Effect of assisted hopping on the formation of local moments in magnetic impurities and quantum dots

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Assisted hopping effects in magnetic impurities and quantum dots are analyzed. The magnitude of the assisted hopping term in a quantum dot in the limit of large level spacing is comparable to other corrections induced by the electron-electron interactions. Assisted hopping leads to differences between conductance peaks associated to the same level, and, when the effect is sufficiently strong, to local pairing correlations.

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I. INTRODUCTION

Electron-electron interactions lead to the formation of local moments and to the Kondo effect in magnetic impurities in metals[1,2] and in quantum dots attached to metallic leads.[3–5] This effect is the direct consequence of the Coulomb repulsion between electrons which occupy the same quantum level of the impurity or quantum dot.

If we assume that the main physical features of the impurity (or the dot) are governed by a single quantum level, the leading correction to the intralevel Coulomb interaction is an assisted hopping term. This interaction induces a dependence of the coupling of the impurity (or the dot) and its environment on the occupancy of the level.[6]

In the following, we estimate the magnitude of such a term for models of large atoms and quantum dots, and analyze its effects on the formation of a local moment on the impurity, or quantum dot. For bulk systems, the inclusion of an assisted hopping term in the electronic Hamiltonian favors the existence of pairing correlations.[7] In the case of an impurity, this tendency towards local pairing quenches the local moment, and, for quantum dots, it can lead to asymmetries in the conductance of peaks associated to the same level, and even to an enhancement of the conductances at low temperatures.

The model is described in the following Sec. II A. Simple estimates of the magnitude of the assisted hopping term for quantum dots are discussed in Sec. II B. A mean field analysis is given in Secs. III A and III B. Extensions of the mean field approach are presented in Sec. III C. Section IV contains the main conclusions.

II. THE MODEL

The Hamiltonian

We analyze a single quantum level, associated to the creation operator $d_s^\dagger$, where $s \equiv \uparrow, \downarrow$ is the spin. This level is coupled to a continuum of non interacting electrons, described by operators $\Sigma_k c_{ks}^\dagger$. For simplicity, we assume that a single channel in the environment interacts with the impurity[8]. The Hamiltonian is

$$\mathcal{H} = \sum_{k,s} \epsilon_k c_{k,s}^\dagger c_{k,s} + \epsilon_d^0 n_d + U n_{d\uparrow} n_{d\downarrow} + (V - \Delta V n_{d\uparrow}) \frac{1}{\sqrt{\mathcal{V}}} \times \sum_k c_{k\downarrow}^\dagger d_\downarrow + (V - \Delta V n_{d\downarrow}) \frac{1}{\sqrt{\mathcal{V}}} \sum_k c_{k\uparrow}^\dagger d_\uparrow + \text{H. c.}, \quad (1)$$

where $\mathcal{V}$ is the volume of the system and

$$n_{d\uparrow} = d_\uparrow^\dagger d_\uparrow ,$$

$$n_{d\downarrow} = d_\downarrow^\dagger d_\downarrow ,$$

$$n_d = n_{d\uparrow} + n_{d\downarrow} . \quad (2)$$

The density of states of the conduction band at the Fermi level is $N(\epsilon_F)$. We assume that $VN(\epsilon_F)$, $\Delta VN(\epsilon_F) \ll 1$. Without loss of generality, we will set $\epsilon_F = 0$, and define $N_0 = N(\epsilon_F)$.

When $\Delta V = 0$ we recover the standard model proposed by Anderson for the study of the formation of local moments in metals.[2] This model is determined by three parameters, the Coulomb repulsion U, the position of the level ϵ_d^0, and its width $\Gamma = V^2 N_0$. The model has electron-hole symmetry around $\epsilon_d = \epsilon_d^0 - U/2$.

We will consider that the interaction effects are mostly due to the existence of localized levels at the impurity site or quantum dot. We further truncate the number of intradot levels to a single spin degenerate state. A simple way to estimate the importance of a given interaction term in the Hamiltonian is by counting the number of operators related to the localized level included in it. Using this criterion, the onsite Coulomb repulsion is the leading term, as all four electronic operators involve the impurity level. The only term with three operators related to the impurity is the assisted hopping term in Eq. (1), so that we expect it to give the next leading correction arising from electron-electron interactions. As discussed in model detail in Sec. III B, this statement can be made more rigorous using perturbation theory in the electron-electron coupling. Note that, in addition, an assisted hopping term requires the existence of intradot interactions only.

The Hamiltonian (1) introduces an additional dimensionless parameter $\Delta V/V$. For small atoms, $\Delta V/V$ is a number of order unity.[6] The inclusion of this term in the Hamiltonian breaks the electron-hole symmetry of the initial Anderson Hamiltonian.

III. CALCULATION OF ΔV

A. Definition of ΔV

We assume that the assisted hopping term in Eq. (1) arises from interactions which involve electronic levels within the dot only. When the Hamiltonian is truncated to the Hilbert space defined by a single state within the dot, and the leads, the electron-electron interactions within the dot can induce, among others, a term of this type.

Our initial Hamiltonian is

$$\mathcal{H}=\mathcal{H}_{\rm dot}+\mathcal{H}_{\rm lead}+\mathcal{H}_{\rm tunn},$$

$$\mathcal{H}_{\rm dot}=\sum_i \epsilon_i c_i^\dagger c_i+\sum_{ijkl} h_{ijkl} c_i^\dagger c_j c_k^\dagger c_l,$$

$$\mathcal{H}_{\rm lead}=t\sum_{n=0}^{\infty} \overline{c_n^\dagger} \overline{c_{n+1}}+\text{H. c.},$$

$$\mathcal{H}_{\rm tunn}=\sum_i V_i c_i^\dagger \overline{c_0}+\text{H. c.} \tag{3}$$

We have assumed that the lead contains a single channel. The index i labels all quantum numbers of the states within the dot, including spin. We are interested in transitions where the charge state of the dot changes from N to $N+1$, and from $N+1$ to $N+2$. In the absence of interactions, they correspond to the filling of a particular level, which we denote i. When the charge state of the dot is N, all levels j such that $j<i$ are occuppied. We use as a basis for the electronic states in the dot the Hartree-Fock wave functions defined when for charge state N. Rearrangements of the electronic levels imply that the corresponding wave functions for charge states $N+1$ and $N+2$ are different.[9] Typically, the tunneling between the dot and the lead takes place in a region of atomic size at some point of the surface of the dot $\vec{\mathbf{r}}_0$. Then, $V_i \propto \Psi_i(\vec{\mathbf{r}}_0)$, where $\Psi_i(\vec{\mathbf{r}})$ is the wave function of state i.

We now assume that the broadening of the levels due to the coupling to the leads $\Gamma=\langle V_i^2 N_0\rangle$ is smaller than the mean level spacing Δ. Then, the effective tunneling can be estimated from the ground state wavefunctions of the dot for different charge states

$$V_{\rm eff}^{N\to N+1}=\langle N+1|\sum_j V_j c_j^\dagger|N\rangle \tag{4}$$

and the difference between adding two electrons to state i, and adding one is

$$\Delta V=V_{\rm eff}^{N+1\to N+2}-V_{\rm eff}^{N\to N+1}. \tag{5}$$

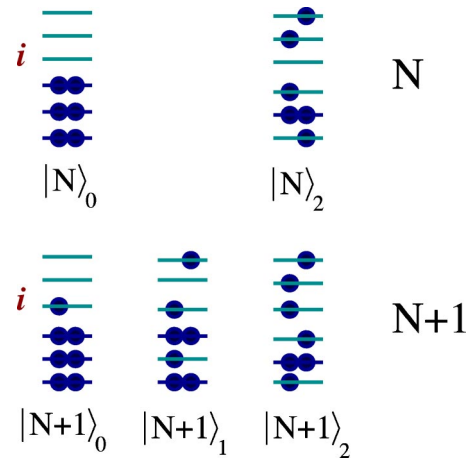

FIG. 1. Sketch of the zeroth order wave functions, and corrections with one and two electron-hole pairs for charge states N and $N+1$. See text for details.

B. Perturbative analysis

For large dots, the interaction terms decrease with the size and conductance of the dot,[10–12] so that a perturbative calculation of ΔV is possible. As mentioned above, we use the electronic basis which diagonalize the Hartree-Fock approximation to $\mathcal{H}_{\rm dot}$ in charge state N, which we denote $\mathcal{H}_{\rm HF}^N$. We can define $\mathcal{H}_{\rm int}=\mathcal{H}_{\rm dot}-\mathcal{H}_{\rm HF}^N$, and the wave functions

$$|N\rangle_0=|N\rangle_{\rm HF},$$

$$|N+1\rangle_0=c_{i\uparrow}^\dagger|N\rangle_{\rm HF},$$

$$|N+2\rangle_0=c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger|N\rangle_{\rm HF}, \tag{6}$$

where $|N\rangle_{\rm HF}$ is the ground state of $\mathcal{H}_{\rm HF}^N$ (note that $|N+1\rangle_0$ and $|N+2\rangle_0$ are not the Hartree-Fock approximations to the wave function of the dot with charge $N+1$ and $N+2$).

The interaction Hamiltonian $\mathcal{H}_{\rm int}$ when acting on $|N\rangle_0$ induces two electron-hole pairs. The occupation of level i in wave functions $|N+1\rangle_0$ and $|N+2\rangle_0$, and the induced interaction between this electron and the rest implies that the basis which diagonalizes $\mathcal{H}_{\rm HF}^N$ is no longer optimal. Then, $\mathcal{H}_{\rm int}$ acting on these wave functions leads to excited states with one and two electron-hole pairs. A sketch of the corrections to the wave functions is shown in Fig. 1.

Matrix elements which involve one and two electron-hole pairs have a different dependence on the size of the dot (see below). We will calculate ΔV to second order in the matrix elements associated to one electron-hole pair $\mathcal{H}_{\rm int,1}$ and to first order in the matrix elements involving two pairs $\mathcal{H}_{\rm int,2}$. We use Eqs. (4) and (5), and we need to calculate the wave functions $|N\rangle, |N+1\rangle$, and $|N+2\rangle$. Generically, we can write

$$|\Psi\rangle=\left(1-\frac{1}{2}\sum_{n_1}\frac{|\langle n_1|\mathcal{H}_{\rm int,1}|0\rangle|^2}{(E_0-E_{n_1})^2}\right)\Bigg(|0\rangle+\sum_{n_1}\frac{|n_1\rangle\langle n_1|\mathcal{H}_{\rm int,1}|0\rangle}{E_0-E_{n_1}}+\sum_{n_2}\frac{|n_2\rangle\langle n_2|\mathcal{H}_{\rm int,2}|0\rangle}{E_0-E_{n_2}}+\sum_{n_2,n_1}\frac{|n_2\rangle\langle n_2|\mathcal{H}_{\rm int,1}|n_1\rangle\langle n_1|\mathcal{H}_{\rm int,1}|0\rangle}{(E_0-E_{n_2})(E_0-E_{n_1})}+\sum_{n_1}\frac{|n_1\rangle\langle n_1|\mathcal{H}_{\rm int,1}|0\rangle\langle 0|\mathcal{H}_{\rm int,1}|0\rangle}{(E_0-E_{n_1})^2}\Bigg),\tag{7}$$

where $|0\rangle$,$|n_1\rangle$, and $|n_2\rangle$ describe states with zero, one, and two electron-hole pairs.

The operator $\Sigma_i V_i c_i^\dagger$ in Eq. (4) can, at most, change by one the number of electron-hole pairs in the wave function. Hence, there are no contributions to Eq. (4) which are of first order in $\mathcal{H}_{\rm int,2}$. In addition, the terms in the second line in Eq. (7) are of second order in $\mathcal{H}_{\rm int,1}$ and lead to wave functions with, at least, one electron-hole pair. Their contributions are of third order in $\mathcal{H}_{\rm int,1}$, and need not be considered. As the basis set used gives the Hartree-Fock solution for charge state N, we have that

$$\mathcal{H}_{\rm int,1}|N\rangle_{\rm HF}=0\tag{8}$$

which implies that the corrections to $V_{\rm eff}^{N\to N+1}$ are of second order in $\mathcal{H}_{\rm int,1}$. Finally, adding all contributions, we find

$$\Delta V\approx\sum_{j<i}\frac{V_j h_{ij}}{\epsilon_j-\epsilon_i}+\sum_{k>i}\frac{V_k h_{ik}}{\epsilon_i-\epsilon_k}-2V_i\sum_{j\leqslant i}^{k>i}\frac{h_{jk}^2}{(\epsilon_j-\epsilon_k)^2}+\sum_{j<i}^{k>i}\frac{V_j h_{jk}h_{ik}}{(\epsilon_i-\epsilon_k)(\epsilon_j-\epsilon_k)}+\sum_{j<i}^{k>i}\frac{V_k h_{jk}h_{ik}}{(\epsilon_j-\epsilon_i)(\epsilon_j-\epsilon_k)},\tag{9}$$

where

$$h_{jk}=\langle j|\mathcal{H}_{\rm int,1}|k\rangle\tag{10}$$

and we assume that all levels are doubly degenerate.

Equation (9) implies that electron-electron interactions within the dot give rise to a first order correction to the hopping, whose sign depends on the nature of the interaction, and a second order correction which tends to suppress the hopping. It is instructive to consider the problem in the opposite limit, where the level spacing within the dot is negligible with respect to the temperature and charging energy. Then, the leading effects of the intredot interaction lead to a Hamiltonian with three simple universal interactions[13] (see also Sec. III D). In that limit, the terms equivalent to assisted hopping give rise to nonequilibrium corrections to the effective tunneling density of states, analyzed in Refs. 14,15.

Note, finally, that in in addition to the correction to the hopping given in Eq. (9), the polarization of the occuppied levels, $j<i$, gives a correction to V which does not depend on the number of electrons in state i. We assume that this correction can be treated as a redefinition of the bare hopping term in Eq. (1).

C. Spherical dot

We now apply the previous analysis to the case of a spherical dot of radius R and $N\gg 1$ electrons. For simplicity, we assume that the positive charge needed to stabilize the system is uniformly distributed within the radius R. The level spacing is

$$\Delta\sim\frac{\hbar^2 k_F}{mR},\tag{11}$$

where $k_F=(9\pi/4)^{1/3}R^{-1}$ is the Fermi wave vector, and m is the mass of the electrons. For sufficently large electronic densities $k_F\gg(me^2)/\hbar^2$, the Coulomb repulsion between electrons can be treated using the Fermi-Thomas approximation. Within this approximation, $\mathcal{H}_{\rm int,1}$ is given by the Fermi-Thomas potential induced by the addition of a unit of of charge to the dot. For a three dimensional spherical dot, this potential is[10]

$$V_{\rm FT}(r)=-\frac{e^2 e^{-k_{\rm FT}(R-r)}}{k_{\rm FT}(R-r)^2},\tag{12}$$

where r is the radial coordinate and $k_{\rm FT}=\sqrt{(4e^2 m k_F)/(\pi\hbar^2)}$ is the Fermi-Thomas wavelength. In addition to this term, we have to include a short range interaction which leads to the excitation of two electron-hole pairs when expanding around the Hertree-Fock solution $\mathcal{H}_{\rm int,2}$ in Eq. (9). The matrix elements of $\mathcal{H}_{\rm int,1}$ decay as R^{-2} for $k_{\rm FT}R\gg 1$, while those of $\mathcal{H}_{\rm int,2}$ decay as R^{-3}, justifying the separation of scales used in obtaining Eq. (9).

The potential $V_{\rm FT}$ is localized within a shell of size $k_{\rm FT}^{-1}$ around the edges of the dot. We assume that the matrix elements $\langle k|V_{\rm FT}|j\rangle$ are roughly constant if $\Delta k\ll k_{\rm FT}$ where $\epsilon_j-\epsilon_k\approx\hbar v_F\Delta k$, and zero otherwise. As the level spacing is given in Eq. (11), the number of levels for which the matrix elements of $V_{\rm FT}$ are not negligible is $k_{\rm FT}R$. Within this energy window, we can also assume that $|\Psi_k(\vec{\mathbf{r}}_0)|\approx|\Psi_i(\vec{\mathbf{r}}_0)|$, so that the the correction to ΔV, using Eq. (9), is the sum of $k_{\rm FT}R$ terms of the same sign. Finally, $V_{\rm FT}$ conserves angular momentum. The maximum angular momentum in a sphere of radius R is approximately $k_F R$.

Defining

$$\overline{V}_{\rm FT}=\langle i|V_{\rm FT}|i\rangle\approx\frac{e^2}{k_{\rm FT}^2R^3}\sim\frac{\hbar^2}{mk_F R^3}\tag{13}$$

we find that the first (linear) and second (quadratic) contributions to ΔV are

$$\Delta V_1 \propto V \frac{\overline{V}_{\rm FT}}{\Delta} \ln(k_{\rm FT} R)$$

$$\Delta V_2 \propto V (k_F R)^2 \frac{\overline{V}_{\rm FT}^2}{\Delta^2} \ln(k_{\rm FT} R), \tag{14}$$

where the $(k_F R)^2$ factor to ΔV_2 arises from the number of angular momentum channels. We have obtained that the two corrections are of similar magnitude, and decay as $(k_F R)^{-2}$.

D. Diffusive dot

The low energy levels and wave functions of quantum dots in the diffusive regime are well described using random matrix theory. We consider a dot of average radius R, mean free path l, and mean level separation Δ. In addition, we assume that the electron density is large $r_s \ll 1$, where $r_s^{-1} = (4/9\pi)^{1/3} (\hbar^2 k_F)/(m e^2)$. The electron-electron interaction can be expanded in powers of the inverse conductance $g = E_T/\Delta$, where $E_T = (\hbar^2 k_F l)/(m R^2)$.[10–12]

As in the case considered in the previous subsection, the leading term in an expansion in g^{-1} arise from the Fermi-Thomas potential (12), upon the addition of electrons. This potential is determined solely by the geometry of the dot and electrostatic constraints, and is independent of the details of the dynamics of the electrons.

We use the matrix elements of $V_{\rm FT}$ calculated for a diffusive dot in Ref. 10. As in Eq. (14), we find two contributions ΔV_1 and ΔV_2. The average over disorder of ΔV_1 is zero, with mean fluctuations

$$\langle \Delta V_1^2 \rangle_{\rm dis} \propto V^2 \frac{c_1}{g} \ln(g), \tag{15}$$

where c_1 is a dimensionless constant of order unity. The $\ln(g)$ correction is due to the summation over states such that $\Delta \leqslant \epsilon_j - \epsilon_k \leqslant E_T$.

To next order in g^{-1}, we find

$$\Delta V_2 \propto V \frac{c_2}{g} \ln(g). \tag{16}$$

For dots of similar radii, ΔV is larger in the diffusive regime than in the regular case. For chaotic, ballistic dots, it seems reasonable to replace g by $k_F R$ in Eqs. (15),(16).

IV. MEAN FIELD ANALYSIS

A. Magnetic solutions

We now consider the Hamiltonian in Eq. (1). We first analyze possible magnetic solutions. The mean field Hamiltonian is

$$\mathcal{H}_{\rm MF} = \sum_{k,s} \epsilon_k c_{k,s}^\dagger c_{k,s} + \epsilon_d^0 n_d + U(\langle n_{d\uparrow}\rangle n_{d\downarrow} + \langle n_{d\downarrow}\rangle n_{d\uparrow}) + V \sum_s \overline{c}_{0,s}^\dagger d_s + \text{H. c.} - \Delta V(\langle n_{d\uparrow}\rangle \overline{c}_{0\downarrow}^\dagger d_\downarrow + \langle n_{d\downarrow}\rangle \overline{c}_{0\uparrow}^\dagger d_\uparrow + \langle \overline{c}_{0\downarrow}^\dagger d_\downarrow + \text{H. c.}\rangle n_{d\uparrow} + \langle \overline{c}_{0\uparrow}^\dagger d_\uparrow + \text{H. c.}\rangle n_{d\downarrow}), \tag{17}$$

where $\overline{c_0}$ is defined in Eq. (3). The sites defined by $c_i, i \neq 0$ can be integrated out. leading to a 2×2 matrix equation for the components of the Green's function for each spin index projected on the c_0 and d sites

$$\mathcal{G}_{ss}^{-1}(\omega) = \begin{pmatrix} -iN_0^{-1} & -V + \Delta V n_s^- \\ -V + \Delta V n_s^- & \omega - \epsilon_d^0 - U n_s^- + \Delta V g_s^- \end{pmatrix}, \tag{18}$$

where s is the spin index and we have defined

$$n_s = \langle n_{ds} \rangle,$$

$$g_s = \langle \overline{c}_{0s}^\dagger d_s + d_s^\dagger c_{0s} \rangle. \tag{19}$$

For the nonmagnetic solution, the different components of the density of states are (omitting spin indices)

$$\text{Im}\, G_{dd}(\omega) = \frac{\Gamma}{(\omega - \epsilon_d)^2 + \Gamma^2},$$

$$\text{Im}\, G_{00}(\omega) = \frac{N_0 (\omega - \epsilon_d)^2}{(\omega - \epsilon_d)^2 + \Gamma^2},$$

$$\text{Im}\, G_{0d}(\omega) = -\frac{N_0 (\omega - \epsilon_d)(V - \Delta V n_0)}{(\omega - \epsilon_d)^2 + \Gamma^2}, \tag{20}$$

where

$$\Gamma = N_0 (V - \Delta V n_0)^2,$$

$$\epsilon_d = \epsilon_d^0 + U n_0 - \Delta V g_0. \tag{21}$$

The self-consistent relations required in Eq. (17), and the Green's functions in Eq. (20) imply that

$$n_0 = \frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{\epsilon_d}{\Gamma}\right),$$

$$\langle c_{0s}^\dagger d_s \rangle = \frac{N_0 (V - \Delta V n_0)}{2\pi} \ln[N_0^2 (\epsilon_d^2 + \Gamma^2)]. \tag{22}$$

For the symmetric Anderson model, we have $\epsilon_d = 0$, and $n_0 = 1/2$. The equations for the magnetic solution, in the limit of small magnetization, are analyzed in the Appendix. Numerical results of the occupancies of the different spin states as function of $U, V, \Delta V$ and ϵ_0 are shown in Fig. 2.

B. Superconducting solutions

Alternatively, we can use the BCS decoupling and write a mean field Hamiltonian

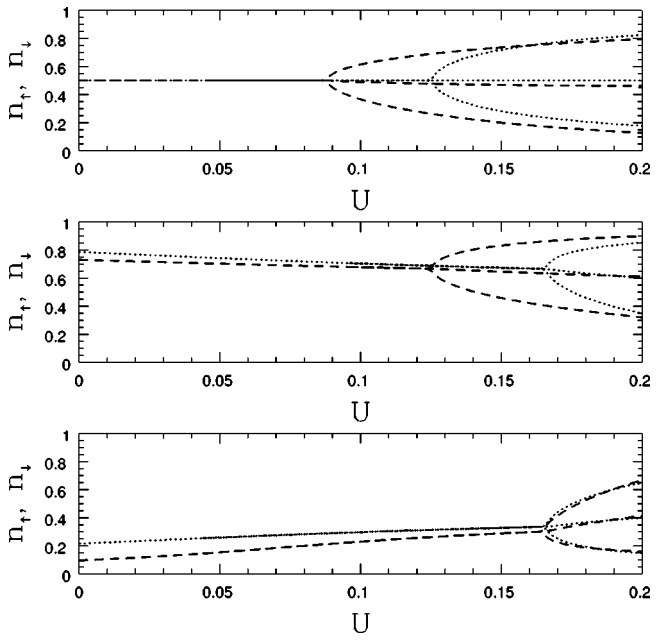

FIG. 2. Number of electrons per spin, as a function of U. Dotted curves: $\Delta V=0$. Broken curves: $\Delta V=0.15$. In all cases, $V=0.2$, in units of $N_{\epsilon_F}^{-1}$. Top: $\epsilon_d^0+U/2=0$. Center: $\epsilon_d^0+U/2=-0.05$. Bottom: $\epsilon_d^0+U/2=+0.05$.

$$\mathcal{H}_{\rm BCS}=\sum_{n,s} t\bar{c}_{n,s}^{\dagger}\bar{c}_{n+1,s}+\epsilon_d n_d+V\sum_s (\bar{c}_{0,s}^{\dagger}d_s+d_s^{\dagger}c_{0,s})$$
$$+U\langle d_\uparrow^{\dagger}d_\downarrow^{\dagger}\rangle d_\uparrow d_\downarrow-\Delta V[\langle d_\uparrow^{\dagger}d_\downarrow^{\dagger}\rangle(d_\downarrow\bar{c}_{0\uparrow}+d_\uparrow c_{0\downarrow})$$
$$+\langle d_\uparrow^{\dagger}\bar{c}_{0\downarrow}^{\dagger}+d_\downarrow^{\dagger}\bar{c}_{0\uparrow}^{\dagger}\rangle d_\uparrow d_\downarrow]+\text{H. c.} \qquad (23)$$

This Hamiltonian couples up spin electrons with down spin holes, and viceversa. The Green's function projected on the electron and hole states at sites c_0 and d can be written in terms of two 4×4 matrices

$$\mathcal{G}(\omega)$$
$$=\begin{pmatrix} -iN_0^{-1} & -V & 0 & \Delta Vn \\ -V & \omega-\epsilon_d & \Delta Vn & -Un+\Delta Vg \\ 0 & \Delta Vn & -iN_0^{-1} & V \\ \Delta Vn & -Un+\Delta Vg & V & \omega+\epsilon_d \end{pmatrix}, \qquad (24)$$

where the two upper (lower) rows correspond to electrons (holes), and we have defined (see Fig. 3)

$$n=\langle d_\uparrow d_\downarrow\rangle,$$
$$g=\langle d_\uparrow c_\downarrow+d_\downarrow c_\uparrow\rangle. \qquad (25)$$

The self-consistency condition implicit in Eq. (24) can be linearized, as outlined in the Appendix.

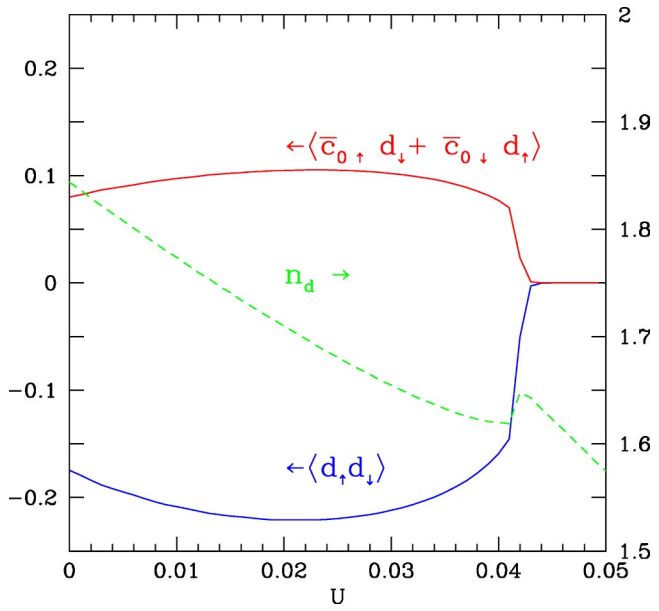

FIG. 3. BCS order parameters, Eq. (25), for $V=0.2$, $\Delta V=0.15$, and $\epsilon_d-U/2=0$ in units of $N(\epsilon_F)^{-1}$. The transition is weakly first order. Broken line: occupancy of the localized level (right scale).

C. Corrections beyond the mean field approximation

The impurity model studied here can be considered as a (0+1)-dimensional model, where fluctuations in time need to be considered (see Fig. 4). In principle, we can integrate out the fermion in the leads, and obtain an effective four state model. The four states correspond to the four occupancies of

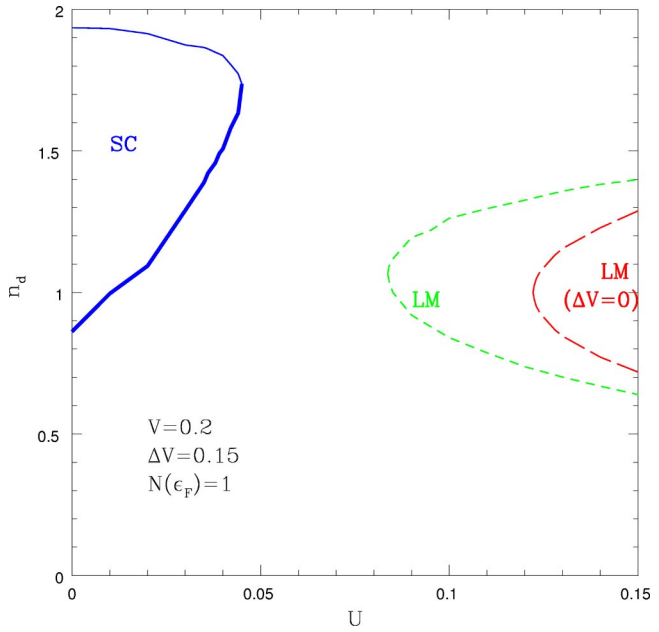

FIG. 4. Mean field phase diagram of the Hamiltonian in Eq. (1). SC: superconducting solution. The thick line is a first order transition (see Fig. 3). The jump in n_d is comparable to the thickness of the line. LM: local moment. For comparison, the results for $\Delta V=0$ are also plotted.

the single state at the impurity, as defined in Eq. (1). These states have long range interactions in time, as in related fermionic and bosonic problems.[16,17] The fluctuations in time will tend to restore the symmetries broken at the mean field level. We will use the mean field results as a guide to infer which type of universality class will determine the low temperature properties. The fact that the reduced Hilbert space associated to the impurity includes only four states greatly restricts the possible low energy fixed points.

The analysis in the two previous subsections suggests that there are two physical regimes: (i) Near $n_d=1$ and for large values of U/Γ, a local magnetic moment is induced and (ii) away from $n_d=1$, and for moderate values of U/Γ, pairing correlations develop near the dot or impurity. We identify the local moment regime studied earlier with the Kondo effect. Note, however, that the relation between the Kondo temperature and the parameters in the Hamiltonian will be changed by the assisted hopping term.

Pairing fluctuations imply that charge states which differ by two are strongly mixed in the ground state. This can be checked by the exact diagonalization of a block containing the impurity and a few sites in the leads. The assisted hopping term leads to an effective negative $U_{\rm eff}$ model, where $U_{\rm eff}=E_N+E_{N+2}-2E_{N+1}$, for certain values of N. These relatively small blocks, when attached to the rest of the leads will act as local defects with a tendency towards pairing. This analysis suggests that the BCS solution identified in the mean field approximation corresponds to a regime approximately described by the negative U Anderson model. The charge state of the impurity will tend to by mostly zero and two, with fast fluctuations between them.

V. CONCLUSIONS

We have analyzed the influence of assisted hopping in correlated impurities embedded in a metal or quantum dots coupled to leads. This type of interaction is the simplest term which can be defined in the restricted basis given by a single quantum level within the dot. Related effects, in the opposite limit where the states within the dot can be treated as a continuum were studied in Refs. 14,15.

We have estimated, in Sec. III, the magnitude of this term for simple models of regular and diffusive dots. In the latter case, we find that the assisted hopping term has a similar dependence on the conductance of the dot as the interaction corrections to the peak spacing.[10,18–21] We have not studied in detail the intermediate case of chaotic dots where the mean free path is larger than the dimensions of the dot (see Sec. III D). The calculations for the cases studied here suggests that assisted hopping terms will also arise as the next leading effects of the interaction term after the onsite Coulomb repulsion.

The assisted hopping term is directly related to the changes of the wave functions within the dot upon the addition of a single electron. We have separated two effects which contribute to this term: (i) The hybridization of the orbital being considered with orbitals associated to excited levels and (ii) the relaxation of occuppied levels (''orthogonality catastrophe''). The second contribution always leads to the suppression of the hopping when the level is already occuppied by one electron. The first contribution, on the other hand, can be of either sign. It can be wiewed as arising from the interference between the direct hopping and hopping through virtual states which becomes allowed when the impurity orbital is occuppied. If the hopping amplitude of all levels being considered is of the same sign, and the hopping through higher energy levels is higher than that through the level at the Fermi energy, the interference is positive, and the hopping is enhanced when the impurity level has one electron. Intuitively, one can say that the orbital is expanded because of the electron repulsion, leading to an increase in the effective hopping. In other situations the sign of contribution (i) to the assisted hopping depends on the interplay between negative interference effects and/or very different hopping elements, and no simple analysis can be given.

This interaction will be larger than estimated in Sec. III in one and two-dimensional geometries as the Fermi-Thomas potential is more extended, and for low electronic density.[9] Note also that the orthogonality catastrophe is expected to be enhanced in disordered two-dimensional systems.[22] We have only taken into account the interactions within the dot. In devices with more than one dot, the interactions between electrons in different dots will also enhance the effects reported here. Assisted hopping can contribute to change the peak height distribution with respect to that predicted by random matrix theory.[23,24]

Our results suggest that assisted hopping can lead to local pairing correlations for reasonable values of the parameters. This implies enhanced conductivity through the dot or impurity, significant deviations from the electron-hole symmetry implicit in the Kondo effect, and measurable differences in the conductance through the two peaks associated to the same quantum level. The existence of these effects does not seem incompatible with present experimental evidence.[25] A detailed analysis of assisted hopping effects quantum dots, in the limit of large level spacing, deserves further investigation.

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APPENDIX

1. Linearization of the magnetic Hartree-Fock equations

We first analyze the magnetic solutions when the magnetization is small. Then, we can write

$$n_{d\uparrow\downarrow}\approx n_0\pm\delta n,$$

$$g_{\uparrow\downarrow}\approx g_0\pm\delta g. \tag{A1}$$

The Hartree Fock approximation introduces four variational parameters $\epsilon_{d\uparrow}$, $\epsilon_{d\downarrow}$, $\Gamma_\uparrow$, and $\Gamma_\downarrow$. We also make the expansion

$$\epsilon_{d\uparrow\downarrow} \approx \epsilon_0 \pm \delta\epsilon,$$
$$\Gamma_{\uparrow\downarrow} \approx \Gamma_0 \pm \delta\Gamma. \tag{A2}$$

The consistency between Eqs. (A1) and (A2) leads to

$$\delta n \approx \frac{\Gamma_0 \delta\epsilon}{\pi(\Gamma_0^2+\epsilon_0^2)} - \frac{\epsilon_0 \delta\Gamma}{\pi(\Gamma_0^2+\epsilon_0^2)},$$

$$\delta g \approx \frac{N_0 \Delta V \delta n}{2\pi} \ln\left(\frac{W^2}{\Gamma_0^2+\epsilon_0^2}\right) + \frac{N_0(V-\Delta V n_0)(\epsilon_0\delta\epsilon+\Gamma_0\delta\Gamma)}{\pi(\Gamma_0^2+\epsilon_0^2)},$$

$$\delta\epsilon \approx -U\delta n + \Delta V \delta g,$$

$$\delta\Gamma \approx 2N_0 V \Delta V \delta n. \tag{A3}$$

Equations (A3) have a nontrivial solution if

$$\mathrm{Det}\begin{vmatrix} 1 & U & 0 & -\Delta V \\ -\dfrac{\Gamma_0}{\pi(\Gamma_0^2+\epsilon_0^2)} & 1 & \dfrac{\epsilon_0}{\pi(\Gamma_0^2+\epsilon_0^2)} & 0 \\ 0 & -2N_0 V\Delta V & 1 & 0 \\ -\dfrac{N_0(V-n_0\Delta V)\epsilon_0}{\pi(\Gamma_0^2+\epsilon_0^2)} & -\dfrac{N_0\Delta V}{2\pi}\ln\left(\dfrac{W^2}{\Gamma_0^2+\epsilon_0^2}\right) & -\dfrac{N_0(V-n_0\Delta V)\Gamma_0}{\pi(\Gamma_0^2+\epsilon_0^2)} & 1 \end{vmatrix} = 0 \tag{A4}$$

For $\Delta V = 0$, Eq. (A4) reduces to

$$\frac{U\Gamma_0}{\pi(\Gamma_0^2+\epsilon_0^2)} = 1. \tag{A5}$$

For $\epsilon_0 = 0$ (symmetric case), and $\Delta V \neq 0$, we find:

$$U = \pi\Gamma_0 - \frac{N_0\Delta V^2}{\pi}\left[\frac{2V}{V-n_0\Delta V} + \ln\left(\frac{W}{\Gamma_0}\right)\right]. \tag{A6}$$

This equation defines the critical value of U at which a solution with a nonzero magnetization appears.

2. Linearization of the BCS equations

We define $\tilde{G}_{dd}(\omega)$ and $\tilde{G}_{dc_0}(\omega)$ as the anomalous Green's functions involving electrons and holes induced by the BCS coupling in Eq. (23). They can be obtained from the implicit Eq. (24). The self-consistency equations are

$$n = \frac{1}{\pi}\int_{-\infty}^{0} \mathrm{Im}\,\tilde{G}_{dd}(\omega)\,d\omega,$$

$$g = \frac{1}{\pi}\int_{-\infty}^{0} \mathrm{Im}\,\tilde{G}_{dc_0}(\omega)\,d\omega. \tag{A7}$$

We can invert Eq. (24) and linearize with respect to n and g, to obtain

$$\mathrm{Im}\,\tilde{G}_{dd}(\omega) = \frac{2V\Delta V N_0(\omega^2-\epsilon_d^2-\Gamma^2)n + 2\Gamma\omega(Un-\Delta V g)}{[(\omega-\epsilon_d)^2+\Gamma^2][(\omega+\epsilon_d)^2+\Gamma^2]},$$

$$\mathrm{Im}\,\tilde{G}_{dc_0}(\omega) = -\frac{2\Gamma^2\Delta V N_0\omega n + (\omega^2-\epsilon_d^2-\Gamma^2)[N_0\Delta V(\omega-\epsilon_d)n - N_0 V(Un-\Delta V g)]}{[(\omega-\epsilon_d)^2+\Gamma^2][(\omega+\epsilon_d)^2+\Gamma^2]}. \tag{A8}$$

We can integrate these expressions, so that

$$n = -\frac{Un-\Delta V g}{\pi\epsilon_d}\arctan\left(\frac{\epsilon_d}{\Gamma}\right),$$

$$g = -\frac{2N_0 \Delta V n}{\pi}\left\{\ln[N_0^2(\epsilon_d^2+\Gamma^2)] + \arctan\left(\frac{\epsilon_d}{\Gamma}\right)\right\}. \tag{A9}$$

Finally, we obtain

$$\left[1+\frac{U}{\pi\epsilon_d}\arctan\left(\frac{\epsilon_d}{\Gamma}\right)\right] + \frac{2N_0\Delta V^2}{\pi^2\epsilon_d}\arctan\left(\frac{\epsilon_d}{\Gamma}\right)\ln[N_0^2(\epsilon_d^2+\Gamma^2)] \leqslant 0, \tag{A10}$$

where we have dropped the arctan term in the second equation in Eq. (A9).

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