Assisted hopping in the Anderson impurity model: A flow equation study

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We investigate the effect of assisted hopping in the Anderson impurity model. We use the flow equation method, which, by means of unitary transformations, generates a sequence of Hamiltonians in order to eliminate the assisted hopping terms. This approach yields a renormalized on-site energy ϵ_d^*, a renormalized correlation energy U^*, and other terms, which include pair hopping. For some parameter values, the initial Hamiltonian flows towards an attractive Anderson model. We argue that this result implies a tendency towards local pairing fluctuations.

I. INTRODUCTION

The properties of magnetic impurities in metals, and of small dots attached to metallic leads share many characteristics, due to the similar role played by electron-electron interactions. The electrostatic repulsion leads to the formation of local moments,[1,2] which are quenched at sufficiently low temperatures. Quantum dots are more complicated structures[3,4] and an effective Kondo Hamiltonian can only be defined in the limit of large spacing between the electronic levels within the dot. Then, the main physical processes at low temperatures are due to the changes of the occupancy of the level closest to the Fermi energy of the leads. Even if we assume this restriction, terms beyond the Kondo Hamiltonian can arise due to the finite extension and inhomogeneities of the electron states inside a mesoscopic quantum dot. The simplest of these additional interactions is an assisted hopping term, extensively studied in relation to bulk correlated systems.[5,6] It can be shown that, within a systematic expansion in the intradot conductance, the leading correction to the intradot capacitance, or averaged Coulomb interaction, has such a form.[7] The inhomogeneous screening and effective "orthogonality catastrophe" which give rise to this term also lead to interesting nonequilibrium effects in the metallic limit, when the level spacing is much less than the temperature.[8,9]

The present work analyzes the model of a correlated impurity, or quantum dot, in the limit where the low-temperature physical properties are determined by a single electronic state within the dot, using the flow equations first proposed in Refs. 10 and 11. The method transforms the initial Hamiltonian into a family of related Hamiltonians by means of a sequence of unitary transformations. If adequately chosen, these transformations lead to simplified models, in a similar way to a renormalization-group transformation. The method has proven useful for a variety of problems,[12,13] and it has also been used to obtain the Kondo Hamiltonian from the Anderson model.[12]

In the following, we will apply the flow equation technique to the Anderson Hamiltonian with assisted hopping. This problem has been analyzed in Ref. 7 using mean-field techniques, but there are no more accurate studies in the literature. Thus, besides the intrinsic interest of the model, this work provides a test case where the flow equation method is used to obtain the information not available by other techniques.

The following section presents the model, and describes how the flow equation method is applied. The results are discussed in Sec. III. Finally, Sec. IV analyzes the main properties of the model, as derived by this method.

II. THE MODEL AND FLOW EQUATIONS

A. The model

We will study the Hamiltonian

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

$$\mathcal{H}_K = \sum_{k,s} \epsilon_k^0 c_{k,s}^\dagger c_{k,s},$$

$$\mathcal{H}_{imp} = \epsilon_d^0 n_d + U^0 n_{d,+} n_{d,-},$$

$$\mathcal{H}_{hyb} = \sum_{k,s} V_k^0 (c_{k,s}^\dagger d_s + d_s^\dagger c_{k,s}),$$

$$\mathcal{H}_{assisted} = \sum_{k,s} W_k^0 n_{d,s} (c_{k,-s}^\dagger d_{-s} + d_{-s}^\dagger c_{k,-s}), \quad (1)$$

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 $n_d = n_{d,+} + n_{d,-}$.

B. The flow equation method

We now perform a sequence of infinitesimal unitary transformations:

$$\partial_\ell \mathcal{H} = [\eta, \mathcal{H}]. \quad (2)$$

These transformations are characterized by the anti-Hermitian generator $\eta = -\eta^\dagger$. The parameters of the initial Hamiltonians become functions of the flow parameter ℓ and, if there are no upper indices on the parameters, it will be implied that they depend on ℓ.

Our main goal is to reduce the initial Hamiltonian, Eq. (1), to another whose physical properties are well under-

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stood. We assume that this is achieved if the assisted hopping term is made to flow to zero. Hence, we impose the requirement

$$\lim_{\ell \to \infty} \mathcal{H}_{assisted}(\ell) \to 0. \tag{3}$$

This condition is satisfied if $\eta = [\mathcal{H}_K, \mathcal{H}_{assisted}]$. More generally, we will employ the following generator:

$$\eta = \sum_{k,s} \eta_k n_{d,s} (c^{\dagger}_{k,-s} d_{-s} - d^{\dagger}_{-s} c_{k,-s}). \tag{4}$$

This expression differs from the generator used to cancel the hybridization with the band, V^0_k in Eq. (1), in that it contains an additional operator related to the localized orbital $n_{d,s}$. It is interesting to note that for the analytic treatment of the flow equations the explicit expression of the parameters η_k is not needed. We only require that Eq. (3) holds.

The physical properties of the impurity are determined by the flow of the on-site energy ϵ^0_d and the correlation energy U^0 as $\ell \to \infty$. Notice that the one particle hybridization in the Hamiltonian, Eq. (1), is not changed during the flow, i.e.,

$$\partial_\ell \mathcal{H}_{hyb} = 0. \tag{5}$$

This is a consequence of our choice of the generator given in Eq. (4).

The commutator $[\eta, \mathcal{H}]$ generates new interactions which have to be included in the Hamiltonian $\mathcal{H}(\ell)$, which, in turn, will lead to other interactions. This infinite hierarchy needs to be decoupled in order for the method to be useful. This point is carefully discussed in Ref. 12, and we will follow the same procedure. We do not include the new operators in the flow, although they will appear in the fixed-point Hamiltonian. The role of these ''marginal'' operators will be discussed in Sec. III C.

The resulting flow equations thus take on the following simple forms:

$$\partial_\ell \epsilon_d = 2 \sum_k \eta_k (V^0_k + W_k) n^0_k, \tag{6}$$

$$\partial_\ell U = -4 \sum_k \eta_k (V^0_k + W_k), \tag{7}$$

$$\partial_\ell W_k = -(\epsilon^0_k - \epsilon_d - U) \eta_k, \tag{8}$$

where we have introduced the occupation number $n^0_k = (e^{\beta \epsilon^0_k} + 1)^{-1}$, which arises from normal ordering of the neglected operators.[14] The procedure used here explicitly breaks particle-hole symmetry. Note that there is no renormalization of the energies of the conduction electrons, ϵ^0_k, which is a typical feature of impurity problems.[15]

From Eq. (8), we obtain the general relation between the flow of the assisted hopping amplitudes and the generator of the infinitesimal transformations,

$$\eta_k = -\frac{\partial_\ell W_k}{\epsilon^0_k - \epsilon_d - U}. \tag{9}$$

Inserting this expression in Eqs. (6) and (7) we obtain

$$\partial_\ell \epsilon_d = -2 \sum_k \frac{(V^0_k + W_k) \partial_\ell W_k}{\epsilon^0_k - \epsilon_d - U} n^0_k, \tag{10}$$

$$\partial_\ell U = 4 \sum_k \frac{(V^0_k + W_k) \partial_\ell W_k}{\epsilon^0_k - \epsilon_d - U}. \tag{11}$$

Note that the above equations imply that

$$\epsilon^*_d - \epsilon^0_d = F(\epsilon^0_d + U^0), \tag{12}$$

$$U^* - U^0 = G(\epsilon^0_d + U^0), \tag{13}$$

where $\epsilon^*_d \equiv \epsilon_d(\ell = \infty)$ and $U^* \equiv U(\ell = \infty)$, and F and G denote universal functions. These functions only depend on the coupling constants V^0_k and W^0_k.

The above flow equations can also be treated semianalytically by substituting the ℓ-dependent parameters ϵ_d and U in the denominator by their fixed-point values ϵ^*_d and U^*. This strategy has proven to be successful in several related models.[12,16] We can then integrate the Eqs. (10) and (11) from $\ell = 0$ to $\ell = \infty$, using the constraint that $\lim_{\ell \to \infty} W_k \to 0$.

We define

$$J(\epsilon) \equiv \sum_k (2|V^0_k W^0_k| - W^0_k W^0_k) \delta(\epsilon - \epsilon^0_k), \tag{14}$$

where we assume that the hybridization V^0_k and the assisted hopping amplitude W^0_k differ in sign.[5] The spectral function is positive for the physically relevant parameter regime, where the hybridization amplitude is larger or comparable to the assisted hopping amplitude. With the above definition we obtain the final result:

$$\epsilon^*_d - \epsilon^0_d = -\int d\epsilon \frac{J(\epsilon)}{\epsilon - \epsilon^*_d - U^*} f(\epsilon), \tag{15}$$

$$U^* - U^0 = 2 \int d\epsilon \frac{J(\epsilon)}{\epsilon - \epsilon^*_d - U^*}, \tag{16}$$

where we have defined the Fermi function $f(\epsilon) \equiv (e^{\beta \epsilon} + 1)^{-1}$.[14]

III. RESULTS

A. Effective parameters

In order to make the analysis more quantitative, we need to specify the density of states in the surrounding medium, described by the function $J(\epsilon)$, Eq. (14). The width of the conduction band in the leads is $2D$, and the Fermi energy is $\epsilon_F = 0$. We also define
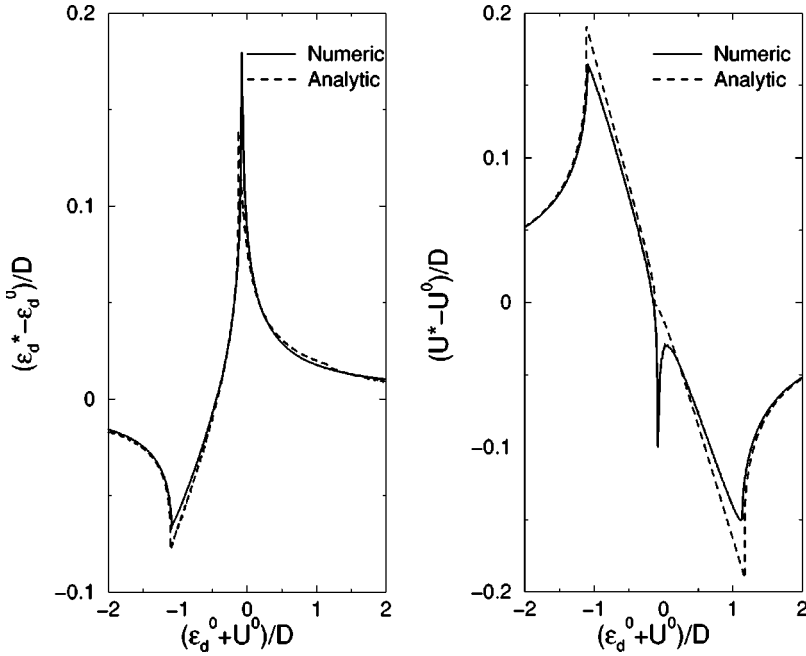
$$V \equiv \sqrt{\sum_k (V^0_k)^2},$$

FIG. 1. The relative fixed point values ϵ_d^* $-\epsilon_d^0$ (left-hand side) and U^*-U^0 (right-hand side) as a function of the scaling variable ϵ_d^0 $+U^0$ for $V/D=0.23$, $W/D=0.17$ at $T=0$. The solid lines follow from the numerically exact solution and the dashed lines from the semianalytical approach.

$$W \equiv \sqrt{\sum_k (W_k^0)^2},$$

$$\Gamma \equiv \pi \rho(\epsilon_F)(2|V_{k_F}^0 W_{k_F}^0| - (W_{k_F}^0)^2) = \pi J(\epsilon_F). \quad (17)$$

We further assume that both coupling functions V_k^0 and W_k^0 are semielliptic. This choice resembles a realistic environment and facilitates the computation.

To obtain the universal functions F and G from Eqs. (12) and (13), we numerically integrate the flow equations (6)–(8) with

$$\eta_k = (\epsilon_k^0 - \epsilon_d - U)W_k. \quad (18)$$

This choice guarantees that W_k vanishes exponentially for $\epsilon_k^0 \neq \epsilon_d^* + U^*$ and algebraically for $\epsilon_k^0 = \epsilon_d^* + U^*$.[12] By this, we introduce an energy-scale dependent decoupling scheme with respect to the renormalized energy of the double occupancy of the dot, $\epsilon_d^* + U^*$.

We now turn to the semianalytical solution. The spectral function of Eq. (14) reads

$$J(\epsilon) \equiv \Theta(D^2 - \epsilon^2)\frac{\Gamma}{\pi D}\sqrt{D^2 - \epsilon^2}, \quad (19)$$

with the resonance $\Gamma = 2(2VW - W^2)/D$. Evaluating Eqs. (15) and (16) we have to distinguish two cases.

For $|\epsilon_d^* + U^*| < D$, we obtain the following self-consistent equations:

$$\epsilon_d^* - \epsilon_d^0 = \frac{\Gamma}{2D}\left[(\epsilon_d^* + U^*) - \frac{2}{\pi}D + \frac{2}{\pi}\sqrt{D^2 - (\epsilon_d^* + U^*)^2}\right.$$

$$\left. \times \ln\frac{|\epsilon_d^* + U^*|}{D - \sqrt{D^2 - (\epsilon_d^* + U^*)^2}}\right], \quad (20)$$

$$U^* - U^0 = -\frac{2\Gamma}{D}(\epsilon_d^* + U^*). \quad (21)$$

For $|\epsilon_d^* + U^*| > D$, we obtain

$$\epsilon_d^* - \epsilon_d^0 = \frac{\Gamma}{2D}\left[(\epsilon_d^* + U^*) - \frac{2}{\pi}D - \text{sgn}(\epsilon_d^* + U^*)\right.$$

$$\times \sqrt{(\epsilon_d^* + U^*)^2 - D^2}$$

$$\left. \times \left(1 - \frac{2}{\pi}\arcsin\frac{D}{(\epsilon_d^* + U^*)}\right)\right], \quad (22)$$

$$U^* - U^0 = -\frac{2\Gamma}{D}[(\epsilon_d^* + U^*) - \text{sgn}(\epsilon_d^* + U^*)$$

$$\times \sqrt{(\epsilon_d^* + U^*)^2 - D^2}]. \quad (23)$$

In Fig. 1, the numerically exact universal functions F and G of Eqs. (12) and (13) are shown as functions of the scaling variable $\epsilon_d^0 + U^0$ (solid line). The coupling strengths were chosen to be $V/D = 0.23$ and $W/D = 0.17$.[17] The semianalytical solution (dashed line) given in Eqs. (20)–(23) qualitatively agrees with the exact solution. The main difference is that the kink in $U^* - U^0$ near $\epsilon_d^0 + U^0 \approx 0$ which is present in the numerical solution is not adequately reproduced by our analytical approach, Eq. (20). This is due to the cruder decoupling scheme which does not incorporate energy-scale separation. It is interesting to note that at this point, the numerical solution yields $\epsilon_d^* + U^* = 0$. It will lead to significant differences for the phase diagram which will be discussed in the following subsection.
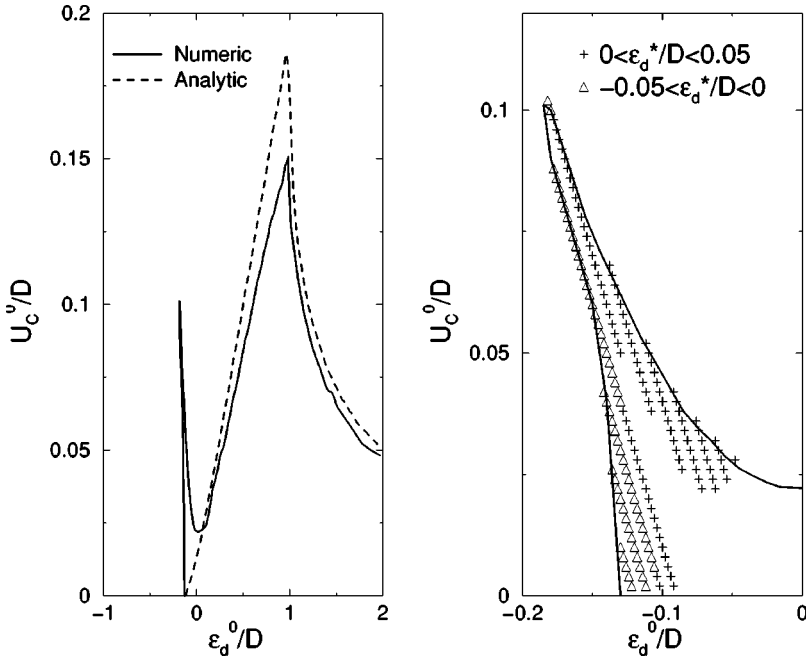
FIG. 2. Left-hand side: The critical correlation energy U_c^0 as a function of ϵ_d^0 following from the numerical (solid line) and semianalytical (dashed line) solutions with $V/D = 0.23$ and $W/D = 0.17$ at $T = 0$. Right-hand side: The critical correlation energy U_c^0 as a function of ϵ_d^0 following from the numerical solution in the regime where $|\epsilon_d^*/D| \leq 0.05$.

B. Critical correlation energy

Equation (21) yields

$$U^* = \frac{U^0 - 2\epsilon_d^* \Gamma/D}{1 + 2\Gamma/D}. \tag{24}$$

Hence, for $\epsilon_d^* > 0$, the renormalized interaction can become negative.

We thus define the critical initial correlation energy U_c^0 such that the renormalized correlation energy U^* becomes zero, i.e.,

$$U^*(U_c^0|\epsilon_d^0) \overset{!}{=} 0. \tag{25}$$

U_c^0 depends on the initial on-site energy ϵ_d^0 and we further restrict U_c^0 to be positive.

The critical correlation energy U_c^0 is enhanced for positive on-site energies $\epsilon_d^0 \geq 0$. This property can most clearly be seen from the analysis of Eqs. (15) and (16) for $T = \infty$.[18] Then, the Fermi function is constant, i.e., $f(\epsilon) = 1/2$, and the integrals yield simple expressions. For the semielliptical coupling function, we obtain for $\epsilon_d^0 < D + \Gamma/2$

$$U_c^0 = \frac{2\Gamma}{D - \Gamma/2} \epsilon_d^0. \tag{26}$$

On the left-hand side of Fig. 2, the critical correlation energy U_c^0 is shown as a function of the initial on-site energy ϵ_d^0 as it follows from the numerical (solid line) and semianalytical (dashed line) solutions. The coupling strengths were again chosen to be $V/D = 0.23$ and $W/D = 0.17$. The main difference between the two curves stems from the spike of $G(\epsilon_d^0 + U^0)$ around $\epsilon_d^0 + U^0 \approx 0$, seen on the right-hand side of Fig. 1.

C. Pairing correlations

It is now interesting to consider the possibility of local pairing correlations. Pair formation does not rely on particle-hole symmetry, in fact, asymmetries can actually enhance this phenomenon.[19] But local pairing can only occur if—in addition to an effective negative correlation energy $U^* < 0$—the renormalized on-site energy ϵ_d^* lies sufficiently close to the chemical potential $\mu = 0$.[20] The local pairing regime is thus determined by the trade-off between a high critical correlation energy U_c^0 and an effective on-site energy ϵ_d^* sufficiently close to the chemical potential.

To discuss the phase diagram of this local pairing regime we will only consider the numerical solution. This approach is more reliable since it incorporates a systematic decoupling of the assisted hopping term, starting with large and ending with small energy differences with respect to $\epsilon_d^* + U^*$. The results are presented on the right-hand side of Fig. 2, where the critical correlation energy U_c^0 is shown as a function of ϵ_d^0 in the regime where $|\epsilon_d^*/D| \leq 0.05$. Furthermore, we distinguish between positive ($+$) and negative ($\triangle$) renormalized on-site energy ϵ_d^*.

Our analysis predicts local pairing for values of ϵ_d^0 which favor double occupancy, and $U_c^0 \lesssim 0.1$. The mean-field analysis in Ref. 7 gives local pairing for $U_c^0 \lesssim 0.05$ and a similar range of values of ϵ_d^0 (note that we are using here comparable hybridization with the band).

It is interesting to note that the strong renormalization of U^* for $\epsilon_d^0 + U^0 \approx 0$ only occurs at large values of $\ell \gg 1/D^2$. Therefore, it is not present in the semianalytical solution which does not incorporate energy-scale separation. Furthermore, there are fixed points for which $\epsilon_d^* \approx U^* \approx 0$, i.e., a degeneracy between the zero-charge and two-charge state of the impurity. Since the marginal interactions also include pseudospin-pseudospin couplings, this might give rise to the Kondo effect in the charge channel, i.e., in the mixed-valence regime.

D. Marginal interactions

We now analyze the marginal terms, which have been neglected so far. One term will be interpreted as a renormalization of the hybridization term V_k^0. This identification is crucial since the assisted hopping term W_k^0 contains an effective hybridization term which must be present in the fixed point Hamiltonian. Another term will explicitly favor local pairing.

As in the Anderson model, the flow generates spin-spin and pseudospin-pseudospin couplings:

$$\mathcal{H}_{SW} = -\sum_{k,k'} V_{k,k'}^*[(:\psi_k^{\dagger\frac{1}{2}}\vec{\sigma}\psi_{k'}:+\text{H.c.})(\psi_d^{\dagger\frac{1}{2}}\vec{\sigma}\psi_d)$$
$$-(:\widetilde{\psi}_k^{\dagger\frac{1}{2}}\vec{\sigma}\widetilde{\psi}_{k'}:+\text{H.c.})(\widetilde{\psi}_d^{\dagger\frac{1}{2}}\vec{\sigma}\widetilde{\psi}_d)]. \quad (27)$$

In addition to this interaction, the following term is also generated:

$$\mathcal{H}_{irr} = \frac{1}{2}\sum_{k,k'} V_{k,k'}^*(:\psi_k^{\dagger}\psi_{k'}:+\text{H.c.})+\widetilde{\epsilon}_d^*(n_d-1). \quad (28)$$

The existence of these terms is independent of the assisted hopping interaction and has been discussed in detail in relation with the Anderson model.[12] There, $\mathcal{H}_{SW}$ gives rise to the well-known Kondo behavior in the spin and charge sectors, respectively.

$\mathcal{H}_{irr}$ is usually neglected in the fixed point Hamiltonian since the first term of Eq. (28) represents potential scattering of the conduction electrons and will be irrelevant for our discussion. The last term renormalizes the on-site energy by $\widetilde{\epsilon}_d^* \equiv \Sigma_k V_{k,k}^*/2$. For the semielliptical coupling function (19), we obtain $\widetilde{\epsilon}_d^*/\epsilon_d^* \approx \Gamma/2D$ according to Eq. (30) within the semianalytical treatment. Our approximation—not to include newly generated coupling terms into the flow of the Hamiltonian—is thus consistent for $\Gamma/D \ll 1$. As in Ref. 12, we will ignore all terms of Eq. (28) in the fixed-point Hamiltonian and assume that they can be taken into account by redefining the initial parameters.

Finally, the commutator $[\eta, \mathcal{H}_{assisted}]$ also gives rise to the following pairing term:

$$\mathcal{H}_{pair} = \sum_{k,k',s} W_{k,k'}^*[c_{k,s}^{\dagger}c_{k',-s}^{\dagger}d_{-s}d_s+\text{H.c.}], \quad (29)$$

which has the same shape as some of the contributions in $\mathcal{H}_{SW}$, Eq. (27).

The additional contributions of Eqs. (27)–(29) need to be included in the flow equation scheme. As these terms contain an even number of operators associated with the localized level, but the generator, Eq. (4), contains an odd number, these terms cannot directly change the flow equations of the parameters U and ϵ_d, Eqs. (6) and (7). They can, however, change the flow of the assisted hopping term, Eq. (8), which will eventually modify Eqs. (6) and (7). We will neglect this second-order modification of the flow equations for U and ϵ_d. This approximation was initially introduced in Ref. 12 and is based on the fact that $V_{k,k'}=0$ and $W_{k,k'}=0$ for ℓ

=0. Note that, provided that the flow equations are unchanged, the presence of these marginal terms in the fixed-point Hamiltonian does not alter the main conclusions of the paper.

We now approximate the magnitude of these terms at the fixed point, neglecting their influence on the flow equations. We obtain

$$V_{k,k'}^* = 2\int_0^{\infty} d\ell\, \eta_k(V_{k'}^0+W_{k'}) \approx -\frac{2|W_k^0 V_{k'}^0|-W_k^0 W_{k'}^0}{\epsilon_{k'}-\epsilon_d^*-U^*}, \quad (30)$$

$$W_{k,k'}^* = \int_0^{\infty} d\ell\, \eta_k W_{k'} \approx \frac{1}{2}\frac{W_k^0 W_{k'}^0}{\epsilon_{k'}-\epsilon_d^*-U^*}. \quad (31)$$

As mentioned earlier, $\mathcal{H}_{SW}$ arises in the analysis of the Anderson Hamiltonian, due to the effects of the hybridization between the state at the impurity and the conduction band, and can be derived by means of a Schrieffer-Wolff transformation.[21] Hence, we can interpret these fixed-point interactions as arising from an effective hopping term in the initial Hamiltonian, which, indeed, can be obtained from a mean-field decoupling of the assisted hopping term. $\mathcal{H}_{pair}$ will enhance the tendency towards pair formation.

IV. CONCLUSIONS

We have studied a model of an impurity, or a quantum dot, with a single electronic level, an on-site repulsion term, hybridization, and assisted hopping. The flow equation method allows us to map the model onto an effective Anderson model without assisted hopping, and with additional Kondo couplings and pair hopping terms.

The most interesting outcome of our calculation is that the value of the on-site electron-electron interaction can become attractive, because of the effect on the flow of the initial assisted hopping term. Although the Anderson model with attractive interactions has not been as extensively studied[19,20] as the repulsive Anderson model, we think that our mapping suffices to give a qualitative description of the physical properties of the model for the interesting case of a relatively strong assisted hopping term. Note that, in addition to a renormalized on-site interaction term, terms which describe pair hopping between the impurity and the conduction band are generated. We expect that significant local pairing correlations will develop in this regime.

This result is in agreement with general arguments which suggest that assisted hopping interactions tend to favor superconducting ground states,[5] and with mean-field studies of the same impurity model.[7] A related tendency towards phase rigidity can be found in the limit where the level spacing within the impurity is negligible with respect to the other parameters.[8,9]

The model does not have electron-hole symmetry, and local pairing is mainly favored when the number of electrons at the impurity exceeds one (half filling), and when the direct hopping and the assisted hoping terms have opposite signs, also in agreement with general properties of bulk systems.

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