

Assisted hopping and interaction effects in impurity models

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We study, using numerical renormalization-group methods, the generalization of the Anderson impurity model where the hopping depends on the filling of the impurity. We show that the model, for sufficiently large values of the assisted hopping term, shows a regime where local pairing correlations are enhanced. These correlations involve pairs fluctuating between on-site and nearest-neighbor positions.

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I. INTRODUCTION

The formation of local moments is the simplest and most extensively studied manifestation of strong electron-electron repulsion in impurities in metals.¹⁻³ This phenomenon can also be observed in mesoscopic systems coupled to metallic leads.^{4,5} In the opposite limit, when the “impurity” becomes a metallic grain whose electronic structure needs to be described by many narrowly spaced levels, the electron-electron repulsion leads to Coulomb blockade.⁶ The intermediate regime when the energy scales of interest (the temperature, the strength of the Coulomb repulsion, and the level spacing) are not too different in magnitude is not so well understood. A similar situation arises in the study of strongly correlated systems. Analogous to the Anderson impurity model is the Hubbard model^{7,8} for extended systems, which leads to a Mott transition and the formation of local moments at half filling. The opposite limit, when many levels within the unit cell have to be included, leads, generically, to ordinary Fermi-liquid behavior.

The simplest modifications of the extended Hubbard model taking into account the multiplicity of levels in the ions in the unit cell lead to assisted hopping terms,^{9,10} which modify substantially the phase diagram and tend to favor superconductivity. Analogously, if the internal degrees of freedom of the metallic grain are included, beyond the constant interaction term which leads to Coulomb blockade, one finds nonequilibrium effects^{11,12} which suppress the Coulomb blockade. These effects are similar to the formation of an excitonic resonance found in the excitation of core electrons.¹³ One can also extend the Anderson impurity model to include the effects associated to the existence of many orbitals. When the influence of these orbitals is described in terms of effective interactions within the restricted Hilbert space of the usual Anderson model, one indeed finds assisted hopping terms.¹⁴ The resulting model has been analyzed using a mean field, BCS-like decoupling of the interaction term¹⁴ and by the flow equation method¹⁵ (for a description of the method, see Refs. 16 and 17), which is well suited to the analysis of impurity models.¹⁸⁻²² These works show a tendency towards local pairing away from half filling, in agreement with the studies of bulk systems.^{9,10} We present here more accurate calculations, using the numerical renormalization-group method,²³ which characterize the low-energy properties of the model in a numerically exact way.

We examine the effect of the assisted hopping term on the local density of states and find that with increasing assisted hopping amplitude the peak characteristic to the mixed valence regime of the Anderson model gets broadened and shifted to negative frequencies. This result is consistent with the fact that the assisted term enhances the occupation of the local level, also found in the calculations. To demonstrate the effect of the new term on the formation of the local moment, we compute the local spin spectral function and find that the spin susceptibility gets suppressed as the assisted hopping term is turned on. This suppression might be interpreted as the trace of the pairing. We also check the pairing correlations in a more direct way and calculate the related spectral functions. Our main result is that although the effect of the assisted term on the pairing correlations on the local level could be explained qualitatively by just considering the renormalization of the level, the so-called off-diagonal correlations (pairing between the d electron and the conduction electrons located at the impurity position) are also enhanced.

The paper is organized as follows. The model and the method of calculation are described in the following section. Then, the main results are presented. Section IV gives the main conclusions of our work.

II. THE MODEL AND METHOD OF CALCULATION

A. The model

We describe the effects of the internal degrees of freedom of the impurity in terms of effective interactions defined within the restricted Hilbert space of the standard Anderson impurity.¹⁴ Using perturbation theory, this approach is justified when the typical level spacing within the impurity, Δ , is much smaller than value of the Coulomb interaction U . Then, it is easy to show that the Anderson model is recovered in the limit $\Delta/U \rightarrow \infty$. We will study the Hamiltonian

$$\mathcal{H} = \mathcal{H}_K + \mathcal{H}_{imp} + \mathcal{H}_{hyb} + \mathcal{H}_{assisted},$$

$$\mathcal{H}_K = \sum_{k,s} \epsilon_k c_{k,s}^\dagger c_{k,s},$$

$$\mathcal{H}_{imp} = \epsilon_d n_d + U n_{d,+} n_{d,-},$$

$$\mathcal{H}_{hyb} = \sum_{k,s} V(c_{k,s}^\dagger d_s + d_s^\dagger c_{k,s}),$$

$$\mathcal{H}_{assisted} = \sum_{k,s} dV n_{d,s} (c_{k,-s}^\dagger d_{-s} + d_{-s}^\dagger c_{k,-s}), \quad (1)$$

where $\mathcal{H}_A = \mathcal{H}_K + \mathcal{H}_{imp} + \mathcal{H}_{hyb}$ is the Anderson Hamiltonian, and the assisted hopping terms are included in $\mathcal{H}_{assisted}$. We have also defined $n_{d,s} = d_s^\dagger d_s$ and $n_d = n_{d,+} + n_{d,-}$. The parameter dV determines the strength of the assisted hopping effects. For the sake of simplicity we consider a flat band with constant density of states for the conduction electrons, with half bandwidth D . In the following we use D as the energy unit.

B. The numerical renormalization-group method

To compute different quantities numerically we use Wilson's numerical renormalization-group (NRG) method.^{23,24} In this method, after the logarithmic discretization of the conduction band, one maps the original impurity Hamiltonian onto a semi-infinite chain with the impurity at the end. One can show that as a consequence of the logarithmic discretization the hopping along the chain decreases exponentially, $t_n \sim \Lambda^{-n/2}$, where Λ is the discretization parameter and n is the index of the site in the chain. The separation of the energy scales due to the decreasing hopping provides the possibility to diagonalize the chain Hamiltonian iteratively and keep the states with the lowest lying energy eigenvalues as most relevant ones. Since we know the energy eigenstates and eigenvalues, we can calculate thermodynamical and dynamical quantities directly (e.g., spectral functions using their Lehman representation).

Since NRG is a well-established numerical method with a quite extended literature, we do not give the details of the calculation here but refer to some important papers.

The numerical renormalization-group method is described in details in Refs. 23 and 25, Krishnamurthy⁸⁰ where it was used to obtain thermodynamical quantities. For the details of calculation of dynamical quantities such as different spectral functions we refer to the paper by Costi *et al.*²⁶ Further details concerning the procedure how to put the discrete information on the spectral density in order to arrive at continuous functions can be found in Ref. 27. The method of calculating dynamical quantities was extended to handle the case of finite magnetic field in a proper way in Ref. 28.

We have performed the calculation using $\Lambda=2$ and keeping $N=1024$ states.

III. RESULTS

The model has four parameters, ϵ_d, U, V , and dV . Previous studies^{14,15} suggest that the most significant deviations from the standard Anderson impurity model take place when the filling of the d orbital is such that $1.2 \leq \langle n_d \rangle \leq 1.8$. We focus our attention to that regime as well. The filling is determined by ϵ_d, U , and also by dV . The mean-field decoupling of the assisted hopping term shows that the latter term contributes to the renormalization of the position of the level. The value

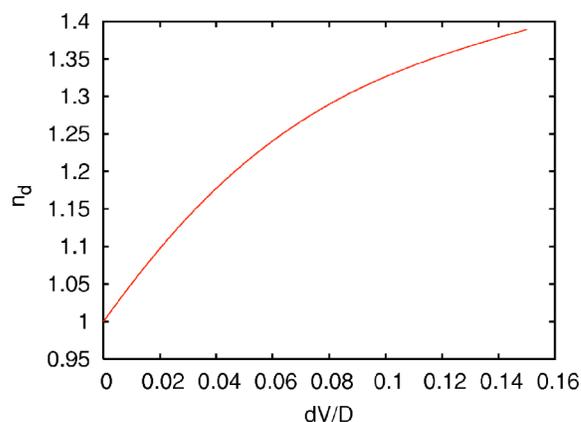


FIG. 1. (Color online) Value of n_d as function of dV for $V=0.2$, $\epsilon_d=-0.025$ and $U=0.05$.

of n_d as function of dV is given in Fig. 1. Since the assisted hopping term renormalizes the impurity level downwards, that term favors the occupancy of the impurity level.

The fact that the assisted hopping term dV and the electron-electron repulsion U have opposite effects can be appreciated in Fig. 2 where the influence of the value of U on n_d , for a fixed value of dV , is shown.

Figure 3 shows the imaginary part of the one-particle Green's function associated to the localized level, defined as

$$\frac{1}{\pi} G_d(\omega) = \sum_{m,\sigma} |\langle 0 | d_\sigma^\dagger | m \rangle|^2 \delta(\omega - \epsilon_m) + \sum_{m,\sigma} |\langle 0 | d_\sigma | m \rangle|^2 \delta(\omega + \epsilon_m), \quad (2)$$

where $|0\rangle$ ($|m\rangle$) is the ground (m th excited) state of the full Hamiltonian with energy $\epsilon_0=0$ (ϵ_m).

In presence of no assisted hopping, the local density of states exhibits a broad peak at the Fermi level which is characteristic to the mixed valence regime of the Anderson impurity model. As dV is increased from zero, the results show a broadening of the resonance, also consistent with the fact that, at the mean-field level, the assisted hopping term modi-

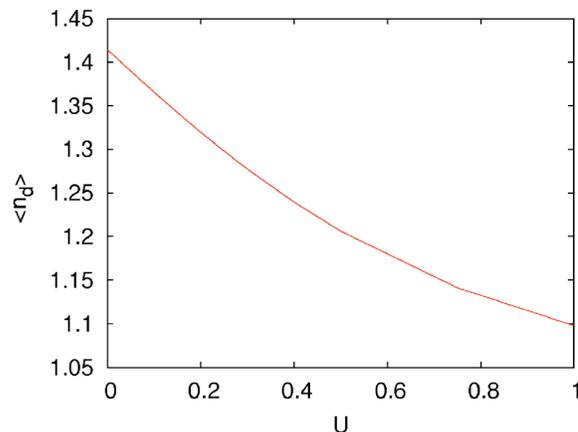


FIG. 2. (Color online) Value of n_d as function of U for $V=0.2$, $\epsilon_d=-0.025$, and $dV=0.15$.

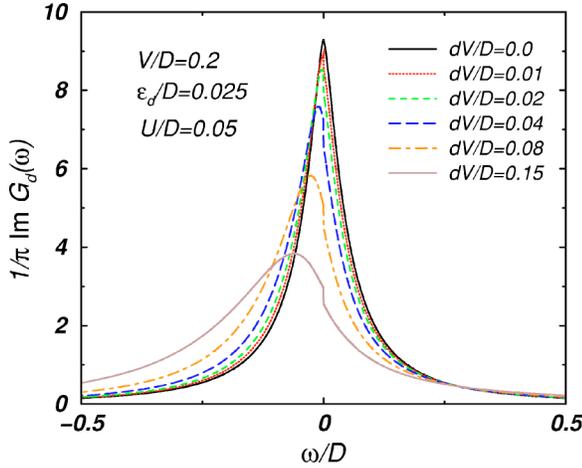


FIG. 3. (Color online) Imaginary part of the impurity one-electron Green's function, $1/\pi G_d(\omega)$, for $V=0.2$, $\epsilon_d=-0.025$, and $U=0.05$.

fies the effective one-particle hopping. As one can see in Fig. 3, the resonance gets not only broadened but also shifted down to negative energies. This fact could already be foreseen from the result for the occupation, since the occupation (at $T=0$) is just the integral of the density of states for negative frequencies. This enhancement of the occupation must leave its trace on the local-moment formation as well.

The influence of the assisted hopping term on the formation of a local moment can be inferred from Fig. 4, which displays the spin-spin correlation function:

$$\text{Im } \rho_S^z(\omega) = \frac{1}{2} \sum_n |\langle 0 | n_{d\uparrow} - n_{d\downarrow} | n \rangle|^2 \delta(\omega - \epsilon_n). \quad (3)$$

This function for $dV=0$ shows a pronounced peak at low energies, which tends to the Kondo temperature below which the local moment is quenched as U increases. At higher energies, $\text{Im} \rho_S^z(\omega) \sim \omega^{-1}$, which corresponds to a Curie susceptibility as function of temperature. This behavior crosses over to a $\text{Im} \rho_S^z(\omega) \sim \omega$ regime, which is characteristic to the

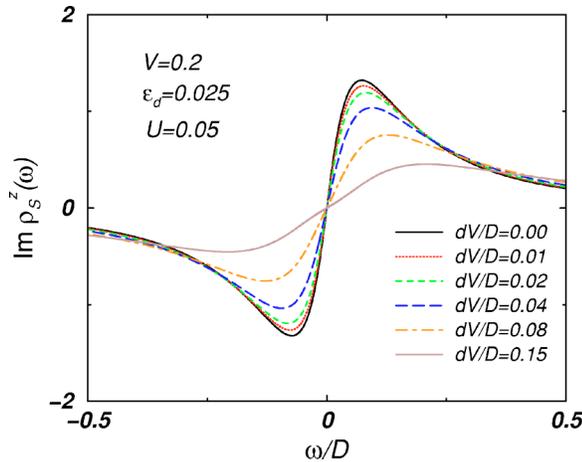


FIG. 4. (Color online) Spin-spin correlation function for $V=0.2$, $\epsilon_d=-0.025$, and $U=0.05$ and different values of dV .

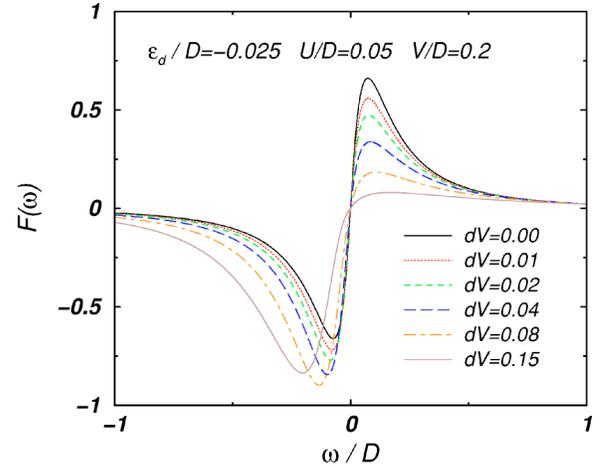


FIG. 5. (Color online) Local pair correlation, $F(\omega)$, in Eq. (4) as function of dV for $\epsilon=-0.025$, $U=0.05$, and $V=0.2$.

compensation of the moment. [Alternatively, one could say that for very high frequencies $\text{Im} \rho_S^z(\omega) \sim \omega^{-1}$ as a consequence of the constant time correlator of the spin for very short times, while for small frequencies $\text{Im} \rho_S^z(\omega)$ shows a linear dependence on ω corresponding to the $\sim t^{-2}$ asymptotics of the correlation. As dV is turned on, this peak becomes broader and it is shifted towards higher energies indicating the suppression of the local moment. This suppression is also consistent with the previous results and might be considered as a fingerprint of the local pairing.

To get a more direct insight to the relation of the assisted hopping and the pairing, we now analyze the possible existence of pairing correlations in the model. Within the reduced Hilbert space of the Anderson's impurity model, we can define two types of such correlations:

$$F(\omega) = \sum_n |\langle 0 | d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger} | n \rangle|^2 \delta(\omega - \epsilon_n) + |\langle 0 | d_{\uparrow} d_{\downarrow} | n \rangle|^2 \delta(\omega + \epsilon_n),$$

$$F'(\omega) = \sum_n \langle 0 | d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger} | n \rangle \langle n | (d_{\uparrow} c_{\downarrow} - d_{\downarrow} c_{\uparrow}) | 0 \rangle \delta(\omega - \epsilon_n)$$

$$+ \langle 0 | d_{\uparrow} d_{\downarrow} | n \rangle \langle n | (d_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} - d_{\downarrow}^{\dagger} c_{\uparrow}^{\dagger}) | 0 \rangle \delta(\omega + \epsilon_n), \quad (4)$$

where $c_{\sigma}^{\dagger} = \sum_k c_{k\sigma}^{\dagger}$, representing the metal orbital closest to the impurity. The function $F(\omega)$ in Eq. (4) gives the magnitude of the on-site pairing, as present, for instance, in the negative- U Anderson's impurity model. The function $F'(\omega)$ describes off-diagonal pairing. Virtual Cooper pairs resonate between the on-site position and that in which one component of the pair is at the impurity and the other is in the metal.

We first analyze the function $F(\omega)$, which is a measure of the on-site pairing. The function $F(\omega)$ is shown in Fig. 5 as a function of the value of dV . For comparison, we plot the same function for $dV=0$ for different values of ϵ in Fig. 6. The two functions show similar behavior, suggesting that the main effect of the assisted hopping term on the *on-site pairing* correlations is the renormalization of the level, since its effect is difficult to be distinguished from the effect of a change in the impurity electron level.

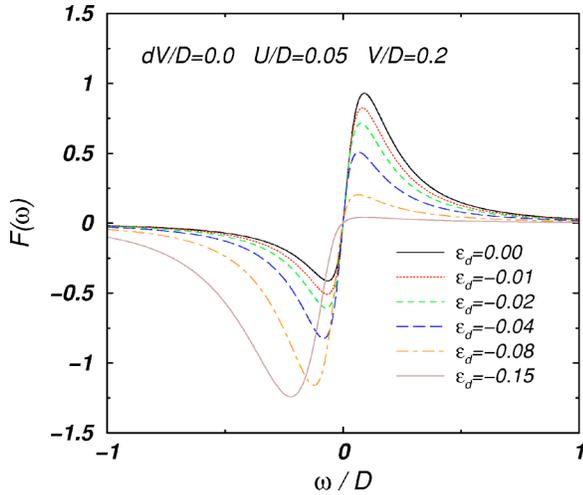


FIG. 6. (Color online) Local pair correlation, $F(\omega)$, in Eq. (4) as function of ϵ for $dV=0$, $U=0.05$, and $V=0.2$.

We estimate the tendency towards pairing by using Eq. (4) to define generalized susceptibilities:

$$\mathcal{F} = \int_0^{\infty} d\omega \frac{F(\omega) + F(-\omega)}{\omega},$$

$$\mathcal{F}' = \int_0^{\infty} d\omega \frac{F'(\omega) + F'(-\omega)}{\omega}. \quad (5)$$

These functions measure the tendency towards the different types of pairing. Figure 7 gives \mathcal{F} as function of ϵ for $dV=0$, and as function of dV for $\epsilon=-0.025$. As it can be appreciated, the inclusion of the assisted hopping term dV does not change significantly the value of this susceptibility. Moreover, its magnitude is not too different from the value ob-

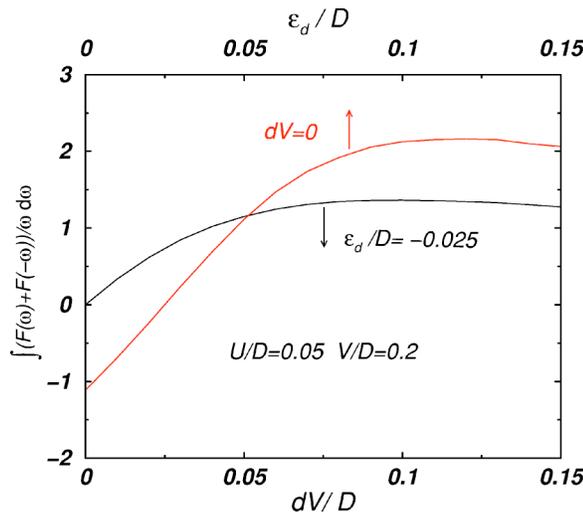


FIG. 7. (Color online) On-site pair susceptibility \mathcal{F} as defined in Eq. (5) as function of ϵ for $dV=0$ (top), and as function of dV for $\epsilon=-0.025$ (bottom).

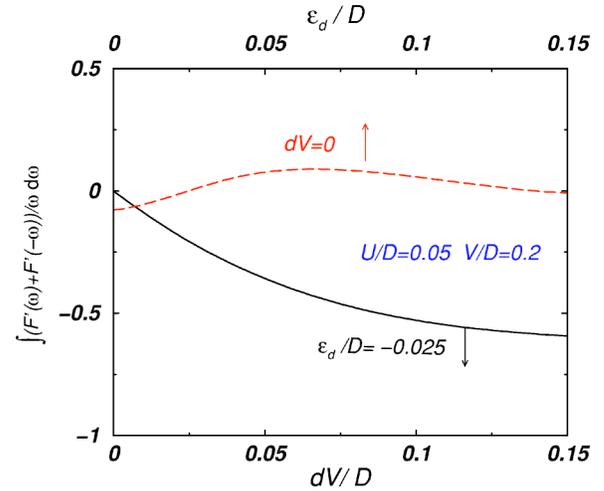


FIG. 8. (Color online) Off-diagonal pair susceptibility \mathcal{F}' as defined in Eq. (5) as function of ϵ for $dV=0$ (top), and as function of dV for $\epsilon=-0.025$ (bottom).

tained for $dV=0$. On the other hand, Fig. 8 gives \mathcal{F}' as function of ϵ for $dV=0$, and as function of dV for $\epsilon=-0.025$. In this case, the effects of dV are quite significant. While of $dV=0$ this susceptibility remains close to zero for the whole range of values of ϵ studied, it raises swiftly as soon as dV is finite. Hence, the assisted hopping term induces an off-diagonal pairing term of the type described by \mathcal{F}' given in Eq. (4).

This is our main result. In contrast to the *local* pairing on the d level—which can be understood as the consequence of the primary effect, the renormalization of the level—the off-diagonal pairing correlations are increased by the enhanced hopping rate which allows stronger fluctuations if the spin of the d electron and the local conduction electron have opposite orientations. There is another interesting feature of this result. Though the formation of the local moment is strongly suppressed and the impurity has no well-defined spin state, the off-diagonal correlations are still enhanced. This would indicate that this type of pairing manifests itself in a dynamical way. The spin state of both the local level and the conduction-electron state fluctuate, but in a correlated way.

IV. CONCLUSIONS

We have studied, using the numerical renormalization-group method, the Anderson impurity model with a hopping, which depends on the charge state of the impurity. This is the simplest model which includes information about the internal structure of the impurity, beyond a single, rigid, electronic state.

Our results indicate that, when the assisted hopping is sufficiently strong, the model shows a crossover to a phase with off-diagonal pairing correlations. It would be interesting to know if this regime could be realized in mesoscopic devices, where the internal structure of a quantum dot can be important.

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