsilon_f) \tag{B18}\]

\[\tilde{R}_9(\epsilon_1, \epsilon_2, \epsilon_3) = [V(\epsilon_1)\tilde{R}_7(\epsilon_2, \epsilon_3) + V(\epsilon_2)\tilde{R}_7(\epsilon_1, \epsilon_3) + V(\epsilon_3)\tilde{R}_7(\epsilon_1, \epsilon_2) ] / (\Delta E_\epsilon + \epsilon_1 + \epsilon_2 + \epsilon_3 - \epsilon_f) \tag{B19}\]

\[\tilde{R}_{10}(\epsilon_1, \epsilon_2, E) = \tilde{V}(E)\tilde{R}_{11}(\epsilon_1, \epsilon_2) \]

\[R_{11}(\epsilon_1, \epsilon_2, E) = V(E)R_6(\epsilon_1, \epsilon_2) / (\Delta E_\epsilon + \epsilon_1 + \epsilon_2 - E - \epsilon_f) \tag{B20}\]

\[R_{12}(\epsilon_1, \epsilon_2, E) = V(E)\tilde{R}_7(\epsilon_1, \epsilon_2) / (\Delta E_\epsilon + \epsilon_1 + \epsilon_2 - E - \epsilon_f) \tag{B21}\]

\[\tilde{R}_{12}(\epsilon_1, \epsilon_2, E) = V(E)\tilde{R}_7(\epsilon_1, \epsilon_2) / (\Delta E_\epsilon + \epsilon_1 + \epsilon_2 - E - \epsilon_f). \tag{B22}\]

where

\[\tilde{R}_2(\epsilon_1, \epsilon_2) = \Theta(\epsilon_1 - \epsilon_2)R_2(\epsilon_1, \epsilon_2) + \Theta(\epsilon_2 - \epsilon_1)R_2(\epsilon_2, \epsilon_1) \tag{B23}\]

\[\tilde{R}_5(\epsilon_1, \epsilon_2) = \Theta(\epsilon_1 - \epsilon_2)R_5(\epsilon_1, \epsilon_2) \]
\[ R = R_0(e_2, e_1) + \Theta(e_2 - e_1)R_5(e_2, e_1) \quad (B24) \]

\[ \hat{R}_7(e_1, e_2) = \Theta(e_1 - e_2)R_7(e_1, e_2) + \Theta(e_2 - e_1)R_7(e_2, e_1) \quad (B25) \]

\[ \hat{R}_8(e_1, e_2) = \Theta(e_1 - e_3)R_8(e_1, e_2, e_3) + \Theta(e_2 - e_1)R_8(e_3, e_1, e_1) \quad (B26) \]

\[ \hat{R}_9(e_1, e_2, e_3) = \Theta(e_1 - e_2)\Theta(e_2 - e_3)R_9(e_1, e_2, e_3) + \Theta(e_1 - e_3)\Theta(e_3 - e_1)R_9(e_2, e_1, e_3) + \Theta(e_1 - e_3)\Theta(e_2 - e_1)R_9(e_3, e_1, e_2) + \Theta(e_1 - e_3)\Theta(e_2 - e_1)R_9(e_3, e_2, e_1) \quad (B27) \]

\[ \hat{R}_{10}(e_1, e_2, E) = \Theta(e_1 - e_2)R_{10}(e_1, e_2, E) + \Theta(e_2 - e_1)R_{10}(e_2, e_1, E) \quad (B28) \]

\[ \hat{R}_{12}(e_1, e_2, E) = \Theta(e_1 - e_2)R_{12}(e_1, e_2, E) + \Theta(e_2 - e_1)R_{12}(e_2, e_1, E) \quad (B29) \]

\[ \text{and } \Delta E_i \text{ is the energy difference between the lowest magnetic state energy and the energy of the filled Fermi sea of the effective conduction band, Eq. (28).} \]

**APPENDIX C: NUMERICS**

A good illustration of the method is provided by the Anderson impurity model with a finite \( U \) \([22,33]\). In our case, putting in Eqs. (22), (23) \( V = 0, \mu = U/2 \) and taking \( V(\epsilon) \) from Figure 3 we obtain the variational principle equations for the singlet state of the symmetric Anderson model which represents the original Hubbard host, Eq. (2). We fix a value of \( \Delta E \) and choose the following functions for starting the iterations: \( r_2 = r_3 = 0 \) and \( r_1(\epsilon) = \sqrt{2V(\epsilon)/(\Delta E + \epsilon + U/2)} \). Then, instead of the normalization we keep \( r_0 = 1 \) on all stages of iterations. The convergence is reached in a few steps and the minimal fixed point of the function \( f \), Eq. (25), is found. The same method was applied to find \( \Delta E_i \) for the symmetric Anderson model. We define \( \Delta E_i - \Delta E_s = T^{AM}_K \) and find that \( T^{AM}_K / D = 0.081, 0.025, 0.011, 0.003 \) for \( U/D = 1.0, 2.0, 2.5, 3.0 \) respectively. We estimate the accuracy of above calculations as \( \pm 10^{-4} \). We may check the credibility of our fixed point iterations by comparing the above values of \( T^{AM}_K \) with the width of the relevant central peak of the DOS in Figure 3. This width has to be proportional to \( T^{AM}_K \) \([22]\) and one can see that it is a fairly good agreement indeed between widths ratios and ratios of \( T^{AM}_K \) for \( U/D = 1, 2, 2.5 \) while for the \( U/D = 3 \) the agreement is less good. The latter is expected because the relative error in this case much larger than in three others. The other check is provided by the expected exponential dependence of \( T^{AM}_K / U \) upon \( U \) \([1]\). The latter is confirmed by an almost linear dependence between the calculated \( lnT^{AM}_K \) and \( U \).

In calculating the singlet ground state energy of the two-impurity Hamiltonian \( H_{\text{eff}} \) we choose as the initial guess for the superposition in Eq. (24) the following functions:

\[ r_4(e_1, e_2) = \delta(e_1)\delta(e_2) \quad r_i = 0 \quad i \neq 4, 5 \quad (C1) \]

The reason for this choice is that in the limit \( V, V \rightarrow 0 \) (i.e. no interaction between the superposition states) the states \( \phi_4(0,0), \phi_5(0,0) \) are the states with lowest energies and therefore the only ones which are occupied. The smaller \( V \) the faster the convergence of the iterations.

For similar reasons the initial guess for the lowest-lying triplet superposition is:

\[ R_5(e_1, e_2) = R_6(e_1, e_2) = \delta(e_1)\delta(e_2) \quad r_i = 0 \quad i \neq 4, 5 \quad (C2) \]

An illustration of the iteration procedure for the singlet case is given in Figure 3. As it is known \([22,32,33]\) the variational wavefunction of the Anderson impurity model sharp varies in the vicinity of zero energy (i.e. Fermi energy). Therefore in order to achieve sufficiently accurate integration with a small number of mesh points we used the dense mesh in the vicinity of zero:

\[ \epsilon_j = \frac{c}{\pi} \ln(1 + g/D) - 1 \quad (C3) \]

where

\[ 0 \leq j \leq n_d \quad (C4) \]

\[ 0 \leq g/D \ll 1 \]

\( g \) is the limit of the dense mesh and \( n_d \) is the number of dense mesh points. In the range \( g \leq E \leq D \) the variational wavefunctions is usually smooth so we used a Gauss-Legendre mesh. The best \( g/D \) was found to be \( 10^{-3} \).

As a criterion for convergence of the iteration procedure we took the inequality

\[ J(i) = |f^{i+1}(\Delta E) - f^i(\Delta E)| < c \quad (C5) \]

where \( f^{i}(\Delta E) \) is the value of the function \( f(\Delta E) \), Eq. (25), in the \( i \)-th iteration and \( c \) is a small number. Surprisingly we found that the inequality

\[ J(i + 2)/J(i + 1) - J(i + 1)/J(i) < c \quad (C6) \]

holds for \( i \) which is much smaller as compared with a needed for the existence of the inequality in Eq. (C5). So after obtaining a convergence of the factor \( J(i + 1)/J(i) \) we calculated \( f(\Delta E) \) by the geometric series sum rule
\[ f(\Delta E) = \frac{f^\prime(\Delta E)}{1 - J(i+1)/J(i)}. \] (C7)

The inequality \( J(i+1)/J(i) > 1 \) indicates divergence of the iterations.

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FIG. 1. A Bethe lattice with the impurity coupled to a lattice site.
FIG. 7. $T_K$ dependence on $U$ for $\epsilon_f = -0.3$ and $V^2 = 0.01$. The cross marks $T_K$ from Eq. (21).

FIG. 8. An illustration of the iteration procedure for the singlet case.
