Friedel artificially inserted resonance magnetic solution to the multichannel Friedel-Anderson problem

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The Friedel artificially inserted resonance (FAIR) magnetic state is extended from the one-channel to the multichannel Friedel-Anderson problem in this paper. The magnetic pseudoground state of the multichannel Friedel-Anderson problem is constructed from a product of one-channel magnetic states of each individual channel. A Hamiltonian that is rotationally invariant in both spin space and real space, which was developed by Dworin, Narath, and Parmenter, is used in the calculation. The magnetic ground-state energy is obtained through optimization of the conduction-band basis and Slater-state coefficients. The FAIR solution yields a considerably lower energy than the mean-field solution and requires a much larger Coulomb energy to form a magnetic moment.

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I. INTRODUCTION

Since the 1930s, a series of experimental results have shown that localized magnetic moments are widespread in iron-group impurities dissolved in nonmagnetic metals.[1] These observations lead to discussions of the interaction between the spins of a localized impurity and the conduction electrons.

To explain the physics of these magnetic impurities Friedel[2] extended the model for a d resonance in an (s,p) host by introducing a Coulomb repulsion between different d electrons on the impurity. Anderson[3] simplified the magnetic impurity problem by removing the orbital degeneracy of the d electrons. This is now called the one-channel Friedel-Anderson (FA) impurity problem while the inclusion of n orbits is denoted as the n-channel impurity problem. In the one-channel FA model the orbital degeneracy is ignored, and only the spin degeneracy of the d impurity is examined. When both the d states are occupied, the two d electrons with opposite spin repel each other due to the Coulomb potential energy U. Thus if the unperturbed energy of one d electron lies below the Fermi level at energy $E_d(E_d < 0)$, then the energy of the other d electron with opposite spin is $E_d + U$, which is above the Fermi energy for $U > |E_d|$. Further, the electrons can hop between the s- and d-electron states via the hopping matrix element V_{sd}. The combination of Coulomb repulsion and s-d hybridization gives the FA impurity its interesting physical properties. Both Friedel and Anderson did a self-consistent mean-field calculation to determine whether a localized moment exists as a function of the values of U and E_d.

Kondo[4] calculated the scattering probability for the conduction electrons due to the s-d exchange interaction in the second order Born approximation. It was shown that the scattering of the conduction electrons by the magnetic impurity yields a divergent contribution to the resistance in perturbation theory. This gives a singular term involving a $-\log T$ dependence for the resistance on temperature T, which increases the resistance at low temperature. Combined with the lattice resistivity, a minimum in the resistance versus temperature curve is observed.

During the last 40 years the properties of the FA impurity have been very intensively studied. However, the overwhelming number of investigations focused on the singlet or Kondo state and its properties below the Kondo temperature. However, in addition a number of sophisticated methods have been developed to calculate the magnetic moment of the impurity. One of these methods is the spin-density-functional theory (SDFT). SDFT calculates the conduction band structure from the first principles, but, like the majority of these methods, the local magnetic moment is still calculated in mean-field theory (MFT).

It is well known that the ground state of the FA impurity problem is a singlet Kondo state which shows no magnetic moment. In many cases the Kondo temperature T_K is very low, in the range of liquid-helium temperature. In this case the impurity is in the magnetic state at relatively low temperature. When the temperature is several times the Kondo temperature one is sufficiently above T_K to destroy the Kondo ground state. On the other hand, one may expect that the properties of the magnetic state are not yet influenced by the thermal excitations due to the finite temperature. Therefore a number of theoretical investigations treat the magnetic state at zero temperature as a magnetic ground state. This approach is probably justified but it leaves the work always vulnerable to the criticism that there is no magnetic moment at zero temperature.

A new numerical method, the Friedel artificially inserted resonance (FAIR) method[5–9] was introduced recently by one of the authors to investigate the Friedel-Anderson and Kondo impurity problems. In the FAIR theory the magnetic state is a building block of the singlet Kondo state. Instead of destroying the singlet state with a magnetic field or raising the temperature above the Kondo temperature in this paper we restrict the solution of the multichannel Friedel-Anderson impurity problem to the magnetic state. We denote this state as the magnetic pseudoground state. One possible interpretation of the pseudoground state is the following: One calculates the ground state in sufficiently large magnetic fields so that the singlet state is destroyed and then extrapolates this state back to zero magnetic field. There is an ambiguity only in the vicinity of the characteristic value of U for the forma-

tion of a magnetic moment, as we explain in the discussion section below.

In this paper the orbital degeneracy of the d impurity is considered in the Friedel-Anderson problem. The different d orbits are coupled with those components of the conduction band that have the same angular symmetry. So the s-d hopping occurs only within the individual channels while the Coulomb coupling occurs between all d orbits. The multichannel FA impurity requires a Hamiltonian that satisfies rotational invariance in both spin and real space. Such a Hamiltonian has been developed by Dworin and Narath[10] and independently by Parmenter[11] [and is denoted as the Dworin-Narath-Parmenter (DNP) Hamiltonian]. The unperturbed d-energy-level structure can be constructed based on the DNP Hamiltonian. In Sec. II we discuss the available states in the two-channel problem. In Sec. III the local magnetic moment is calculated from mean field theory for two, three, four, and five channels. In Sec. IV, the FAIR method is extended to the three-channel Friedel-Anderson problem. A FAIR magnetic multichannel ansatz is constructed from the product of the FAIR magnetic solutions of each individual channel. Then the FAIR ground state and magnetic moment are derived by minimizing the ground-state energy. In Sec. V the physical meaning of the results is discussed. Sec. VI is the conclusion.

II. MULTICHANNEL IMPURITY PROBLEM

Friedel and Anderson considered a d impurity dissolved in an s-band host. When the orbital degeneracy of the d impurity is ignored, the tenfold degeneracy of a real d impurity is simplified to a twofold degeneracy for electron spin up and spin down. The Coulomb repulsion energy U is introduced when both the spin-up and spin-down d states are occupied. The one-channel Friedel-Anderson Hamiltonian H_{FA} is expressed as follows:

$$H_{FA} = \sum_\sigma \left\{ \sum_{\nu=0}^{N-1} \varepsilon_\nu c_{\nu\sigma}^\dagger c_{\nu\sigma} + E_d d_\sigma^\dagger d_\sigma \right. $$
$$\left. + \sum_{\nu=0}^{N-1} V_{sd}(\nu)[d_\sigma^\dagger c_{\nu\sigma} + c_{\nu\sigma}^\dagger d_\sigma] \right\} + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow, \quad (1)$$

where N Wilson states are used in the Hamiltonian to express the conduction band. σ represents the spin direction, $c_{\nu\sigma}^\dagger$ and $d_\sigma^\dagger$ are the creation operators of the Wilson s electrons and the d-impurity electrons, ε_ν and E_d are the energies of the $c_{\nu\sigma}^\dagger$ and $d_\sigma^\dagger$ states, $V_{sd}(\nu)$ is the hopping matrix element between $c_{\nu\sigma}^\dagger$ and the $d_\sigma^\dagger$ impurity, and U is the Coulomb energy between two d-impurity electrons with opposite spins. The details of how to construct the Wilson states can be found in Ref. 12.

The one-channel model did not include the orbital degeneracy (l) of the d impurity. When $l \neq 0$, there are $(2l+1)$ degenerate spatial orbits and $2(2l+1)$ degenerate d-impurity states after including the spin effect, which creates $(2l+1)$ channels to couple with the s-band electrons. Both the Coulomb repulsion potential and the exchange energy should be included when considering the interaction among d-impurity electrons. As Anderson suggested, a Hamiltonian can be written as follows:

$$H = \sum_{m,\sigma} H_{m,\sigma} + H_c,$$

$$H_{m,\sigma} = \sum_{\nu=0}^{N-1} \varepsilon_\nu c_{\nu\sigma}^{m\dagger} c_{\nu\sigma}^m + E_d^m n_\sigma^m + \sum_{\nu=0}^{N-1} V_{sd}^m(\nu)[d_\sigma^{m\dagger} c_{\nu\sigma}^m + c_{\nu\sigma}^{m\dagger} d_\sigma^m],$$

$$H_c = \frac{1}{2} U \sum_{m,m',\sigma} n_\sigma^m n_{-\sigma}^{m'} + \frac{1}{2}(U - U_{ex}) \sum_{m,m',\sigma} (1 - \delta_{m,m'}) n_\sigma^m n_\sigma^{m'},$$
$$(2)$$

where $n_\sigma^m = d_\sigma^{m\dagger} d_\sigma^m$; $H_{m,\sigma}$ is the kinetic energy term in channel m and spin σ; and H_c represents the potential energy term. $U n_\sigma^m n_{-\sigma}^{m'}$ represents the Coulomb interaction between two opposite-spin d electrons from any two channels. When two d electrons have the same spin, an extra exchange energy $-U_{ex}$ is included. According to the Pauli exclusion principle, two d electrons cannot have the same orbital quantum number and spin quantum number simultaneously. If the two d electrons have the same quantum numbers, $m = m'$ and $\sigma = \sigma'$, we will have $\delta_{m,m'} = 1$ and $(1 - \delta_{m,m'}) n_\sigma^m n_\sigma^{m'} = 0$, and the contribution to Hamiltonian will be zero.

Caroli *et al.*[13] and also Lucas and Mattis[14] pointed out independently that the above Hamiltonian potential, H_c in Eq. (2), is not rotationally invariant in spin space. Later Dworin and Narath[10] and independently Parmenter[11] pointed out that the Hamiltonian suggested by Caroli *et al.* is not rotationally invariant in real space. Instead they suggested the following Hamiltonian, which is simultaneously rotationally invariant in both spin and real space:

$$H_c = \frac{1}{2} U \sum_{m,m',\sigma} n_\sigma^m n_{-\sigma}^{m'} + \frac{1}{2}(U - U_{ex}) \sum_{m,m',\sigma} (1 - \delta_{m,m'}) n_\sigma^m n_\sigma^{m'}$$
$$- \frac{1}{2} U_{ex} \sum_{m,m',\sigma} (1 - \delta_{m,m'}) d_\sigma^{m\dagger} d_{-\sigma}^m d_{-\sigma}^{m'\dagger} d_\sigma^{m'}$$
$$+ \frac{1}{2} U_{ex} \sum_{m,\sigma} n_\sigma^m n_{-\sigma}^m. \quad (3)$$

This DNP Hamiltonian commutes with the total spin angular momentum operator and total orbital angular momentum operator. Therefore, it is rotationally invariant in both real and spin space. We start our analysis of the DNP Hamiltonian by considering the possible states and energies of the d electrons in the absence of interaction with the s electrons.

In the nondegenerate d-impurity problem, there are only two d states, spin up and spin down. If only one d state is occupied, the state energy is E_d, where $E_d < 0$. If both the spin-up and spin-down d states are occupied simultaneously, a Coulomb energy U is introduced by the two antiparallel spins and the total energy is $2E_d + U$, which is analogous to the second d-electron state having an effective energy $E_d + U > 0$. For convenience of calculation, the Fermi energy is placed right in the middle of the two d-electron energies, which makes the energy of the two electrons symmetric

TABLE I. States and energies for different numbers of d electrons on the two-channel impurity.

No. of d electrons	State composition	ΔE	Total energy
First	$\uparrow_x$	E_d	E_d
Second (a)	$\uparrow_x\uparrow_y$	E_d+U-U_{ex}	$2E_d+U-U_{ex}$
Second (b)	$\uparrow_x\downarrow_y$	E_d+U	$2E_d+U$
Second (c)	$\uparrow_x\downarrow_x$	E_d+U+U_{ex}	$2E_d+U+U_{ex}$
Third	$\uparrow_x\downarrow_x\uparrow_y$	E_d+2U+U_{ex}	$3E_d+3U$
Fourth	$\uparrow_x\downarrow_x\uparrow_y\downarrow_y$	E_d+3U	$4E_d+6U$

around the Fermi energy, and the sum of the energies of the two d electrons is zero. Therefore, we have the relation $2E_d+U=0$ and $E_d=-U/2$.

In the multichannel case, the problem becomes more complicated because of the exchange energy U_{ex}. Let us consider as an example the two-channel problem, where we name the two channels channel x and channel y. There are totally four d states after including spin up and spin down. The possible multielectron states are listed in Table I and explained below.

Without losing generality, we can assume that the first electron is located in the channel x spin-up state ($\uparrow_x$), which has energy E_d. The second electron has three options, (a) channel y spin up ($\uparrow_y$), (b) channel y spin down ($\downarrow_y$), and (c) channel x spin down ($\downarrow_x$). For case (a), ($\uparrow_x\uparrow_y$) are occupied, and the total energy is $2E_d+U-U_{ex}$, which means the effective energy of the second electron is E_d+U-U_{ex}. For case (b), ($\uparrow_x\downarrow_y$) are occupied, the total energy is $2E_d+U$, and the effective energy of the second electron is E_d+U. For case (c), ($\uparrow_x\downarrow_x$) are occupied, the total energy is $2E_d+U+U_{ex}$, and the effective energy of the second electron is E_d+U+U_{ex}. From the above discussion, one can see that the energy of case (a) ($\uparrow_x\uparrow_y$) is lower than that of the other two cases and the combination in case (a) is most energetically favorable. When a third electron is introduced based on the two-electron occupation in case (a), the state composition looks like ($\uparrow_x\downarrow_x\uparrow_y$), and the total energy is $3E_d+3U$, which implies the third electron has the effective energy E_d+2U+U_{ex}. All states with three d electrons have the same energy. It will be a full shell d state when a fourth electron is added. The state is then ($\uparrow_x\downarrow_x\uparrow_y\downarrow_y$), the total energy is $4E_d+6U$, and the fourth electron has energy E_d+3U. The number of electrons that are below the Fermi energy can be manipulated by changing the relation between E_d, U, and U_{ex}.

Figure 1 shows the effective energy of the four d electrons in the two-channel Friedel-Anderson problem. When the relation $2E_d+U-U_{ex}=0$ is satisfied, the Fermi energy lies cen-
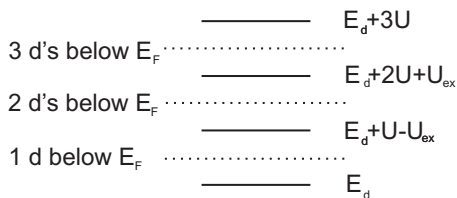

FIG. 1. Manipulation of the number of occupied d states by changing the location of the Fermi level.

tered between the first and the second d electrons, and there is only one d electron below the Fermi level. If $2E_d+3U=0$ is satisfied, the Fermi energy is centered between the second and the third d electrons, and there are two d electrons below the Fermi level. If $2E_d+5U+U_{ex}=0$ is satisfied, three d electrons are below the Fermi energy.

For simplicity we have discussed the two-channel problem as an example in this section. The energy level scheme for a larger number of channels follows the same principles but is slightly more complicated.

III. MAGNETIC MOMENT IN MEAN-FIELD THEORY

Because the Coulomb and exchange interaction terms in the DNP Hamiltonian are not single-body operators, an exact solution cannot be obtained analytically. The mean field method is one of the simplest approaches to many-body theory problems, and it can provide us with a number of meaningful results. In the DNP Hamiltonian, the $H_{m,\sigma}$ term is a single-body Hamiltonian, which can be written directly as a Hamiltonian matrix. The H_c term is a two-body problem, which cannot be simply expressed as a Hamiltonian matrix. By assuming that the state occupation has a small variation around the expectation value, the two-body problem can be transformed into a one-body problem by the following substitutions:

$$n_\sigma^m n_{\sigma'}^{m'} = n_\sigma^m \langle n_{\sigma'}^{m'}\rangle + \langle n_\sigma^m\rangle n_{\sigma'}^{m'} - \langle n_\sigma^m\rangle\langle n_{\sigma'}^{m'}\rangle,$$

$$d_\sigma^{m\dagger} d_{-\sigma}^m d_{-\sigma}^{m'\dagger} d_\sigma^{m'} = d_\sigma^{m\dagger} d_{-\sigma}^m \langle d_{-\sigma}^{m'\dagger} d_\sigma^{m'}\rangle + \langle d_\sigma^{m\dagger} d_{-\sigma}^m\rangle d_{-\sigma}^{m'\dagger} d_\sigma^{m'}$$
$$- \langle d_\sigma^{m\dagger} d_{-\sigma}^m\rangle\langle d_{-\sigma}^{m'\dagger} d_\sigma^{m'}\rangle, \quad (4)$$

where $n_\sigma^m = d_\sigma^{m\dagger} d_\sigma^m$, and $\langle n_\sigma^m\rangle$ is the expectation value of the d occupation for channel m and spin σ. As Eq. (4) shows, one obtains a spin-flip term in the mean-field Hamiltonian. This term is a consequence of the rotational invariance of the original DNP Hamiltonian.

After substituting these expressions into the DNP Hamiltonian the mean-field Hamiltonian becomes

$$H = \sum_{m,\sigma} H'_{m,\sigma} - \frac{1}{2}U \sum_{m,m',\sigma} \langle n_\sigma^m\rangle\langle n_{-\sigma}^{m'}\rangle - \frac{1}{2}(U-U_{ex})\sum_{m,m',\sigma}^{m\neq m'} \langle n_\sigma^m\rangle$$

$$\times\langle n_\sigma^{m'}\rangle - \frac{1}{2}U_{ex}\sum_{m,\sigma} \langle n_\sigma^m\rangle\langle n_\sigma^m\rangle + \frac{1}{2}U_{ex}\sum_{m,\sigma}^{m\neq m'} \langle d_{m,\sigma}^\dagger d_{m,-\sigma}\rangle$$

$$\times\langle d_{m',-\sigma}^\dagger d_{m',\sigma}\rangle, \quad (5)$$

$$H'_{m,\sigma} = \sum_{\nu=0}^{N-1}\varepsilon_\nu c_{\nu,\sigma}^{m\dagger} c_{\nu,\sigma}^m + \sum_{\nu=0}^{N-1}V_{sd}^m(\nu)[d_\sigma^{m\dagger}c_{\nu,\sigma}^m + c_{\nu,\sigma}^{m\dagger}d_\sigma^m]$$

$$+\left[E_d^m + U\sum_{m'}\langle n_{-\sigma}^{m'}\rangle + (U-U_{ex})\sum_{m'\neq m}\langle n_\sigma^{m'}\rangle\right.$$

$$\left.+ U_{ex}\langle n_{-\sigma}^m\rangle\right]n_\sigma^m - U_{ex}\left(\sum_{m'\neq m}\langle d_\sigma^{m'\dagger} d_{-\sigma}^{m'}\rangle\right)d_{-\sigma}^{m\dagger} d_\sigma^m. \quad (6)$$

All the terms in H except for $H'_{m,\sigma}$ are numbers instead of variables. The last term in $H'_{m,\sigma}$ generates spin flips. There is no transition matrix element between different channels. We define

$$\langle E^m_{d,\sigma}\rangle = E^m_d + U\sum_{m'}\langle n^{m'}_{-\sigma}\rangle + (U - U_{ex})\sum_{m'\neq m}\langle n^{m'}_{\sigma}\rangle + U_{ex}\langle n^m_{-\sigma}\rangle,$$

$$V^m_{dd} = -U_{ex}\left(\sum_{m'\neq m}\langle d^{m'\dagger}_{\sigma}d^{m'}_{-\sigma}\rangle\right). \qquad (7)$$

Because of the spin-flip transition process between $H'_{m,\uparrow}$ and $H'_{m,\downarrow}$, they are coupled together and can be expressed by a $(2N+2)\times(2N+2)$ Hamiltonian matrix for each channel as follows:

$$
\begin{array}{c}
c^\dagger_{0\uparrow} \\[4pt]
c^\dagger_{N-1\uparrow} \\
c^\dagger_{0\downarrow} \\[6pt]
c^\dagger_{N-1\downarrow} \\
d^\dagger_{\uparrow} \\
d^\dagger_{\downarrow}
\end{array}
\left[
\begin{array}{cccccc}
\varepsilon_0 & 0 & 0 & 0 & V_{sd}(0) & 0 \\[4pt]
0 & \varepsilon_{N-1} & 0 & 0 & V_{sd}(N-1) & 0 \\
0 & 0 & \varepsilon_0 & 0 & 0 & V_{sd}(0) \\[6pt]
0 & 0 & 0 & \varepsilon_{N-1} & 0 & V_{sd}(N-1) \\
V_{sd}(0) & V_{sd}(N-1) & 0 & 0 & \langle E_{d\uparrow}\rangle & V_{dd} \\
0 & 0 & V_{sd}(0) & V_{sd}(N-1) & V_{dd} & \langle E_{d\downarrow}\rangle
\end{array}
\right]
$$

$$
\begin{array}{cccccc}
c_{0\uparrow} & c_{N-1\uparrow} & c_{0\downarrow} & c_{N-1\downarrow} & d_{\uparrow} & d_{\downarrow}
\end{array}
$$

The ground state of each channel can be simply obtained from separate matrix diagonalization. The eigenstates are mixtures of spin-up and spin-down states

$$\phi^\dagger_i = \sum_{j=0}^{N-1}[c^\dagger_{j\uparrow}A_{j,i} + c^\dagger_{j\downarrow}A_{j+N,i}] + d^\dagger_{\uparrow}A_{2N,i} + d^\dagger_{\downarrow}A_{2N+1,i}. \qquad (8)$$

Therefore the expectation value $\langle d^{m\dagger}_{\uparrow}d^m_{\downarrow}\rangle$ is not zero.

If the s-electron band is half filled, where $N/2$ electrons have spin up and $N/2$ electrons have spin down for each channel, then the ground state for each channel Ψ_{ground} listed below is constructed from those N eigenstates ϕ_i that have the lowest eigenenergies

$$\Psi_{ground} = \prod_{i=0}^{N-1}\phi^\dagger_i\Phi_0,$$

where Φ_0 is the vacuum state.

The expectation values can be calculated in the ground state as

$$\langle n_\uparrow\rangle = \langle\Psi_{ground}|d^\dagger_\uparrow d_\uparrow|\Psi_{ground}\rangle = \left\langle\prod_{i=0}^{N-1}\phi_i\left|d^\dagger_\uparrow d_\uparrow\right|\prod_{i=0}^{N-1}\phi_i\right\rangle$$

$$= \sum_{i=0}^{N-1}|A_{2N,i}|^2, \qquad (9)$$

$$\langle d^\dagger_\uparrow d_\downarrow\rangle = \langle\Psi_{ground}|d^\dagger_\uparrow d_\downarrow|\Psi_{ground}\rangle = \sum_{i=0}^{N-1}A_{2N,i}A_{2N+1,i} = \langle d^\dagger_\downarrow d_\uparrow\rangle. \qquad (10)$$

We can give an initial value to each expectation value and substitute these initial values into the Hamiltonian matrix. After diagonalizing the Hamiltonian matrix, the new expectation values can be calculated. The ground state can be approached by repeating this procedure until these expectation values reach self-consistency. Then the electron occupation and magnetic moment can also be calculated.

Figure 2 shows the magnetic moment transition curve when there is only one d state below the Fermi energy for the two-, three-, four- and five-channel problems with $|V^0_{sd}|^2 = 0.1$ and $U_{ex} = 0.1$. Because there is only one d-impurity electron below the Fermi energy, the magnetic moment approaches μ_B when the Coulomb potential U is larger than the
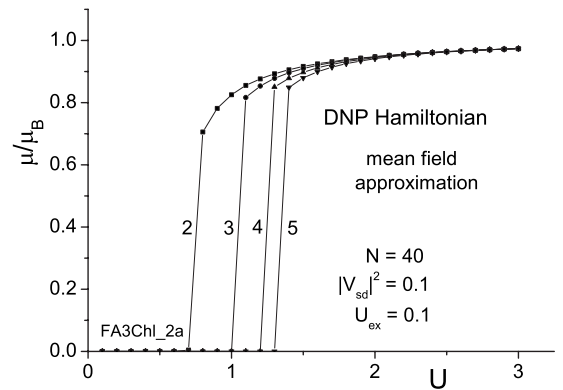

FIG. 2. Calculation of the magnetic moment in mean-field theory for a multichannel Friedel-Anderson impurity as a function of the Coulomb energy U. One d electron lies below the Fermi level. The number of channels (2,3,4,5) is labeled beside each curve.

characteristic value. In Fig. 2 one clear moment transition can be observed. The Friedel-Anderson impurity which has more channels has a larger characteristic Coulomb potential U.

IV. MAGNETIC MOMENT IN THE FAIR SOLUTION OF THE MULTICHANNEL IMPURITY PROBLEM

Now the FAIR method is applied to solve the DNP Hamiltonian. The FAIR method uses a series of discrete Wilson-band states[15] to represent a continuous conduction electron band, where the large number of states in a macroscopic metal, such as $N = 10^{23}$, is reduced to a small number, such as $N = 40$. A FAIR state, which is constructed from s-band Wilson states, hybridizes with the d electron to approach the ground state. After optimization of the FAIR state by rotation in the Hilbert space an impressively good result for the ground-state energy is obtained. For details see Refs. 5–7.

The one-channel FAIR magnetic solution for half filling of the s band is composed of four Slater states

$$\Psi_{MS} = (Aa_{0\uparrow}^{\dagger}b_{0\downarrow}^{\dagger} + Ba_{0\uparrow}^{\dagger}d_{\downarrow}^{\dagger} + Cd_{\uparrow}^{\dagger}b_{0\downarrow}^{\dagger} + Dd_{\uparrow}^{\dagger}d_{\downarrow}^{\dagger})\prod_{i=1}^{n-1}a_{i\uparrow}^{\dagger}\prod_{i=1}^{n-1}b_{i\downarrow}^{\dagger}\Phi_0,$$

(11)

where $a_{0\uparrow}^{\dagger}$ and $b_{0\downarrow}^{\dagger}$ are the FAIR states for the spin-up and spin-down bases, and $n = N/2$. Both the FAIR states can be constructed from linear combinations of the Wilson conduction-band states.

$$a_{0\uparrow}^{\dagger} = \sum_{\nu=0}^{N-1}\alpha_{\nu}^{0}c_{\nu\uparrow}^{\dagger},$$

$$b_{0\downarrow}^{\dagger} = \sum_{\nu=0}^{N-1}\beta_{\nu}^{0}c_{\nu\downarrow}^{\dagger}.$$

(12)

The details of the construction of the FAIR states and the calculation of coefficients α_{ν}^{0} and β_{ν}^{0} have been shown in Refs. 6 and 12. $(a_{0\uparrow}^{\dagger}, a_{1\uparrow}^{\dagger}, a_{2\uparrow}^{\dagger}, \ldots, a_{N-1\uparrow}^{\dagger})$ and $(b_{0\downarrow}^{\dagger}, b_{1\downarrow}^{\dagger}, b_{2\downarrow}^{\dagger}, \ldots, b_{N-1\downarrow}^{\dagger})$ are both orthogonal bases, and the $a_{i\uparrow}^{\dagger}$ and $b_{i\downarrow}^{\dagger}$ states can be uniquely determined by the FAIR states $a_{0\uparrow}^{\dagger}$ and $b_{0\downarrow}^{\dagger}$.

Using the basis $(a_{0\uparrow}^{m\dagger}, a_{1\uparrow}^{m\dagger}, a_{2\uparrow}^{m\dagger}, \ldots, a_{N-1\uparrow}^{m\dagger})$ and $(b_{0\downarrow}^{m\dagger}, b_{1\downarrow}^{m\dagger}, b_{2\downarrow}^{m\dagger}, \ldots, b_{N-1\downarrow}^{m\dagger})$ the multichannel Friedel-Anderson DNP Hamiltonian can be written as follows:

$$H = \sum_{m}(H_{m\uparrow}' + H_{m\downarrow}') + H_c,$$

$$H_{m\uparrow}' = \sum_{i=0}^{N-1}E^{am}(i)a_{i\uparrow}^{m\dagger}a_{i\uparrow}^{m} + \sum_{i=1}^{N-1}V_{fr}^{am}(i)[a_{0\uparrow}^{m\dagger}a_{i\uparrow}^{m} + a_{i\uparrow}^{m\dagger}a_{0\uparrow}^{m}]$$

$$+ E_d d_{\uparrow}^{\dagger}d_{\uparrow} + \sum_{i=0}^{N-1}V_{sd}^{am}(i)[d_{\uparrow}^{\dagger}a_{i\uparrow}^{m} + a_{i\uparrow}^{m\dagger}d_{\uparrow}^{m}],$$

$$H_{m\downarrow}' = \sum_{i=0}^{N-1}E^{bm}(i)b_{i\downarrow}^{m\dagger}b_{i\downarrow}^{m} + \sum_{i=1}^{N-1}V_{fr}^{bm}(i)[b_{0\downarrow}^{m\dagger}b_{i\downarrow}^{m} + b_{i\downarrow}^{m\dagger}b_{0\downarrow}^{m}]$$

$$+ E_d d_{\downarrow}^{\dagger}d_{\downarrow} + \sum_{i=0}^{N-1}V_{sd}^{bm}(i)[d_{\downarrow}^{\dagger}a_{i\downarrow}^{m} + a_{i\downarrow}^{m\dagger}d_{\downarrow}^{m}],$$

$$H_c = \frac{1}{2}U\sum_{m,m',\sigma}n_{\sigma}^{m}n_{-\sigma}^{m'} + \frac{1}{2}(U - U_{ex})\sum_{m,m',\sigma}^{m\neq m'}n_{\sigma}^{m}n_{\sigma}^{m'}$$

$$- \frac{1}{2}U_{ex}\sum_{m,m'}^{m\neq m'}d_{\sigma}^{m\dagger}d_{-\sigma}^{m}d_{-\sigma}^{m'\dagger}d_{\sigma}^{m'} + \frac{1}{2}U_{ex}\sum_{m,\sigma}n_{\sigma}^{m}n_{-\sigma}^{m},$$

(13)

where m represents the channel index. Here

$$E^{am}(i) = \sum_{\nu}\alpha_{\nu}^{mi}\varepsilon_{\nu}\alpha_{\nu}^{mi},$$

$$V_{sd}^{am}(i) = \sum_{\nu}V_{sd}(\nu)\alpha_{\nu}^{mi},$$

$$V_{fr}^{am}(i) = \sum_{\nu}\alpha_{\nu}^{mi}V_{sd}(\nu)\alpha_{\nu}^{m0}$$

(14)

and corresponding expressions for the b basis.

Because there is no transition process among the different channels in the DNP Hamiltonian, all the channels are independent. The multichannel magnetic FAIR state Ψ_{MS}^{M} is the product of one-channel FAIR magnetic solutions for each individual channel.

$$\Psi_{MS}^{M} = \prod_{m}(Aa_{0\uparrow}^{m\dagger}b_{0\downarrow}^{m\dagger} + Ba_{0\uparrow}^{m\dagger}d_{\downarrow}^{m\dagger} + Cd_{\uparrow}^{m\dagger}b_{0\downarrow}^{m\dagger}$$

$$+ Dd_{\uparrow}^{m\dagger}d_{\downarrow}^{m\dagger})\prod_{i=1}^{n-1}a_{i\uparrow}^{m\dagger}\prod_{i=1}^{n-1}b_{i\downarrow}^{m\dagger}\Phi_0.$$

(15)

There are $4^2 + 2 = 18$ Slater states in a two-channel FAIR magnetic state, $4^3 + 24 = 88$ Slater states in a three-channel FAIR magnetic state. The 2 and 24 additional states are due to spin-flip processes. Take the three-channel FAIR magnetic state case as an example. Similar to the procedure in the one-channel Friedel-Anderson problem, the FAIR states $a_0^{m\dagger}$ and $b_0^{m\dagger}$, and the 88 coefficients can be obtained by minimizing the ground-state energy. The 88 coefficients are optimized under the normalization constrain condition, $\langle\Psi_{MS}^{M}|\Psi_{MS}^{M}\rangle = 1$

$$E_{gs} = \frac{\langle\Psi_{MS}^{M}|H|\Psi_{MS}^{M}\rangle}{\langle\Psi_{MS}^{M}|\Psi_{MS}^{M}\rangle}.$$

(16)

The quasivacuum energy E_{quasi} is defined as the ground-state energy when there is no interaction between the s-conduction electrons and d-impurity electrons. We define $E_{00} = E_{gs} - E_{quasi}$ to remove the dependence of the ground-state energy on the construction of the conduction band. In Fig. 3 the numerical results for E_{00} are plotted as a function of the Coulomb repulsion U for the three-channel Friedel-
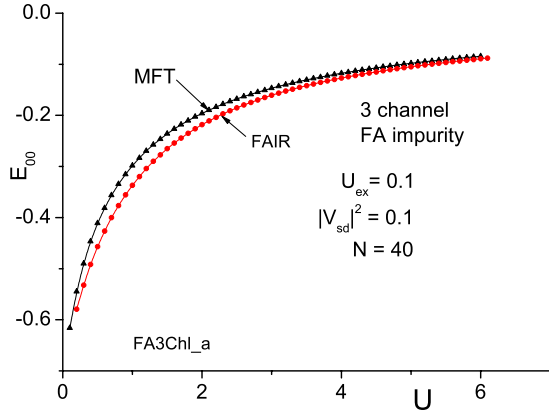
FIG. 3. (Color online) Ground-state energy comparison between the FAIR magnetic state and the mean-field approach in the three-channel Friedel-Anderson problem with three d electrons below the Fermi level.

Anderson problem with three d electrons below the Fermi energy. The s-d interaction is fixed as $|V_{sd}|^2 = 0.1$, the exchange energy among d-impurity electrons is chosen as $U_{ex} = 0.1$, and the Coulomb repulsion U varies from 0 to 6. The third d electron has the energy $E_d + 2U - 2U_{ex}$, and the fourth d electron has energy $E_d + 3U + U_{ex}$. The Fermi energy is centered between the third and the fourth d electron so that the sum of the energies of these two electrons is zero, $(2E_d + 5U - U_{ex} = 0)$, which implies that the d-state energy $E_d = (U_{ex} - 5U)/2$. Figure 3 shows that the ground-state energy of the FAIR magnetic state is lower than that of the mean-field approach in this three-channel Friedel-Anderson problem, which means the FAIR magnetic state is closer to the ground state than is the mean-field-theory state.

In Fig. 4 the magnetic moments obtained from the FAIR magnetic and the mean-field approach are plotted as a function of the Coulomb repulsion U for the three-channel Friedel-Anderson problem. The cases of one d, two d, and
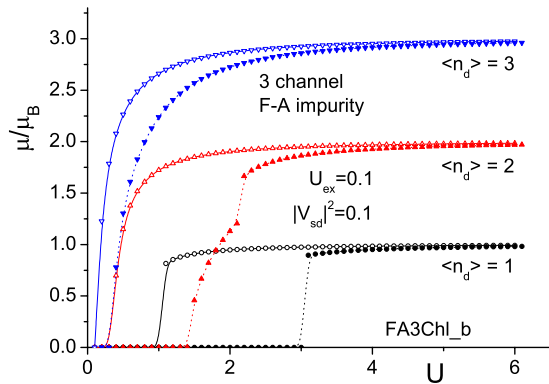

FIG. 4. (Color online) Magnetic moments as a function of the Coulomb energy U for the three-channel Friedel-Anderson impurity. The open symbols represent the results of the mean-field approximation and the filled symbols are calculated with the FAIR magnetic state. The three different sets of data are for different positions of the Fermi level. The number of d levels below the Fermi level is one for circles, two for up triangles, and three for down triangles.

three d electrons below the Fermi energy are compared in this graph. To obtain the different d occupations one has to fulfill conditions similar to those for the two-channel case, as discussed below Table I. For the three-channel case the corresponding conditions for one, two, and three occupied d states are: (1) $2E_d + U - U_{ex} = 0$, (2) $2E_d + 3U - 3U_{ex} = 0$, and (3) $2E_d + 5U - U_{ex} = 0$. The meaning of the various symbols in the graph is explained in the figure caption. Both the mean-field approach and the FAIR magnetic approach show similar phenomenon: the magnetic moment does not show up until the Coulomb repulsion U is larger than a characteristic value. Most of the FAIR calculations show some hysteresis near the characteristic value of U. This causes the discontinuities shown in Fig. 4 for one and two d electrons below the Fermi energy. The filled symbols correspond to the states with the lowest energies. When the Coulomb repulsion U is large, the spin-up and spin-down subbands are fully split, and the magnetic moment value in units of μ_B approaches the number of d-impurity electrons below the Fermi energy.

However, one can observe that the FAIR magnetic solution has a much larger transition Coulomb repulsion than in the mean-field approach. For example, when the Fermi energy lies centered between the first d electron and the second d electron, the mean-field solution develops a magnetic moment when $U > 1.0$, while the FAIR magnetic solution does not show a magnetic moment until a considerably larger Coulomb repulsion $U = 3.0$, which is three times larger than the characteristic value predicted by the mean-field method. In the Friedel-Anderson problem, the d impurities prefer to keep the symmetry between spin up and spin down until the symmetry is broken by the increasing Coulomb repulsion U. The FAIR solution has much more flexibility in approaching the ground state than the mean-field method, therefore the symmetry can survive for a longer time than the mean-field approach. The more d electrons there are below the Fermi energy, the easier it is to observe a magnetic moment. When there are three d electrons below the Fermi energy, the characteristic Coulomb potential is only $U = 0.3$, which is much smaller than for the case of one d electron below the Fermi level.

V. DISCUSSION

The ground state for the FA-impurity problem is the singlet state, which is nonmagnetic. Only if one destroys the singlet state, either by raising the temperature above the Kondo temperature or by applying a magnetic field larger than $k_B T_K / \mu_B$, does the magnetic moment become visible. In the parameter range of large $U (U \gg \Gamma = \pi |V_{sd}|^2 g_F)$ (g_F = density of states in the s subband at the Fermi level) the Kondo energy is very small. In this region the singlet state is built from a well-defined magnetic moment. This was demonstrated by Krishna-murthy, Wilkins, and Wilson.[16] Reference 16 showed that the renormalization-group flow diagram passes close to the (unstable) fixed point for a local moment. In this range of U the FAIR singlet ground state is essentially built from the magnetic pseudoground state and its spin-reversed sibling. Since the Kondo temperature is low the same moment is observed above T_K.

With decreasing value of U the magnetic moment decreases and the Kondo temperature increases. In the range of U where the moment of the magnetic pseudoground state disappears the Kondo temperature has a maximum. Here the concept of a rigid magnetic moment breaks down. This means that the value of μ shows an increasing variance depending on the external parameters such as temperature and magnetic field and on the internal structure. (At the characteristic value of U the singlet ground state (in the FAIR theory) is still composed of a magnetic state and its sibling but they strongly interfere since they are not orthogonal). The characteristic value of U indicates the parameter range where the magnetic moment is no longer well defined and changes strongly with magnetic field or temperature.

In complete analogy the MFT magnetic ground state is also a pseudoground state. One can use it to construct a Kondo state by pairing it with its spin-reversed sibling.[17] In this paper we confirm for the multichannel FA impurity problem a previous result that we observed for the single-channel impurity:[5] the energy of the magnetic FAIR state is considerably lower than the energy of the corresponding MFT state. Furthermore in the FAIR calculation the formation of magnetic moment requires a much larger Coulomb energy than in the mean field theory. This means the MFT strongly overestimates the tendency for a magnetic moment. The difference is rather dramatic, up to a factor of 5 in the three-channel case.

We assume that the reason for this failure of the MFT is the fact that it generally yields an incorrect resonance width of the impurity d states. This can be seen with the following argument for an impurity with n_d occupied d states. If an electron is injected into an empty d state then all the occupied d states are coupled by the Coulomb interaction and experience a collective increase in energy. Every d electron can perform a transition into its conduction subband with the same angular wave function. This yields (n_d+1) decay channels for the excited multi-d-electron state. In MFT only the injected d electron can decay because MFT freezes all the other d electrons in their mean-field expectation values. Therefore in MFT one obtains a decay rate and resonance width which are much too small. Actually the resonance width in MFT is the same as for a Friedel d resonance: $\Gamma = \pi|V_{sd}|^2 g_F = \hbar/(2\tau_d)$, where τ_d is the lifetime of the electron in the d state, $1/\tau_d = (2\pi/\hbar)|V_{sd}|^2 g_F$. This broadening of the d resonances has been known for several decades in the singlet state of the one-channel impurity.[18,19] However, the conclusion that this reduces the formation of a magnetic moment has been only made recently.[5,20]

It should be emphasized that the majority of numerical procedures for the calculation of an impurity magnetic moment use some kind of MFT in the last step. One example is spin-density-functional theory. Therefore one would expect that it strongly overestimates the formation of a magnetic moment. Even more important is the fact that the MFT misses the dynamic broadening of the density of states and yields d-resonance widths that are much too small.

VI. CONCLUSION

In this paper we extend the FAIR method from a one-channel FA-impurity to a three-channel impurity. The orbital degeneracy of the d impurity is included in the s-d interaction. The DNP Hamiltonian is applied in the calculation to satisfy rotational invariance in both spin and real spaces. The magnetic moment of the impurity is calculated in MFT and in the magnetic FAIR state. Like the case of a one-channel impurity, the energy of the FAIR state lies considerably below the MFT energy. Both approaches yield a characteristic Coulomb energy U that must be interpreted carefully. The first important result is that the MFT strongly overestimates the tendency to form a magnetic moment.

The FAIR magnetic state is constructed as a product of the FAIR magnetic states of each individual channel. The FAIR magnetic state of each channel m can be expressed as a compact form in a rotated Hilbert space $\{a_{0\uparrow}^{m\dagger}, a_{i\uparrow}^{m\dagger}\}$ and $\{b_{0\downarrow}^{m\dagger}, b_{i\downarrow}^{m\dagger}\}$. The whole basis can uniquely be determined by the FAIR states $a_{0\uparrow}^{m\dagger}$ and $b_{0\downarrow}^{m\dagger}$. The ground-state energy can be calculated through the optimization of the FAIR state composition of each channel and the coefficients of all the Slater states. The energy of the FAIR magnetic method clearly shows a lower value than that of the mean-field approach. The magnetic moment obtained by the FAIR magnetic method approaches the same value as the mean-field solution, however with a much larger characteristic Coulomb repulsion U. The FAIR magnetic state shows much more flexibility in keeping the impurity symmetry as the Coulomb repulsion increases.

A further analysis for the FAIR solution is planned. A rotationally invariant singlet state, which is a better approximation of the real ground state, can be constructed from the FAIR magnetic state. We are analyzing the singlet state together with the magnetic state for the two-channel problem and will present our results separately. These calculations are only an initial step to approach a realistic FA impurity. Another interesting challenge is to add a spin-orbit interaction. However, fortunately the spin-orbit interaction is strongly suppressed in a cubic lattice. This FAIR method can also be applied to the multichannel Kondo problem, which can contribute to understanding the formation condition of the Kondo resonance in the multichannel Kondo problem.

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