Hybridization versus Local Exchange Interaction in the Kondo Problem: A Two-Band Model

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The competition between local exchange and hybridization in Kondo systems is investigated by studying a model in which a localized spin $1/2$ has an exchange interaction with two bands with a ferromagnetic coupling $J_{\mathrm{sf}} > 0$ and an antiferromagnetic coupling $J_{\mathrm{hyb}} < 0$, respectively. It is shown that a Kondo effect takes place even for large values of the ratio $|J_{\mathrm{sf}}/J_{\mathrm{hyb}}|$. The results should be applicable to real systems when orbital degeneracy is taken into account, and indicate that the Kondo effect can occur even in the presence of a strong local exchange. Consequences on the picture of the competition between the two effects are discussed. [S0031-9007(96)01202-1]

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The magnetic interaction in normal rare-earth compounds originates from local exchange between the f shell and conduction electrons through the Ruderman-Kittel-Kasuya-Yosida (RKKY) mechanism. In anomalous rare-earth compounds (Kondo systems and heavy fermions) the electronic hybridization between f and band electrons gives rise to the Kondo effect and tends to produce the nonmagnetic heavy Fermi liquid ground state [1].

The observation of Kondo-like phenomena suggests that hybridization dominates over local exchange; this is usually taken for granted in the study of Kondo systems, and, in fact, local exchange is neglected in the commonly adopted Anderson model. However, electronic structure calculations suggest that in several Ce compounds (like CeTe, CeSe, CeAg) the magnetic interaction is determined essentially by local exchange, rather than by the hybridization-induced pair coupling: in fact, the magnetic ordering temperature calculated by keeping hybridization only is an order of magnitude smaller than the experimental value [2,3], while agreement with experiment is obtained when local exchange is accounted for [2].

This behavior cannot be understood within a simple spin $1/2$ one-band model. In such a model the local exchange coupling J_{sf} [which is usually ferromagnetic (FM), $J_{\mathrm{sf}} > 0$] competes with the antiferromagnetic (AFM) coupling $J_{\mathrm{hyb}} < 0$ generated from hybridization through the Schrieffer-Wolff transformation [4]: the relevant coupling is $J_{\mathrm{sf}} + J_{\mathrm{hyb}}$, so that the Kondo effect occurs only when $|J_{\mathrm{hyb}}| > J_{\mathrm{sf}}$ [5]. However, more subtle effects can take place in the presence of orbital degeneracy. Under the usual assumption that hybridization is spherically symmetric and local exchange is a spin-only interaction, hybridization couples the f shell with conduction electrons in a partial wave $l = 3$ around the impurity site [6], while local exchange couples the f shell to band electrons in a $l = 0$ state. Thus the Kondo and local exchange interactions involve two different conduction electron channels.

In this Letter we model this situation by studying a two-band (or two-channel) Hamiltonian in which a localized spin $1/2$ interacts with two distinct bands, with a FM coupling $J_{\mathrm{sf}} > 0$ and an AFM coupling $J_{\mathrm{hyb}} < 0$, respectively. Since a FM coupling is known to scale to weak coupling for the one-band model at low temperatures, while AFM coupling scales always to strong coupling, it can be expected that the Kondo effect persists even when the ratio $|J_{\mathrm{sf}}/J_{\mathrm{hyb}}|$ is large. This is shown explicitly in this paper, and leads to a picture of the competition between Kondo effect and magnetic ordering which is quite different from the commonly assumed one.

The model Hamiltonian is

$$H = \sum_{\nu\sigma} \epsilon_\nu c^\dagger_{\nu\sigma} c_{\nu\sigma} + \sum_{q\sigma} \epsilon_q c^\dagger_{q\sigma} c_{q\sigma} - J_{\mathrm{sf}} \vec{s}_F(0) \cdot \vec{S}_f - J_{\mathrm{hyb}} \vec{s}_{AF}(0) \cdot \vec{S}_f , \qquad (1)$$

where ϵ_ν (ϵ_q) is the energy of an FM-band (AF-band) conduction electron with wave vector $\vec{\nu}$ ($\vec{q}$). The FM-band (AF-band) cutoff is B_F (B_{AF}). The exchange interaction between the localized spin $\vec{S}_f$ and the FM-band (AF-band) spin density at the impurity site, $\vec{s}_F(0)$ [$\vec{s}_{AF}(0)$], is FM [AFM] with a coupling constant $J_{\mathrm{sf}} > 0$ [$J_{\mathrm{hyb}} < 0$].

We adopt the nonperturbative method developed by Yoshimori and Yosida [7] for the one-band Kondo model, in which the ground-state wave function is expanded in a many-body basis with electron-hole excitations [see Fig. 1(a)] and $S_{\mathrm{tot}} = 0$. An integral equation for the lowest-order expansion coefficient (d_q) is derived by a resummation to infinite order in J_{hyb}, keeping only the (logarithmically) most divergent terms. The equation can be solved analytically, and its solution describes the formation of a many-body singlet ground state. The nonperturbative energy gain is defined to be the Kondo temperature and is given by $T_K^0 = B_{AF} \exp(1/\rho J_{\mathrm{hyb}})$, where ρ is the

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band density of states (assumed to be constant). T_K^0 has the correct exponent, but is higher than the exact Kondo temperature, $T_K^{\text{exact}} \sim \sqrt{|\rho J_{\text{hyb}}|}\, B_{AF} \exp(1/\rho J_{\text{hyb}})$ [8].

The basis for the two-band model is illustrated in Fig. 1(b). The lowest-order state on the left has one electron on the impurity level, one electron with wave vector $\vec{\nu}$ over the FM-band Fermi sea, and one electron with wave vector $\vec{q}$ over the AF-band Fermi sea. The higher order states on the right have an additional electron-hole excitation in either the FM band or the AF band. The ground-state wave function is found in the subspace $S_{\text{tot}} = 1/2$, which allows for a singlet state between localized spin and one of the conduction spins. The integral equations resulting from the Yosida procedure for the two-band Kondo model are given by (setting $\rho J \rightarrow J$ for simplicity)

$$
\begin{aligned}
&[\epsilon_q + \epsilon_\nu - \epsilon + \Delta E(\epsilon_q, \epsilon_\nu)]\left(d_{q\nu} + \frac{1}{2} c_{q\nu}\right) \\
&\quad = -3\left(\frac{J_{\text{hyb}}}{4}\right) \int d\epsilon_{q'} \left(d_{q'\nu} + \frac{1}{2} c_{q'\nu}\right) - \frac{3}{2}\left(\frac{J_{\text{sf}}}{4}\right) \int d\epsilon_{\nu'}\, c_{q\nu'} \\
&\quad - 3\left(\frac{J_{\text{hyb}}}{4}\right)^2 \int d\epsilon_{q'} \ln\left(\frac{\epsilon_{q'} + \epsilon_q + \epsilon_\nu - \epsilon}{B_{AF}}\right)\left[1 - J_{\text{hyb}} \ln\left(\frac{\epsilon_{q'} + \epsilon_q + \epsilon_\nu - \epsilon}{B_{AF}}\right)\right]^{-1}\left(d_{q'\nu} + \frac{1}{2} c_{q'\nu}\right) \\
&\quad + 3\left(\frac{J_{\text{sf}}}{4}\right)^2 \int d\epsilon_{\nu'} \ln\left(\frac{\epsilon_{\nu'} + \epsilon_q + \epsilon_\nu - \epsilon}{B_F}\right)\left[1 - J_{\text{sf}} \ln\left(\frac{\epsilon_{\nu'} + \epsilon_q + \epsilon_\nu - \epsilon}{B_F}\right)\right]^{-1}\left(d_{q\nu'} - \frac{1}{2} c_{q\nu'}\right) \\
&\quad + 6\left(\frac{J_{\text{hyb}}}{4}\right)^3 \int d\epsilon_{q'}\, I_{AF}(\epsilon_{q'}, \epsilon_q, \epsilon_\nu)\left(d_{q'\nu} + \frac{1}{2} c_{q'\nu}\right) + 3\left(\frac{J_{\text{hyb}}}{4}\right)^2\left(\frac{J_{\text{sf}}}{4}\right) \int d\epsilon_{\nu'}\, I_{AF}(\epsilon_{\nu'}, \epsilon_\nu, \epsilon_q) c_{q\nu'} \\
&\quad + 6\left(\frac{J_{\text{sf}}}{4}\right)^2\left(\frac{J_{\text{hyb}}}{4}\right) \int d\epsilon_{q'}\, I_F(\epsilon_{q'}, \epsilon_q, \epsilon_\nu)\left(d_{q'\nu} + \frac{1}{2} c_{q'\nu}\right) + 3\left(\frac{J_{\text{sf}}}{4}\right)^3 \int d\epsilon_{\nu'}\, I_F(\epsilon_{\nu'}, \epsilon_\nu, \epsilon_q) c_{q\nu'}\,, \qquad (2)
\end{aligned}
$$

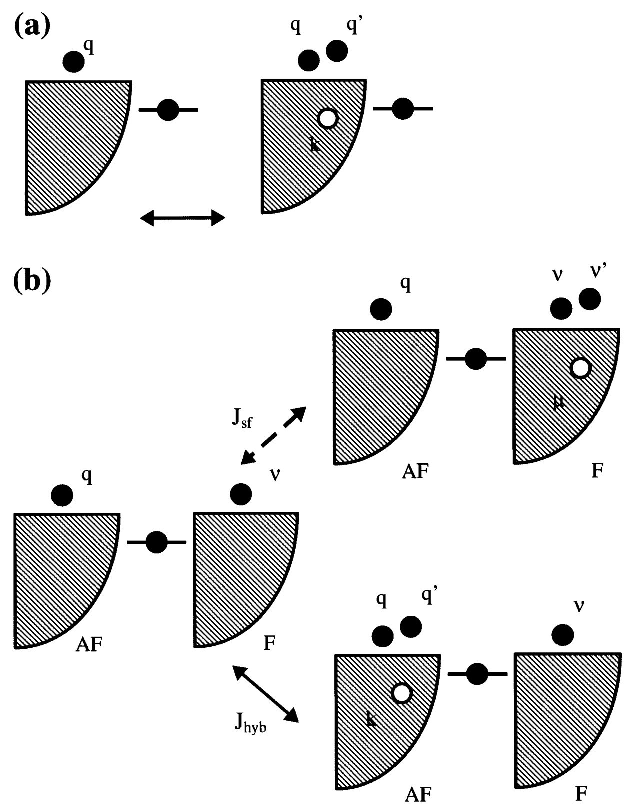

FIG. 1. Schematic representation of the many-body basis used in the Yosida method for (a) the one-band Kondo problem and (b) the present two-band Kondo model.

where

$$
I_\alpha(x, y, t) = -\frac{h_\alpha(x + t) - h_\alpha(y + t)}{x - y}\,, \qquad \alpha = \text{AF}, \text{FM}\,, \qquad (3)
$$

$$
h_\alpha(x) = f_\alpha(x) - 2 f_\alpha(x + B_\alpha) + f_\alpha(x + 2B_\alpha)\,, \qquad (4)
$$

$$
f_\alpha(x) = (-\epsilon + x) \ln\left(\frac{-\epsilon + x}{B_\alpha}\right), \qquad (5)
$$

and by another equation, which can be derived from (2) with the interchanges $J_{\text{sf}} \leftrightarrow J_{\text{hyb}}$ and AF band $\leftrightarrow$ FM band. ΔE is the perturbative correction to the ground-state energy, which is the same for the $S_{\text{tot}} = 1/2$ and $S_{\text{tot}} = 3/2$ states, and to leading order is given by

$$
\Delta E = -6\left(\frac{J_{\text{sf}}}{4}\right)^2 h_F(\epsilon_q + \epsilon_\nu) - 6\left(\frac{J_{\text{hyb}}}{4}\right)^2 h_{AF}(\epsilon_q + \epsilon_\nu). \qquad (6)
$$

The right-hand side contains two first order terms, followed by two second order terms, which include a resummation in the most divergent approximation. The third order terms are nondivergent and two of them (those proportional to $J_{\text{sf}}^2 J_{\text{hyb}}$ and to $J_{\text{hyb}}^2 J_{\text{sf}}$) are crossed. For the AF band alone, keeping the third order nondivergent term (which was neglected by Yosida) in the integral equation for d_q can be shown to yield a lowering of T_K towards the exact value T_K^{exact}. The integral equations for the two-band model do not seem to admit analytical solutions:

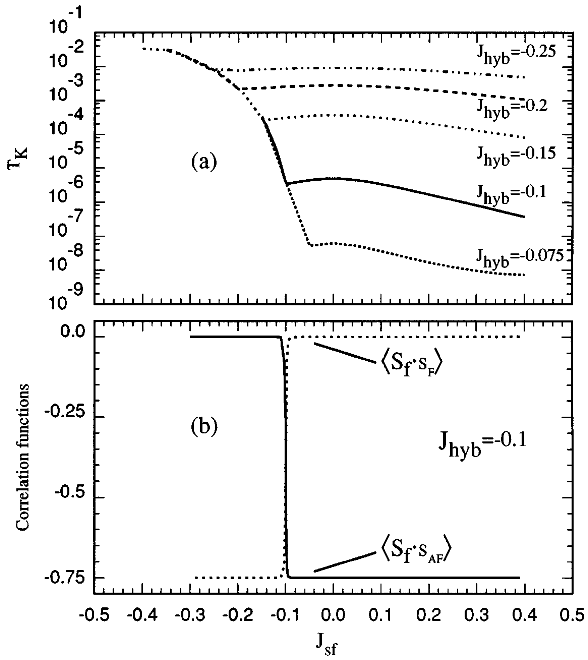

FIG. 2. (a) Kondo temperature as a function of J_{sf} for different values of J_{hyb} ($B_F = B_{AF} = 1$) and (b) correlation function $\langle \vec{S}_f \cdot \vec{s}_{AF} \rangle$ (solid line), $\langle \vec{S}_f \cdot \vec{s}_F \rangle$ (dotted line), as a function of J_{sf} for $J_{\mathrm{hyb}} = -0.1$ from the Yosida method.

we therefore adopt a numerical technique based on logarithmic discretization of the band energies and Gaussian integration. The equations are then solved by a scanning procedure which yields the ground-state energy to great accuracy. T_K is defined as the energy gain of the $S_{\mathrm{tot}} = 1/2$ ground state with respect to the $S_{\mathrm{tot}} = 3/2$ ground state.

In Fig. 2 we show the Kondo temperature and correlation functions as a function of J_{sf}. It can be seen from Fig. 2(a) that T_K first decreases when $|J_{\mathrm{sf}}|$ is finite and small ($|J_{\mathrm{sf}}| \ll |J_{\mathrm{hyb}}|$). When J_{sf} is negative (AFM) and $J_{\mathrm{sf}} < J_{\mathrm{hyb}}$, T_K starts to increase again: this is due to the fact that the role of the two bands is interchanged, and T_K is now determined by J_{sf}. The most interesting region for us is where $J_{\mathrm{sf}} > 0$: here T_K decreases continuously. In Fig. 2(b) we plot the ground-state correlation between the f spin and the total spin in each one of the two bands for $J_{\mathrm{hyb}} = -0.1$. This is calculated by keeping the lowest-order basis state in the ground state, which can be shown to be the dominant one. Figure 2(b) proves that a (Kondo) singlet is formed with the AF band for all values of J_{sf}, except when J_{sf} is more negative than J_{hyb}, in which case the singlet is formed with the FM band. The results of Fig. 2 confirm the expectations discussed at the beginning: the Kondo effect persists even when $J_{\mathrm{sf}} \gg |J_{\mathrm{hyb}}|$ (provided, of course, both couplings are $\ll 1$, which is the physically relevant region). This behavior is very different from that of a one-band model with hybridization and local exchange, where the Kondo effect disappears as soon as $J_{\mathrm{sf}} > |J_{\mathrm{hyb}}|$ [5].

The decrease of T_K for increasing J_{sf} can be understood as follows. For $J_{\mathrm{sf}} \to \infty$, the hopping in the FM band becomes negligible, and the localized spin is locked in a triplet state with the FM band at the impurity site. We call $\vec{S}_{\mathrm{eff}} = \vec{S}_f + \vec{s}_F$ this effective spin one. In the limit $J_{\mathrm{sf}} \to \infty$ the two-band model can therefore be mapped onto the model

$$H = \sum_{q\sigma} \epsilon_q c_{q\sigma}^\dagger c_{q\sigma} - \frac{J_{\mathrm{hyb}}}{2} \vec{s}_{AF}(0) \cdot \vec{S}_{\mathrm{eff}} . \tag{7}$$

This is the Hamiltonian of a localized spin 1 interacting through AFM exchange interaction with a spin $1/2$ band. The AFM coupling constant is $J_{\mathrm{hyb}}/2$. The model (7) describes an undercompensated Kondo effect: the related expression of T_K (apart from the prefactor) is $T_K^\infty \sim B_{AF} \exp(2/J_{\mathrm{hyb}})$. Thus the Kondo temperature is expected to decrease monotonically from the value T_K^0, found for $J_{\mathrm{sf}} = 0$, to the value T_K^∞, found for $J_{\mathrm{sf}} \to \infty$ ($T_K^0 > T_K^\infty$). The impurity susceptibility remains finite for all finite values of J_{sf} and diverges for $J_{\mathrm{sf}} \to \infty$.

We have studied the two-band model also by perturbative scaling [9]. We calculate the change of the effective coupling constants as the two-band cutoffs B_F and B_{AF} are reduced. The scaling equations up to third order in the coupling constants (which in the one-band case yield the correct expression for T_K [1]) are

$$\delta J_{\mathrm{hyb}} = [J_{\mathrm{hyb}}^2 + \tfrac{1}{2} J_{\mathrm{hyb}}^3] \delta \ln(B_{AF}) + \tfrac{1}{2} J_{\mathrm{hyb}} J_{\mathrm{sf}}^2 \delta \ln(B_F), \tag{8}$$

$$\delta J_{\mathrm{sf}} = [J_{\mathrm{sf}}^2 + \tfrac{1}{2} J_{\mathrm{sf}}^3] \delta \ln(B_F) + \tfrac{1}{2} J_{\mathrm{sf}} J_{\mathrm{hyb}}^2 \, \delta \ln(B_{AF}). \tag{9}$$

We take $B_F = B_{AF}$ and reduce the two cutoffs simultaneously. There are four fixed points: (1) $J_{\mathrm{sf}} = J_{\mathrm{hyb}} = 0$. This is a trivial, unstable fixed point, which is the end of all trajectories when the starting point of the scaling procedure falls in the quadrant ($J_{\mathrm{sf}} > 0, J_{\mathrm{hyb}} > 0$). (2) $J_{\mathrm{sf}} = J_{\mathrm{hyb}} = -1$. This is an unstable, non-Fermi-liquid fixed point, already discussed in Refs. [10,11] in the context of the multichannel Kondo problem. (3) $J_{\mathrm{sf}} = 0, J_{\mathrm{hyb}} = -2$. This is a stable fixed point of the scaling equations. Of course, the scaling equations are valid only for $|J_{\mathrm{hyb}}|, |J_{\mathrm{sf}}| \ll 1$: in fact, for the full model the corresponding fixed point will be moved to $(0, J_{\mathrm{hyb}} \to -\infty)$, as for the one-band model [10]. Since the effective interaction J_{hyb} scales to strong coupling, a Kondo effect must occur at low temperature. This strong coupling fixed point is the end of all trajectories starting in the ($J_{\mathrm{sf}} > 0, J_{\mathrm{hyb}} < 0$) quadrant: this shows that a Kondo effect eventually takes place for all values of the couplings in this quadrant. (4) $J_{\mathrm{sf}} = -2, J_{\mathrm{hyb}} = 0$. This is the obvious counterpart of $(0, -2)$ discussed above. The resulting scaling trajectories for the full model (1) are shown in Fig. 3.

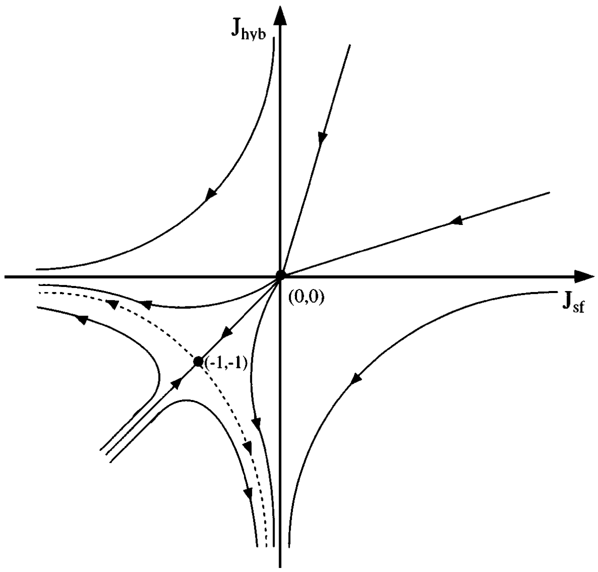

FIG. 3. Sketch of the scaling trajectories for the two-band model (1).

Thus the study of the scaling equations confirms that a Kondo effect (namely, a crossover to strong coupling) takes place for $J_{\mathrm{sf}} > 0$, $J_{\mathrm{hyb}} < 0$, irrespective of the ratio $J_{\mathrm{sf}}/J_{\mathrm{hyb}}$. Although the scaling equations are derived only for $|J_{\mathrm{hyb}}|, |J_{\mathrm{sf}}| \ll 1$, the conclusions inferred from the flux diagram should remain valid also beyond the perturbative procedure, as discussed by Nozières and Blandin [10].

It is interesting to calculate the variation of T_K as a function of J_{sf} (at fixed J_{hyb}) by means of the scaling trajectories. This can be done by reducing both band cutoffs simultaneously starting from $B_F = B_{AF} = 1$ and defining T_K as the value of the cutoff at which J_{hyb} equals a given value, which we have taken to be $J_{\mathrm{hyb}} = -1/2$, for a given pair of starting values $(J_{\mathrm{hyb}}, J_{\mathrm{sf}})$. The resulting T_K are found to be quite similar to those of Fig. 2(a): the results of the scaling procedure are therefore in fair agreement with those from the Yosida approach.

The main result of the present study is that even in the regime $|J_{\mathrm{hyb}}| \ll J_{\mathrm{sf}} \ll 1$ a Kondo effect (i.e., a quenching of the impurity moment) takes place at low temperature; the relevant scale T_K decreases on increasing J_{sf}. This shows that within the present one-impurity model, local exchange is essentially ineffective in eliminating the Kondo effect, which persists for all physically relevant values of the parameters.

The mechanism for competition between hybridization and local exchange must therefore be studied within a periodic model. Here an additional effect occurs, namely, a pair interaction between localized spins originating from both hybridization and local exchange [2]. Competition between Kondo effect and magnetic ordering is well described by treating the magnetic interaction at a mean-field level [12,13]: such a treatment shows that the condition for the onset of magnetic ordering is that the magnetic coupling be larger than T_K. Therefore the Kondo effect persists even when local exchange is much larger than hybridization, provided the pair coupling $I_{\mathrm{RKKY}} < T_K$. Thus it is fully possible that the indirect interaction be determined by local exchange, while the Kondo effect still takes place due to the presence of a small hybridization. These conclusions might help in explaining why rare-earth materials with f-band hybridization are so frequently found in a nonmagnetic state, even when local exchange is large: basically, the relevant quantities to be compared are not hybridization and local exchange in a single-impurity model, but rather the Kondo temperature with the pair coupling in a lattice framework.

The above conclusions are, of course, born out of a simplified spin $1/2$ model. The next step will be to study a realistic model with orbital degeneracy and to look at the effect of the different interactions involving spin and orbital degrees of freedom.

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[1] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1993).
[2] N. Kioussis, B. R. Cooper, and J. M. Wills, Phys. Rev. B **44**, 10 003 (1991); Q. G. Sheng and B. R. Cooper, Phys. Rev. B **50**, 965 (1994).
[3] P. Monachesi, L. C. Andreani, A. Continenza, and A. K. McMahan, J. Appl. Phys. **73**, 6634 (1993).
[4] J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966).
[5] R. Freytag and J. Keller, Z. Phys. B **85**, 87 (1991).
[6] B. Coqblin and J. R. Schrieffer, Phys. Rev. **185**, 847 (1969).
[7] A. Yoshimori and K. Yosida, Prog. Theor. Phys. **39**, 1413 (1968).
[8] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[9] P. W. Anderson, J. Phys. C **3**, 2436 (1970).
[10] P. Nozières and A. Blandin, J. Phys. **41**, 193 (1980).
[11] H. B. Pang and D. L. Cox, Phys. Rev. B **44**, 9454 (1991); T.-S. Kim and D. L. Cox, Phys. Rev. Lett. **75**, 1622 (1995).
[12] D. L. Cox, Phys. Rev. B **35**, 4561 (1987).
[13] L. C. Andreani, E. Liviotti, P. Santini, and G. Amoretti, Z. Phys. B **100**, 95 (1996).