PHYSICAL REVIEW B VOLUME 33, NUMBER 9 1 MAY 1986

Integrability of a general model for intermediate valence

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(Received 25 February 1985)

We study the integrability by means of the Bethe ansatz of a model which consists of two $4f$ configurations of total angular momentum J_0 and J_1 hybridized through the promotion of an electron of total angular momentum j_e to a conduction band. For $J_0=0$ the model reduces to the degenerate Anderson model, while for $J_0J_1\neq0$ it describes valence fluctuators between two magnetic configurations. We find that in addition to the case $J_0J_1=0$, and any j_e, the model is also exactly solvable for $j_e=\frac{1}{2}$ and any $J_0,J_1=J_0\pm\frac{1}{2}$. We present several static ground-state properties for the latter case.

I. INTRODUCTION

In 1980 Andrei[1] and Wiegmann[2] independently diagonalized the spin-$\frac{1}{2}$ Kondo model by means of the Bethe ansatz. Since then, the Bethe hypothesis and integrability conditions have been shown to be valid for several models for magnetic impurities in metals, allowing them to be solved exactly.[3]

These models include the nondegenerate[4] and orbital degenerate Anderson model.[5,6] Using the exact solution, several properties of these intermediate-valence (IV) models have been calculated: energy, valence, and magnetoresistance at zero temperature, and specific heat and magnetic susceptibility at arbitrary temperatures.[3] A modified version of the periodic Anderson Hamiltonian has also been solved exactly.[7]

While the nondegenerate Anderson model describes qualitatively the properties of IV systems (IVS) fluctuating between a magnetic and a nonmagnetic configuration, and the degenerate Anderson model is more realistic for Ce or Yb systems, none of the so far Bethe-ansatz solved model for IVS describe valence fluctuators between two magnetic configurations, as Tm or Pr systems.

The magnetic properties of IV compounds and alloys in which the two accessible configurations are magnetic are quite different from those of the other known IVS: the magnetic susceptibility of TmSe (Ref. 8) and $Tm_xY_{1-x}Se$ (Ref. 9), the existence of magnetic order at low temperatures in TmSe (Ref. 10), the spin-glass behavior in $Tm_xY_{1-x}Se$ (Ref. 11), and the specific heat of TmSe and its dependence on magnetic field (Ref. 12) suggest that the ground state of these systems is magnetic in contrast to what is observed in the Ce, Eu, Sm, or Yb systems and to the result of a nonmagnetic ground state for the above mentioned exactly solved Anderson models.[5,7,13] The magnetic neutron spectrum of IV Tm systems shows a narrow elastic line and an inelastic line at low temperatures[14] instead of the broad quasielastic line observed in the other rare-earth IVS.[15]

In Ref. 16 a model for valence fluctuations between two magnetic configurations has been proposed to explain qualitatively the main properties of Tm systems in the IV as well as in the exchange regimes. The total angular momenta of the $4f$ configurations are $\frac{1}{2}$ and 1 and the f states are hybridized with band states of total angular momentum $j_e=\frac{1}{2}$. Though the model does not include a realistic description of both $4f$ configurations, it provides an explanation of the peculiar neutron spectrum of IV Tm systems.[16] Wilson's renormalization-group calculations show that the ground state of the model is degenerate leading to a divergent magnetic susceptibility for vanishing temperature[17] in agreement with the experimental results.

A simplification of this model that allowed it to be solved exactly[18] without use of the Bethe hypothesis and its extension to a lattice[19] explains qualitatively the ground-state magnetic order, insulator or metallic character, static and dynamical magnetic susceptibility, magnetoresistance, and specific heat of dilute IV Tm systems.[18,19]

In this paper we consider an isotropic impurity model which includes two configurations of arbitrary angular momentum J_0 and J_1 hybridized through the promotion of an electron of total angular momentum j_0 to a conduction band. It contains as particular cases the Anderson model of arbitrary degeneracy and the model of Ref. 16. Preliminary results about the exact solution of the latter[20] and its thermodynamics[21] were presented elsewhere.

In Sec. II we describe the model and its exchange limits. In Sec. III we develop the Bethe-ansatz formalism for the model. In Sec. IV we show that the model is not integrable by means of the Bethe ansatz for $j_e>\frac{1}{2}$ if both configurations are magnetic ($J_0J_1>0$). In Sec. V we diagonalize the model for $j_e=\frac{1}{2}$ and calculate the zero-temperature impurity energy, valence, and impurity magnetization. Section VI contains the conclusions and a discussion.

II. MODEL

The intermediate valence rare-earth impurities can be described in terms of the Hamiltonian[22,23]

$$H=\sum_{M_0} E_{J_0}\,|J_0M_0\rangle\langle J_0M_0\,| + \sum_{M_1}(E_{J_0}+\Delta)\,|J_1M_1\rangle\langle J_1M_1\,| + \sum_{k,m}\epsilon_{kj_e}c^\dagger_{kj_em}c_{kj_em}$$

$$+V\sum_{k,m,M_0,M_1}\langle J_0j_eM_0m\,|J_1M_1\rangle(c^\dagger_{kjm}\,|J_0M_0\rangle\langle J_1M_1\,|+\text{H.c.})\;. \tag{2.1}$$

Here the first (second) term represents the energy of the Hund's rule ground multiplet of the $4f^n$ ($4f^{n+1}$) configuration. J_0 (J_1) is the total angular momentum of this multiplet and M_0 (M_1) is its projection over the quantization axis. The third term describes a conduction band in terms of Bloch states with wave number k, total angular momentum j and projection m. The last term represents the hybridization energy. The angular brackets denote Clebsh-Gordan coefficients.

The main hypothesis involved in (2.1) as a realistic model for rare-earth impurities are the following.

(1) Due to the large $4f$ intra-atomic Coulomb repulsion energy, only two neighboring configurations $4f^n$ and $4f^{n+1}$ are considered.

(2) The excited multiplets of each configuration are neglected because of the strong spin-orbit coupling.

(3) Crystal-field splittings are neglected.

(4) For rare-earth impurities $j_e=\frac{5}{2}$ or $\frac{7}{2}$. $j_e=\frac{5}{2}$ $(\frac{7}{2})$ dominates the hybridization effects in light (heavy) rare earths and only one of these terms is included.

(5) The hybridization is assumed k independent.

Hamiltonian (2.1) is invariant under rotations. Another symmetry property is that the model that associates the angular momentum J_0 (J_1) to the $4f^{n+1}(4f^n)$ configuration can be mapped into Hamiltonian (2.1) by means of the transformation

$$c_{kj_em}\rightarrow(-1)^{J_0-J_1+2j_e+m}c_{kj_e-m}\;, \tag{2.2a}$$

$$\epsilon_{kj_e}\rightarrow-\epsilon_{kj_e}\;, \tag{2.2b}$$

$$V\rightarrow V\left[\frac{2J_1+1}{2J_0+1}\right]^{1/2}. \tag{2.2c}$$

For $|\Delta-\epsilon_F|\gg\pi\rho(\epsilon_F)V^2$, where ϵ_F is the Fermi energy and $\rho(\epsilon)$ the unperturbed density of band states, the model reduces to exchange like Hamiltonians. Due to the symmetry transformation (2.2) we can restrict ourselves to $\Delta-\epsilon_F>0$ and project out of the space of interest the configuration with angular momentum J_1. In this case, a canonical transformation of the Schrieffer-Wolff type[23,24] on Hamiltonian (2.1) leads to the exchange interaction model

$$H=\sum_{k,m}\epsilon_{kj_e}c^\dagger_{kj_em}c_{kj_em}$$
$$-K\sum_{k,k'M_0,M_0',m,m'}\langle J_0j_eM_0'm'\,|P_{J_1}|\,J_0j_eM_0m\rangle$$
$$\times c^\dagger_{k'j_em'}c_{kj_em}\,|J_0M_0'\rangle\langle J_0M_0\,|\;, \tag{2.3}$$

where $\hat{P}_{J_1}$ is the projection operator over total angular momentum J_1:

$$\hat{P}_{J_1}=\sum_{M_1}|J_1M_1\rangle\langle J_1M_1\,| \tag{2.4}$$

and the coupling constant is given by

$$K=\frac{V^2}{\Delta-\epsilon_F}\;. \tag{2.5}$$

In the derivation of Hamiltonian (2.3), $V^2/(\Delta-\epsilon_k)$ has been approximated by K and constant terms were neglected.

Model (2.3) generalizes the usual Kondo interaction, which is obtained for $j_e=\frac{1}{2}$. In this case calling $\boldsymbol{\sigma}=\mathbf{j}_e$ we have[23]

$$\hat{P}_{J_1}=\frac{1}{2}+\frac{\text{sgn}(J_1-J_0)}{2J_0+1}(\tfrac{1}{2}+2\boldsymbol{\sigma}\cdot\mathbf{J}_0)\;. \tag{2.6}$$

The first term of Eq. (2.6) gives a potential scattering term after replacement in Eq. (2.3). The second term gives an s-d antiferromagnetic (ferromagnetic) interaction if $J_1=J_0-\frac{1}{2}$ $(J_0+\frac{1}{2})$. Thus, disregarding potential scattering and using transformation (2.2), we see that for $j_e=\frac{1}{2}$ in the limit $|\Delta-\epsilon_F|\gg\pi\rho(\epsilon_F)V^2$, model (2.1) reduces to a spin $J_{\max}$ if the configuration of greater angular momentum $J_{\max}$ is the ground-state configuration, and to a ferromagnetic s-d exchange model with spin $J_{\min}=J_{\max}-\frac{1}{2}$ in the opposite situation. In both situations the magnitude of the exchange coupling constant is given by $2|K|/(2J_0+1)$.

III. BETHE HYPOTHESIS

The steps and assumptions necessary to describe the system in terms of a wave function of the Bethe-ansatz form are similar to those followed in the solution of the Anderson model.[25]

Linearizing the dispersion relation about the Fermi energy, the Hamiltonian can be put in the form (dropping the subindex j_e of the band operators)

$$H=E_{J_0}\sum_{M_0}|J_0M_0\rangle\langle J_0M_0|+(E_{J_0}+\Delta)\sum_{M_1}|J_1M_1\rangle\langle J_1M_1|$$
$$+\int dx\left[-i\sum_m c_m^\dagger(x)\frac{\partial}{\partial x}c_m(x)+V\delta(x)\left[\sum_{m,M_0,M_1}\langle J_0j_eM_0m\,|\,J_1M_1\rangle[c_m^\dagger(x)\,|J_0M_0\rangle\langle J_1M_1|+\text{H.c.}]\right]\right]. \quad (3.1)$$

The eigenstates of H with N particles and total angular momentum projection M are of the form

$$|\psi\rangle=\sum_{M_0,m_1,m_2,\dots,m_N}{}' \int\left[\prod_{i=1}^N dx_i\right]g_{M_0,m_1m_2\cdots m_N}(x_1,x_2,\dots,x_N)\left[\prod_{i=1}^N c_{m_i}^\dagger(x_i)\right]|J_0M_0\rangle$$
$$+\sum_{M_1,m_1,m_2,\dots,m_{N-1}}{}' \int\left[\prod_{i=1}^{N-1} dx_i\right]e_{M_1m_2m_2\cdots m_{N-1}}(x_1,x_2,\dots,x_{N-1})\left[\prod_{i=1}^{N-1} c_{m_i}^\dagger(x_i)\right]|J_1M_1\rangle\ , \quad (3.2)$$

where the prime over the summation indicates that only states with total angular momentum projection M are included.

Inserting Eq. (3.2) into the Schrödinger equation

$$H|\psi\rangle=E|\psi\rangle \quad (3.3)$$

we obtain first quantization equations relating the functions g and e:

$$N!\left[-i\sum_{j=1}^N\frac{\partial}{\partial x_j}+E_{J_0}-E\right]g_{M_0m_1m_2\cdots m_N}(x_1,x_2,\dots,x_N)$$
$$+V\sum_{P_1,M_1}(-1)^P\langle J_0j_eM_0m_{PN}\,|\,J_1M_1\rangle\delta(x_{PN})e_{M_1m_{P1}m_{P2}\cdots m_{P(N-1)}}(x_{P1},x_{P2},\dots,x_{P(N-1)})=0\ , \quad (3.4)$$

$$\left[-i\sum_{j=1}^{N-1}\frac{\partial}{x_j}+E_{J_0}+\Delta-E\right]e_{M_1m_1m_2\cdots m_{N-1}}(x_1,x_2,\dots,x_{N-1})$$
$$+VN\sum_{M_0,m_N}\langle J_0j_eM_0m_N\,|\,J_1M_1\rangle g_{M_0m_1m_2\cdots m_N}(x_1,x_2,\dots,x_{N-1},0)=0\ , \quad (3.5)$$

where P is a permutation of the N numbers $1,2,\dots,N$.

As explained by Wiegmann[26] the space should be divided into $(N+1)!$ regions defined by the different permutations Q of the numbers $1,2,3,\dots N$:

$$X_Q=\{x_{Q0}<x_{Q1}<\cdots<x_{QN}\}\ ,$$

where $x_0=0$ is the impurity position. According to Bethe hypothesis the function g that satisfies Eqs. (3.4) and (3.5) has the following form in each region X_Q:

$$g_{M_0m_1m_2\cdots m_N}(x_1,x_2,\dots,x_N)$$
$$=\sum_P A_{M_0m_1m_2\cdots m_N}(Q;P)\exp\left[i\sum_{j=1}^N k_{P_j}x_j\right]\ , \quad (3.6)$$

where the k_i are N different numbers that give the energy of the state $|\psi\rangle$

$$E=E_{J_0}+\sum_{j=1}^N k_j \quad (3.7)$$

and P labels a permutation of these numbers.

The antisymmetry of g relates the coefficients A for any P to those corresponding to $P=1$ (identity permutation) by

$$A_{M_0m_1m_2\cdots m_N}(Q;P)=(-1)^PA_{M_0m_{P1}m_{P2}\cdots m_{PN}}(PQ;I)\ . \quad (3.8)$$

Equations (3.4) and (3.5) relate the coefficients $A(Q;I)$ of neighboring regions X_Q and $X_{\tilde Q}$. The equations for the discontinuities at $x_j=0$ $(j\neq0)$ take the form of a one-particle problem since the remaining coordinates can be kept fixed. Consequently, the corresponding coefficients are related by a matrix involving only two pairs of indices,

$$A_{M_0\cdots m_j\cdots}(\tilde Q;I)=\sum_{M_0',m_j'}(\hat R_{j0})_{m_jm_j'}^{M_0M_0'}A_{M_0'\cdots m_j'\cdots}(Q,I)\ \text{ with } X_{\tilde Q}=\{\cdots<0<x_j<\cdots\}\ ;\ X_Q=\{<x_j<0<\cdots\}\ . \quad (3.9)$$

The equations for the discontinuities at $x_i=x_j$ $(i,j\neq0)$ involve two particles and the impurity. It is essential for the validity of Bethe hypothesis that the corresponding matrix relating the coefficients of both neighboring regions does not depend on the impurity indices.[27] In this case we can write

$$A_{\cdots m_i \cdots m_j \cdots}(\widetilde{Q};I)=\sum_{m_i',m_j'}(\hat{S}_{ji})^{m_i m_i'}_{m_j m_j'}A_{\cdots m_i' \cdots m_j' \cdots}(Q;I)$$

$$\text{with } X_{\widetilde{Q}}=\{\cdots<x_i<x_j<\cdots\};\quad X_Q=\{\cdots<x_j<x_i<\cdots\}\ . \tag{3.10}$$

There are many ways of expressing the coefficients $A(\widetilde{Q},I)$ in terms of the $A(Q;I)$ for two arbitrary regions $X_{\widetilde{Q}}$ and X_Q by repeated application of Eqs. (3.9) and (3.10). The requirement that all these ways should lead to an identical result leads to the unitary and triangular conditions.[28] With the imposition of periodic boundary conditions, the whole problem is reduced to the solution of N eigenvalue equations similar to those found in other Bethe-ansatz-solved problems:[3]

$$(e^{ik_jL}-\hat{T}_j)A(I',I)=0,\quad j=1,2,\ldots,N\ , \tag{3.11}$$

where

$$\hat{T}_j=\hat{S}_{j+1,j}\hat{S}_{j+2,j}\cdots\hat{S}_{N,j}\hat{R}_{0j}\hat{S}_{1j}\hat{S}_{2j}\cdots\hat{S}_{j-1,j}\ . \tag{3.12}$$

Here and in what follows the angular momentum projection indices are omitted for simplicity and in all multiplications the sum over repeated indices is understood.

The matrix $\hat{R}_{j0}$ and its inverse can be calculated replacing Eq. (3.6) in Eqs. (3.4) and (3.5). One obtains a set of linear equations for the $A(Q;I)$ which has the same form for any value of N. As in Ref. 29 we take the value of a function at a discontinuity as half the sum of both limiting values. The solution of this system gives us

$$\hat{R}_{j0}=\hat{I}+\frac{iK_j}{1-iK_j/2}\hat{P}_{J_1}\ , \tag{3.13}$$

where $\hat{I}$ is the identity matrix, $\hat{P}_{J_1}$ is given by Eq. (2.4), and

$$K_j=\frac{V^2}{\Delta-k_j}\ . \tag{3.14}$$

In the exchange limit given by Hamiltonian (2.3) the states of the system are described by the function g only, and making the same approximations that lead to (2.3), the matrix $\hat{R}_{j0}$ is given the same expression (3.13) with K_j replaced by K [Eqs. (2.5)].

The calculation of the matrices $\hat{S}_{ji}$ is more involved as we shall see in Sec. V. Nevertheless its general form can be determined by the condition of continuity of the function g at the boundaries $x_i=x_j$ $(i,j\neq 0)$. Using Eq. (3.8), these conditions are seen to be satisfied if and only if the matrix $\hat{S}_{ji}$ has the following form

$$\hat{S}_{ji}=b_{ji}\hat{I}+(1-b_{ji})\hat{P}_{ji}\ , \tag{3.15}$$

where b_{ji} is a complex constant and $\hat{P}_{ji}$ interchanges the momentum projections of both particles:

$$(\hat{P}_{ji})^{m_i m_i'}_{m_j m_j'}=\delta_{m_i m_j'}\delta_{m_j m_i'}\ . \tag{3.16}$$

In the exchange limit, since the matrices $\hat{R}$ do not depend on wave vector, one can choose a totally antisymmetric form for the function g in *each* region of space.[30] In this case, using the antisymmetry conditions (3.8) we have

$$\hat{S}_{ji}=\hat{P}_{ji};\quad |\Delta-\epsilon_F|\to\infty\ . \tag{3.17}$$

This form of the matrix $\hat{S}_{ji}$ can be easily seen to satisfy the unitary and triangular conditions for any form of $\hat{R}_{j0}$. Then, the coordinate Bethe ansatz is valid in the exchange limit for any total angular momenta J_0, J_1, j_e. Diagonalization of Hamiltonian (2.3) is reduced to solving a problem of a linear chain of interacting spins given by (3.11) to (3.14) and (3.17) with $K_j=K$.

This is not the case for $J_0J_1<0$, $j_e>\frac{1}{2}$ in the intermediate valence regime, as we show in Sec. IV.

IV. THE INTEGRABILITY OF THE MODEL

Eigenvalue problems of the form (3.11) and (3.12) have been solved using a so-called second Bethe ansatz or the related quantum inverse-scattering method.[3] To apply this method, the matrices $\hat{R}_{j0}$ and $\hat{S}_{ji}$ should be generalized to a family of matrices $\widetilde{R}_{j0}(\alpha)$ and $\widetilde{S}_{ji}(\alpha)$ depending on one parameter α. These matrices should coincide with the previous ones for certain values of their parameters:

$$\hat{R}_{jo}=\widetilde{R}_{j0}(\alpha_{j0})\ , \tag{4.1}$$

$$\hat{S}_{ji}=\widetilde{S}_{ji}(\alpha_{ji})\ . \tag{4.2}$$

For the model to be integrable, the new matrices should satisfy parametric equations that generalize the unitary and triangular conditions

$$\widetilde{R}_{j0}(\alpha)\widetilde{R}_{j0}(-\alpha)=\hat{I}\ , \tag{4.3}$$

$$\widetilde{S}_{ji}(\alpha)\widetilde{S}_{ji}(-\alpha)=\hat{I}\ , \tag{4.4}$$

$$\widetilde{S}_{jk}(\alpha)\widetilde{R}_{j0}(\alpha+\alpha')\widetilde{R}_{k0}(\alpha')=\widetilde{R}_{k0}(\alpha')\widetilde{R}_{j0}(\alpha+\alpha')\widetilde{S}_{jk}(\alpha)\ , \tag{4.5}$$

$$\widetilde{S}_{jk}(\alpha)\widetilde{S}_{ji}(\alpha+\alpha')\widetilde{S}_{ki}(\alpha')=\widetilde{S}_{ki}(\alpha')\widetilde{S}_{ji}(\alpha+\alpha')\widetilde{S}_{jk}(\alpha)\ . \tag{4.6}$$

For those equations to imply the unitary and triangular conditions as a particular case one should have

$$\hat{R}_{0j}=\widetilde{R}_{j0}(-\alpha_{j0})\ , \tag{4.7}$$

$$\hat{S}_{ij}=\widetilde{S}_{ji}(-\alpha_{ji})\ , \tag{4.8}$$

$$\alpha_{j0}=\alpha_{jk}+\alpha_{k0}\ , \tag{4.9}$$

$$\alpha_{ji}=\alpha_{jk}+\alpha_{ki}\ . \tag{4.10}$$

The solution of Eqs. (4.4) and (4.6) in terms of $\hat{I}$ and $\hat{P}_{ij}$ is (within a factor irrelevant of our discussion[3])

$$\widetilde{S}_{ji}(\alpha)=b(\alpha)\hat{I}+[1-b(\alpha)]\hat{P}_{ji} \tag{4.11}$$

with

$$b(\alpha)=\frac{\alpha}{\alpha+ig}\,, \tag{4.12}$$

where g is a constant. This matrix satisfies (4.2) for $\hat{S}_{ji}$ given by (3.15) or (3.17) and some α_{ji}.

Similarly, the solution of Eq. (4.3) with the condition (4.1) with (3.13) in terms of $\widetilde{I}$ and $\hat{P}_{J_1}$ is (within other unimportant factors)

$$\widetilde{R}_{j0}(\alpha)=\hat{I}+\frac{2f(\alpha)}{1-f(\alpha)}\hat{P}_{J_1}\,, \tag{4.13}$$

where the function $f(\alpha)$ satisfies

$$f(\alpha_{j0})=iK_j/2\,, \tag{4.14}$$

$$f(-\alpha)=-f(\alpha)\,, \tag{4.15}$$

being otherwise arbitrary.

To satisfy all the parametric equations it remains to check if the triangular condition (4.5) is satisfied for matrices of the form (4.11) and (4.13). We show below that failure of this condition for $J_0J_1>0$, $j_e>\frac{1}{2}$ and $\alpha\neq 0$ implies for these angular momenta, that (1), the Bethe hypothesis is not valid in the intermediate valence regime and (2) in the exchange limit, though that hypothesis works, the model is not integrable with the parametrization (4.11) and (4.13) of the matrices $\widetilde{R}_{j0}$ and $\hat{S}_{ji}$.

Using Eqs. (4.11) and (4.13), Eq. (4.5) takes the form

$$2b(\alpha)h(\alpha')h(\alpha+\alpha')\hat{O}_1+[1-b(\alpha)][h(\alpha+\alpha')-h(\alpha')]\hat{O}_2=0\,, \tag{4.16}$$

where

$$h(\alpha)=\frac{f(\alpha)}{1-f(\alpha)} \tag{4.17}$$

and the operators $\hat{O}_1$ and $\hat{O}_2$ are given by

$$(\hat{O}_1)^{M_0m_1m_2}_{M_0'm_1'm_2'}=(\hat{Q}_1)^{M_0m_1m_2}_{M_0'm_1'm_2'}-(\hat{Q}_1)^{M_0m_2m_1}_{M_0'm_2'm_1'}\,, \tag{4.18}$$

$$(\hat{O}_2)^{M_0m_1m_2}_{M_0'm_1'm_2'}=(\hat{Q}_2)^{M_0m_1m_2}_{M_0'm_1'm_2'}-(\hat{Q}_2)^{M_0m_2m_1}_{M_0'm_2'm_1'}\,, \tag{4.19}$$

with

$$(\hat{Q}_1)^{M_0m_1m_2}_{M_0'm_1'm_2'}=\delta_{M_0+m_1+m_2,M_0'+m_1'+m_2'}\langle J_0M_1j_em_1\,|\,\hat{P}_{J_1}\,|\,J_0(M_0+m_1-m_1')j_em_2'\rangle \times\langle J_0M_0'+m_2'-m_2)j_em_2\,|\,\hat{P}_{J_1}\,|\,J_0M_0'j_em_2'\rangle\,, \tag{4.20}$$

$$(\hat{Q}_2)^{M_0m_1m_2}_{M_0',m_1'm_2'}=\delta_{m_2m_1'}\langle J_0M_0j_em_1\,|\,\hat{P}_{J_1}\,|\,J_0M_0'j_em_2'\rangle\,. \tag{4.21}$$

For Eq. (4.16) to be satisfied for any values of the parameters, the operators $\hat{O}_1$ and $\hat{O}_2$ should be proportional. This is not the case for $J_0J_1>0$, $j_e>\frac{1}{2}$ since one can find particular nonvanishing matrix elements of $\hat{O}_1$, while the corresponding ones of $\hat{O}_2$ do vanish. Hence the parametric equation (4.5) is not satisfied for these total angular moments.

We also see from the foregoing discussion that if the triangular condition implied by Eq. (4.5) with (4.1) and (4.2) holds for $J_0J_1>0$, $j_e>\frac{1}{2}$, the coefficients of the operators $\hat{O}_i$ in Eq. (4.16) should vanish for the parameters α_{j0} and α_{ji}. Using Eqs. (4.5), (4.12), and (4.14) we see that this happens if and only if $\alpha_{jk}=0$. This is the case in the exchange limit [compare Eqs. (3.17) and (4.11)], but in the intermediate valence regime since we have $K_j\neq K_k$ [see Eq. (3.14)] because all the k numbers are different, Eq. (4.14) implies $\alpha_{j0}\neq\alpha_{k0}$ and then from Eq. (4.9) we have $\alpha_{jk}\neq 0$.

We conclude that for two magnetic configurations and $j_e>\frac{1}{2}$, the Bethe hypothesis is not valid for model (2.1) in the intermediate valence regime. In the exchange limit we believe that the model is not integrable by means of the quantum inverse-scattering method, since a parametrization of the matrices $\hat{R}_{j0}$ and $\hat{S}_{ji}$ including other operators as those involved in (4.11) and (4.13) and satisfying Eqs. (4.3) to (4.6) does not seem physically plausible (we were not able to prove it).

The remaining cases are integrable and can be classified as follows.

(1) For a nonmagnetic $4f^n$ configuration ($J_0=0$) the model reduces to the SU($2j_e+1$) Anderson model solved in Refs. 5 and 6. The operator $\hat{P}_{J_1}$ is equivalent to the identity and the matrices $\hat{R}_{0j}$ and $\hat{R}_{0j}(\alpha)$ reduce to scalars [see Eqs. (3.13) and (4.13)]. Equation (4.5) reduces to an identity and $\hat{R}_{0j}$ enters the problem only as a phase shift in Eq. (3.12).

(2) For a nonmagnetic $4f^{n+1}$ configuration ($J_1=0$) we can apply transformation (2.2) and we return to the preceding case. For $J_1=0$ we have $\hat{O}_2=(2j_e+1)\,\hat{O}_1$ and Eq. (4.5) can also be satisfied.

(3) For $j_e=0$ the impurity angular momentum is conserved. For each projection $M_0=M_1$ the model takes the form of a one-particle problem and can then be solved exactly without use of the Bethe method. For $J_0=J_1=\frac{1}{2}$ the model is equivalent to that studied in Ref. 18.

(4) For $J_0J_1>0$, $j_e=\frac{1}{2}$. The Bethe ansatz solution of the model for $j_e=\frac{1}{2}$, including these cases and the nondegenerate Anderson model, is presented in Sec. V.

To close this section we note that, as we have shown in Sec. II, for $j_e=\frac{1}{2}$ the exchange limits of our model are similar to usual spin-S s-d exchange models which have been solved exactly.[29,31] The solution of the parametric triangular equations is presented in Ref. 31. Following our scheme, for $j_e=\frac{1}{2}$, we have

$$\hat{O}_2 = -(2J_0+1)\mathrm{sgn}(J_1-J_0)\hat{O}_1 \ . \tag{4.22}$$

Replacing this, (4.12), and (4.17) in Eq. (4.16) we obtain

$$\frac{1}{f(\alpha+\alpha')} = \frac{1}{f(\alpha')} + \frac{2\alpha}{ig(ZJ_0+1)}\mathrm{sgn}(J_1-J_0) \ . \tag{4.23}$$

The solution of this equation with condition (4.15) is

$$f(\alpha) = \frac{ig(2J_0+1)}{2\alpha}\mathrm{sgn}(J_1-J_0) \ . \tag{4.24}$$

Thus, for $j_e=\frac{1}{2}$, the parametric equations (4.3) to (4.6) are satisfied by the matrices given by (4.11) and (4.13) with (4.12) and (4.24).

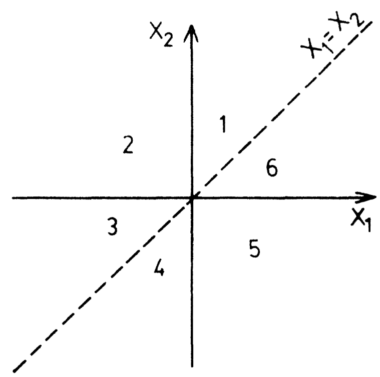

FIG. 1. The 3! regions X_Q in which the space is divided to set up the Bethe hypothesis for two particles.

V. EXACT SOLUTION FOR $j_e=\frac{1}{2}$

We restrict ourselves to $J_1=J_0+\frac{1}{2}$. The case $J_1=J_0-\frac{1}{2}$ can be reduced to the former using transformation (2.2).

A. The matrix $\hat{S}_{ji}$

As explained in Sec. III, the matrix $\hat{S}_{ji}$ is determined by the equations for the discontinuities of the coefficients $A(Q,I)$ at $x_i=x_j$ $(I,j\neq 0)$ obtained replacing (3.6) into (3.4) and (3.5). These take the form of a problem with two particles and the impurity. Thus, for simplicity we perform the calculations for $N=2$. The result is independent of $N\geq 2$. We number the permutations Q defining the different regions of the two-dimensional space according to Fig. 1.

Replacing (3.6) into (3.4) and equating to zero the coefficients of $\delta(x_2)$ we obtain (taking $j_e=\frac{1}{2}$, $m_i=\sigma_i$)

$$V\langle J_0\tfrac{1}{2}M_0\sigma_2\,|\,J_1M_1\rangle e_{M_1\sigma_1}(x) = 2\sum_P \exp(ik_{P1}x)\{[A_{M_0\sigma_1\sigma_2}(2;P)-A_{M_0\sigma_1\sigma_2}(3;P)]\Theta(-x)$$
$$+[A_{M_0\sigma_1\sigma_2}(6;P)-A_{M_0\sigma_1\sigma_2}(5;P)]\Theta(x)\} \ , \tag{5.1}$$

where the unit step function $\Theta(x)$ is defined as

$$\Theta(x) = \begin{cases} 0 & \text{if} \quad x<0 \\ \frac{1}{2} & \text{if} \quad x=0 \\ 1 & \text{if} \quad x>0 \ . \end{cases} \tag{5.2}$$

When replacing Eq. (5.1) into (3.5) we obtain terms with factors $\exp(ik_jx)\Theta(\pm x)$ $(j=1,2)$ and other terms in $\delta(x)$. The former terms give four equations for the discontinuities at $x_j=0$, the solution of which is given by (3.9) and (3.13) with (3.8). Equating to zero the terms in $\delta(x)$ and using (3.8) we obtain

$$A_{M_0\sigma_1\sigma_2}(6;I)+A_{M_0\sigma_1\sigma_2}(3;I)-A_{M_0\sigma_1\sigma_2}(5;I)-A_{M_0\sigma_1\sigma_2}(2;I)$$
$$+A_{M_0\sigma_2\sigma_1}(5;I)+A_{M_0\sigma_2\sigma_1}(2;I)-A_{M_0\sigma_2\sigma_1}(1;I)-A_{M_0\sigma_2\sigma_1}(4;I)=0 \ . \tag{5.3}$$

All these coefficients can be expressed in terms of those of regions 3 and 4 for example (one could also choose regions 1 and 6) using the matrices $\hat{R}_{j0}$. If the triangular conditions are satisfied, the result for $\hat{S}_{ji}$ does not depend on the choice of regions.

The resulting equations and particular continuity conditions

$$A_{M_0\sigma\sigma}(3;I)=A_{M_0\sigma\sigma}(4;I) \tag{5.4}$$

determine $\hat{S}_{ji}$ for each value of the total angular momentum M_t.

For $J_0>0$ and $|M_t|\leq J_0$, Eqs. (5.3) are not all independent since some discontinuities of the $A(Q;P)$ across the boundaries $x_j=0$ are related with others.

Solving the system of linear equations and using Eq. (3.10) we find, after a lengthy algebraic analysis, that for all values of M_t the matrix S_{ji}, can be represented by

$$\hat{S}_{ji}=\tilde{S}_{ji}(k_i-k_j) \ , \tag{5.5}$$

where

$$\tilde{S}_{ji}(\alpha)=\frac{\alpha\hat{I}+ig\hat{P}_{ji}}{\alpha+ig} \ , \tag{5.6}$$

and

$$g=\frac{V^2}{2J_0+1}\ . \tag{5.7}$$

B. The Bethe ansatz equations

In analogy to Eqs. (5.5) to (5.7), we can write Eq. (3.13) in the form

$$\hat{R}_{j0}=\tilde{R}_{j0}(\Delta-k_j) \tag{5.8}$$

with

$$\tilde{R}_{j0}(\alpha)=\hat{I}+\frac{ig(2J_0+1)}{\alpha-ig(2J_0+1)/2}\hat{P}_{J_1}\ . \tag{5.9}$$

We have seen in the preceding section that the matrices $\tilde{S}_{ji}(\alpha)$ and $\tilde{R}_{jo}(\alpha)$ satisfy the parametric equations (4.3) to (4.6). Taking particular values of the parameters these equations imply the validity of the Bethe hypothesis. Then, the model is integrable.

Using a procedure similar to that employed for the Kondo model with arbitrary spin[3] we obtain that for total angular momentum $J=J_0+N/2-M$, the N different numbers k_j and M different numbers Λ_γ satisfy the set of coupled equations

$$e^{ik_jL}=\frac{k_j-\Delta+i\frac{V^2}{2}}{k_j-\Delta-i\frac{V^2}{2}}\prod_{\beta=1}^{M}\frac{\Lambda_\beta+k_j+\frac{iV^2}{4J_0+2}}{\Lambda_\beta-k_j-i\frac{V^2}{4J_0+1}}\ ,$$

$$j=1,2,\ldots,N \tag{5.10}$$

$$\prod_{\beta=1}^{M}\frac{\Lambda_\alpha-\Lambda_\beta+i\frac{V^2}{2J_0+1}}{\Lambda_\alpha-\Lambda_\beta-i\frac{V^2}{2J_0+1}}=-\frac{\Lambda_\alpha-\Lambda+\frac{iV^2J_0}{2J_0+1}}{\Lambda_\alpha-\Delta-\frac{iV^2J_0}{2J_0+1}}\prod_{j=1}^{N}\frac{\Lambda_\alpha-k_j+i\frac{V^2}{4J_0+2}}{\Lambda_\alpha-k_j+i\frac{V^2}{4J_0+2}}\ ,$$

$$\alpha=1,2,\ldots,M\ . \tag{5.11}$$

For $J_0=0$, these equations are identical to those corresponding to the nondegenerate Anderson model in the limit of infinite $4f$ intra-atomic Coulomb repulsion.[6,13]

In the exchange limit $\Delta-\epsilon_F\gg V^2$, making the same approximations that led to (2.3) we should take $k_j=\epsilon_F$, $j=1$ to N, in the right-hand side of Eqs. (5.10) and (5.11).[25] Replacing Λ_B for $\epsilon_F+V^2\lambda_B/(2J_0+1)$ and neglecting a constant shift of all levels, these equations take the form of the Bethe ansatz equations for an s-d exchange model with ferromagnetic coupling between a localized spin of magnitude J_0 and conduction-electron spins.[29,31]

For $|\Delta|\gg V^2$ and $\Delta<0$, we take $N+1$ particles and $k_{N+1}=\Delta$ in the right-hand side of Eqs. (5.10) and (5.11). Following the same procedure as before and making the approximation

$$\frac{\Lambda_\alpha-\Delta+\frac{iV^2J_0}{2J_0+1}}{\Lambda_\alpha-\Delta+\frac{iV^2J_0}{2J_0+1}}\ \frac{\Lambda_\alpha-\Delta+\frac{iV^2}{4J_0+2}}{\Lambda_\alpha-\Delta-\frac{iV^2}{4J_0+2}}\cong\frac{\Lambda_\alpha-\Delta+i\frac{V^2}{2}}{\Lambda_\alpha-\Delta-i\frac{V^2}{2}}$$

we get the Bethe ansatz equations of a spin-$J_0+\frac{1}{2}$ Kondo model.[29,31]

In both cases the magnitude of the coupling constant is $2V^2/[(2J_0+1)|\Delta-\epsilon_F|]$ in agreement with the results of the canonical transformation on model (2.1) (Sec. II).

C. The ground-state densities of k's and Λ's

As in the Anderson models[5,13] the electrons with opposite spin of our system tend to bind and form bound pairs. These are described by pairs of complex conjugated k numbers.

Similarly to Ref. 13, the ground state of our system for total angular momentum $J=J_0+N/2-M$ is described by $2M$ complex k's, $N-2M$ real k's (corresponding to unpaired electrons) and M real Λ's.

If k_j is complex, the first member of Eq. (5.10) vanishes or diverges in the thermodynamic limit $L\to\infty$. Thus, one of the factors in the numerator or denominator, respectively, of the second member of the equation should vanish. This implies that each pair of complex conjugated k's are associated with one of the numbers Λ_β and we can write choosing a particular order for the k_j (the real with the smallest subindices).

$$\begin{aligned}k_{N-2M+2\beta-1}&=\Lambda_\beta+i\frac{g}{2}+a_\beta\ ,\\ k_{N-2M+2\beta}&=\Lambda_\beta-i\frac{g}{2}+\bar{a}_\beta\ ,\end{aligned} \tag{5.12}$$

where g is given by (5.7), $\beta=1,2,\ldots,M$, and a_β is a complex number that vanishes in the thermodynamic limit which we henceforth assume. $\bar{a}_\beta$ is the complex conjugate of a_β.

Dividing member by member Eqs. (5.10) for $j=N-2M+2\alpha-1$ and $j=N-2M+2\alpha$ we obtain an expression for $|a_\alpha|$ which shows that it is exponentially small.

Replacing (5.12) in (5.10) and (5.11), neglecting exponentially small terms, and taking logarithms we obtain, in the continuous limit,

$$\begin{aligned}\sigma(\Lambda)=&\frac{1}{\pi}+\frac{1}{L}\frac{(J_0+1)g/\pi}{(\Lambda-\Delta)^2+(J_0+1)^2g^2}\\ &-\int_D^Q d\Lambda'\sigma(\Lambda')\frac{g/\pi}{(\Lambda-\Lambda')^2+g^2}\\ &-\int_D^B dk\,\rho(k)\frac{g/2\pi}{(\Lambda-k)^2+g^2/4}\ ,\end{aligned} \tag{5.13}$$

where

$$\Gamma=\frac{V^2}{2}=g(J_0+\tfrac{1}{2})\ . \tag{5.14}$$

Analogously, Eq. (5.10) for $j=1$ to $N-2M$ takes the form

$$\rho(k)=\frac{1}{2\pi}+\frac{1}{L}\frac{\Gamma/\pi}{(k-\Delta)^2+\Gamma^2}-\int_D^Q d\Lambda'\,\sigma(\Lambda')\frac{g/2\pi}{(\Lambda'-k)^2+g^2}\ . \tag{5.15}$$

D is a cutoff that bounds the energy spectrum from below, and the upper limits Q and B are determined by the number of spin-paired $(2M)$ and unpaired $(N-2M)$ electrons

$$\frac{M}{L}=\int_D^Q \sigma(\Lambda)d\Lambda\ , \tag{5.16}$$

$$\frac{N-2M}{L}=\int_D^B \rho(k)dk\ . \tag{5.17}$$

Due to the assumption of a linear dispersion relation in Hamiltonian (3.1), the spectrum of k and Λ is unbounded. The cutoff D is introduced to make the integrals convergent and simulates the bottom of a square conduction band.

The densities $\sigma(\Lambda)$ and $\rho(k)$ are split into host (order 1) impurity (order $1/L$) parts. The former $[\sigma_h(\Lambda)$ and $\rho_h(k)]$ are the only ones that contribute significantly to Eq. (5.16) and (5.17) and then determine the integration limits. The impurity contributions $\sigma_i(\Lambda)/L$ and $\rho_i(k)/L$ determine the physical properties of the impurity.

The results for the host and impurity densities obtained solving numerically Eqs. (5.13) to (5.17) are represented in Figs. 2 and 3, respectively, for several values of the parameters. The host densities depend only on N/L, M/L, and g. $\sigma_h(\Lambda)$ and $\rho_h(k)$ are similar to the unperturbed spectral densities per spin of spin-paired and unpaired conduction electrons, respectively. The only significant differences are in intervals of energy of width of order g at the Fermi energy and at the bottom of the band. For $g=0$ we have the unperturbed structure.

We take the zero of energy as $(Q+D)/2$ with the value of Q corresponding to $N=2M$. For this value of M/N, the host densities are even functions of their arguments in the interval $[D,Q]$.

The structure of the densities near D is an artifact of the finite cutoff. It leads to a spontaneous host magnetization which is obviously wrong. To avoid this problem, in our numerical calculations we have placed the host densities for their unperturbed values for negative values of their respective arguments. In this way we reproduce the correct Pauli susceptibility within our precision.

As seen in Fig. 3, $2\sigma_i(\Lambda)$ has a resonant-level-like form of intermediate width between Γ and $\Gamma+g/2$ for $\Lambda-B>\Gamma$. It decreases for increasing B and vanishes for $B-\Lambda\gg\Gamma$. $\rho_i(k)$ has always a resonant-level-like form of width Γ. Both impurity densities have a small structure at their respective upper integration limits.

For $J_0\to\infty$, g goes to zero and Eqs. (5.13) and (5.15) can be solved analytically. We obtain for $1\ll J_0\ll L$ in the interval of interest $[D,\max(B,Q)]$

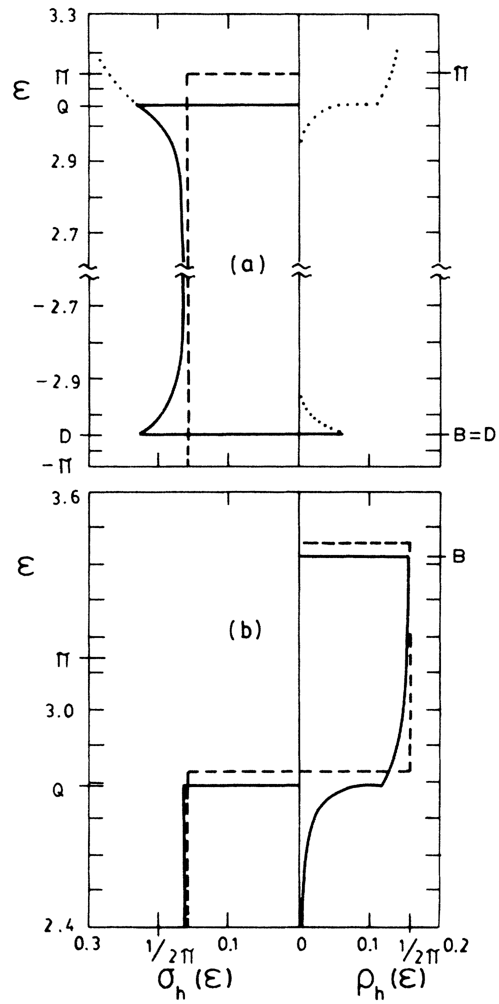

FIG. 2. Host densities or $N=2L$, $g=0.1$, and (a) $N-2M=0$, (b) $N-2M=0.1L$. The dashed lines show the densities per spin of spin-paired (left) and unpaired (left) and unpaired (right) unperturbed electrons for a rectangular band. The dotted lines in (a) show the densities beyond their respective upper limits of integration.

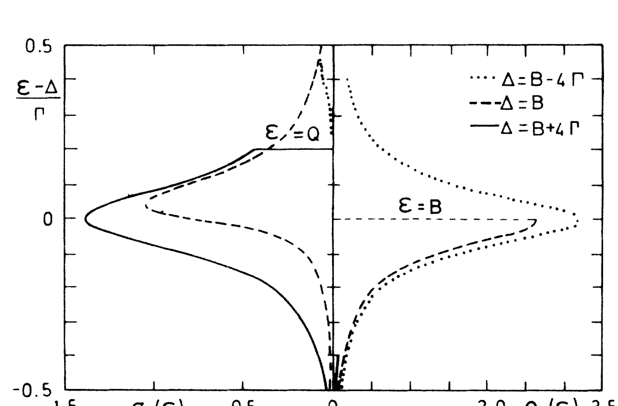

FIG. 3. Impurity densities for $J_0=\frac{1}{2}$, $\Gamma=0.1$, $B=Q-6\Gamma$, $Q=3.0526$ [as in Fig. 2(a)] and different values of Δ.

$$\sigma(\Lambda)=\frac{1}{2\pi}+\frac{1}{2L}\Theta(\Lambda-B)\frac{\Gamma/\pi}{(\Lambda-\Delta)^2+\Gamma^2}\ , \tag{5.18}$$

$$\rho(k)=\frac{1}{2\pi}\Theta(k-Q)+\frac{1}{L}\frac{\Gamma/\pi}{(\Lambda-\Delta)^2+\Gamma^2}\ . \tag{5.19}$$

D. The ground-state properties

Since the physical properties do not depend on the parity of N, we can assume N even. We find that for zero magnetic field ($H=0$) the energy given by (3.7) is minimum for $M=N/2$. This means that the ground state has total angular momentum J_0, and then except for the Anderson model ($J_0=0$) it is degenerate. This agrees with the predictions made by Anderson[32] and Mazzaferro *et al.*[16] with the renormalization-group calculations for $J_0=\frac{1}{2}$ (Ref. 17) and with the results for the spin-$J_0+\frac{1}{2}$ Kondo model (Refs. 29 and 31), which corresponds to the limit $\epsilon_F-\Delta\gg\Gamma$ of our model as explained in Sec. III.

For $H=0$, $B=D$ for the ground state and Eqs. (5.13) and (5.15) can be solved analytically for $D=-\infty$. To do this it is convenient to introduce the quantities

$$\mu=-\frac{\Lambda-Q}{g},\ \ q=\frac{k-Q}{g},\ \tilde{\Delta}=\frac{\Delta-Q}{g},\ \ \tilde{B}=\frac{B-Q}{g}\ , \tag{5.20}$$

and the densities of μ and q

$$\Sigma(\mu)=g\sigma(-\mu\Gamma+Q),\ \ R(q)=g\rho(q\Gamma+Q)\ . \tag{5.21}$$

In terms of these quantities, Eqs. (5.13) and (5.15) for $D=-\infty$ take the form

$$\Sigma(\mu)=\frac{g}{\pi}+\frac{1}{L}a_{2J_0+2}(\mu+\tilde{\Delta})-\int_0^{+\infty}d\mu'\,\Sigma(\mu')a_2(\mu-\mu') -\int_{-\infty}^{\tilde{B}}dq\,R(q)a_1(\mu+q)\ , \tag{5.22}$$

$$R(q)=\frac{g}{2\pi}+\frac{1}{L}a_{2J_0+1}(q-\tilde{\Delta})-\int_0^{\infty}d\mu\,\Sigma(\mu)a_1(\mu+q)\ , \tag{5.23}$$

where

$$a_n(x)=\frac{1}{\pi}\frac{n/2}{x^2+n^2/4}\ . \tag{5.24}$$

For $B=-\infty$, Eq. (5.22) is solved by the Wiener-Hopf method.[33] The result in terms of the Fourier transforms of the functions

$$\Sigma^{\pm}(\mu)=\Theta(\pm\mu)\Sigma(\mu)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{-1\omega\mu}\Sigma^{\pm}(\omega)d\omega \tag{5.25}$$

is given by

$$\Sigma_0^{-}(\omega)=-\frac{ig}{\sqrt{2\pi}}\frac{G^{-}(\omega)}{\omega-i0}+\frac{1}{L}\frac{i}{(2\pi)^{3/2}}G^{-}(\omega)I(\omega)\ , \tag{5.26}$$

where the subindex 0 indicates that the result is for zero magnetic field ($\tilde{B}=-\infty$) and

$$G^{-}(\omega)=\frac{(2\pi)^{1/2}[(i\omega/2\pi+0)/e]^{i\omega/2\pi}}{\Gamma[\frac{1}{2}+(i\omega/2\pi)]}\ , \tag{5.27}$$

$$I(\omega)=\int d\omega'\frac{\Gamma(\frac{1}{2}+i\omega')[(0-i\omega')/e]\exp[-2\pi i\omega'\tilde{\Delta}+(J_0+\frac{1}{2})\,|\,\omega'\,|\,]}{\omega'+i0-\omega/2\pi}\ . \tag{5.28}$$

$\Sigma^{+}(\omega)$ is obtained from $\Sigma^{-}(\omega)$ by Fourier transforming (5.22). In terms of this analytical solution one obtains an integral expression for the number of $4f$ electrons at zero field:

$$n_f=n+2\int_D^0\sigma_i(\Lambda)d\Lambda+\int_D^B\rho_i(k)dk =n+1-\frac{i}{2\pi^{3/2}}I(\omega=0)\ . \tag{5.29}$$

The expression generalizes the result for the nondegenerate Anderson model [Eq. (8.2.56) of Ref. 3 for $U\to\infty$]. n_f varies smoothly from $n+1$ for $\tilde{\Delta}\ll-J_1$ to n for $\tilde{\Delta}\gg J_1=J_0+1/2$ as shown in Fig. 4(a). To compare the values of n_f for the same Δ and different J_0 we have calculated Q solving numerically Eqs. (5.13) and (5.16) for $\sigma_h(\Lambda)$ with a finite cutoff and $M=N/2=L$. (We have used these values in all numerical calculations.)

The impurity energy is given by

$$E_i=2\int_D^Q\Lambda\sigma_i(\Lambda)d\Lambda+\int_D^B k\rho(k)dk+E_{J_0}\ . \tag{5.30}$$

For $H=0$ the second term vanishes. Since this expression diverges for $D\to-\infty$, we cannot use the Wiener-Hopf expression for $\sigma_i(\Lambda)$. The numerical results for a finite cutoff are shown in Fig. 4(b). The asymptotic limits for E_i are E_{J_0} for $\Delta-\epsilon_F\gg\Gamma$ and $E_{J_0}+\Delta-\epsilon_F$ for $\Delta-\epsilon_F\ll-\Gamma$.

An external magnetic field H removes the ground-state degeneracy. For small H, the impurity magnetization can be calculated analytically following similar arguments to those employed in Ref. 3 to calculate the magnetic susceptibility of the degenerate Anderson model.

Replacing the result for $\Sigma^{+}(u)$ obtained by means of the Fourier transform of Eq. (5.22) into (5.23) we obtain an equation with an integrable inhomogeneous term for $D=-\infty$. It is

$$R(q)=R'(q-\tilde{B}) . \tag{5.31}$$

This equation takes the form

$$R'(k)=\frac{1}{L}S_{2J_0+1}(k+\tilde{B}-\tilde{\Delta})+f(k) + \int_{-\infty}^{0} dk\, S_2(k-k')R'(k')dk' , \tag{5.32}$$

where

$$f(k)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} S_1(\omega)e^{i\omega(k+\tilde{B})}\Sigma^-(\omega)d\omega \tag{5.33}$$

and

$$S_n(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i\omega\lambda}\frac{e^{-n|\omega|/2}}{1+e^{-|\omega|}}d\omega . \tag{5.34}$$

Neglecting terms in H^2 [see Eq. (5.41)] we can replace $\Sigma^-(\omega)$ in Eq. (5.33) by $\Sigma_0^-(\omega)$ given by (5.26). The resulting integrand is analytical in the lower half plane. For $B \rightarrow -\infty$ the integral can be evaluated by residues using a contour that encircles only the pole in $-i\pi$ of the integrand. Neglecting terms in H^2 the result is

$$f(k)=\left[\frac{ge^{\pi\tilde{B}}}{(2\pi^3 e)^{1/2}}+\frac{C}{L}\frac{e^{\pi\tilde{B}}}{2\pi\sqrt{(2e)}}\right]e^{\pi k} , \tag{5.35}$$

where

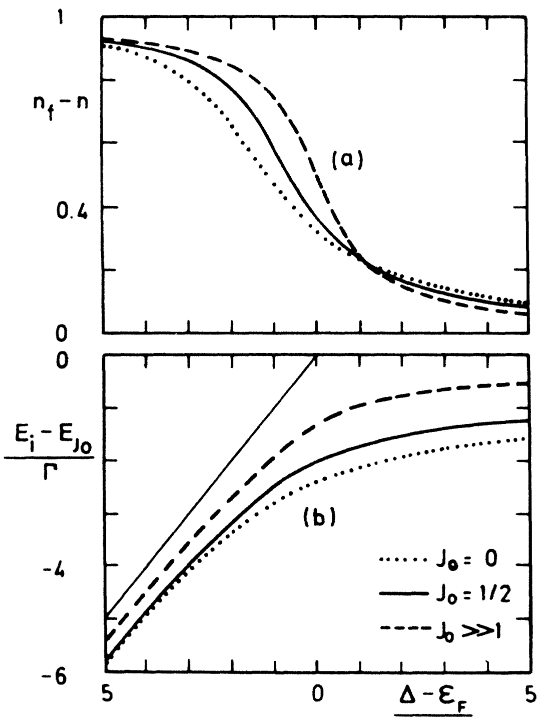

FIG. 4. (a) Valence and (b) impurity energy as functions of Δ for $H=0$, $\Gamma=0.1$, and different values of J_0. The straight line in (b) shows the asymptotic behavior for $\epsilon_F-\Delta \gg \Gamma$.

$$C=\int d\omega \frac{\Gamma(\frac{1}{2}+i\omega)\left[\frac{0-i\omega}{e}\right]^{-i\omega}\exp\{-2\pi[i\omega\tilde{\Delta}+(J_0+\frac{1}{2})|\omega|]\}}{\frac{1}{2}-i\omega} . \tag{5.36}$$

Applying the Wiener-Hopf method[33] to Eqs. (5.32) and (5.35) we obtain

$$R'^-(\omega)=\frac{ge^{\pi\tilde{B}}}{\sqrt{2}\pi e}\frac{G^-(\omega)}{i\omega+\pi} -\frac{i}{2\pi L}G^-(\omega)\int_{-\infty}^{+\infty} d\omega' \frac{G^-(-\omega')}{\omega-\omega'-i0}\frac{\exp[i\omega'(\tilde{\Delta}-\tilde{B})-(J_0+\frac{1}{2})|\omega'|]}{1+e^{-|\omega'|}}+\frac{C}{L}\frac{e^{\pi\tilde{B}}}{2e\sqrt{(2\pi)}}\frac{G^-(\omega)}{i\omega+\pi} . \tag{5.37}$$

With this expression we can evaluate the host and impurity magnetizations (we take $g\mu_B=1$ for all states) by

$$\frac{M_n}{L}=\frac{1}{2}\int_D^B \rho_h(k)dk=\frac{1}{2}R_h'^-(\omega=0) , \tag{5.38}$$

$$M_i=J_0+\frac{1}{2}\int_D^B \rho_i(k)dk=J_0+\frac{1}{2}R_i'-(\omega=0) . \tag{5.39}$$

Equations (5.26)—(5.29) and (5.37) and (5.39) are used in the calculation of the low-temperature expansion of the thermodynamic potential.[21]

To leading order in $1/L$ the magnetization of the system should be that of a free conduction band.

$$\frac{M_h}{L}=\frac{H}{4\pi} . \tag{5.40}$$

From Eqs. (5.38), (5.39), and (5.41) one can determine B as a function of H by

$$H=\frac{2g}{e\pi}e^{\pi\tilde{B}} . \tag{5.41}$$

Replacing the term in $1/L$ (5.37) in (5.39) and using (5.41) we finally obtain

$$M_i=M_i^K+\frac{HC}{8\sqrt{\pi}g} , \tag{5.42}$$

where C is given by (5.36) and

$$M_i^K=J_0+\frac{i}{4\pi^{3/2}}\int d\omega \frac{\exp[2i\omega\ln(T_\Delta/H)]}{\omega+i0} \times\Gamma(\tfrac{1}{2}+i\omega)e^{-J_0|\omega|}[(0-i\omega)/e]-i\omega , \tag{5.43}$$

where

$$T_\Delta = \frac{2g}{e\pi} e^{\pi\tilde{\Delta}} . \tag{5.44}$$

Since C behaves as $e^{\pi\tilde{\Delta}}$ for $\tilde{\Delta} \to -\infty$, M_i^K gives the impurity magnetization in the limit $\Delta - \epsilon_F \ll \Gamma$. In fact (5.43) is the expression for the impurity magnetization of a spin-$J_0 + \frac{1}{2}$ Kondo model[31] with Kondo temperature given by[3]

$$T_K = \left[\frac{e}{2\pi} \right]^{1/2} T_\Delta . \tag{5.45}$$

For $J_0 = 0$ the magnetic susceptibility of the nondegenerate Anderson model is reproduced.[3] The impurity magnetization varies from J_0 for $H \to 0$ to $J_0 + \frac{1}{2}$ for large fields. For $\Delta - \epsilon_F \ll \Gamma$ ($\tilde{\Delta} \ll J_0 + \frac{1}{2}$), Eq. (5.43) gives the impurity magnetization for all fields and for $J_0 \neq 0$ the intermediate values of M_i occur for fields of order T_Δ.

In the intermediate valence region, for intermediate or large values of the field and for J_0 of the order of 1, the Eqs. (5.13) and (5.15) cannot be solved analytically with standard methods. The numerical result for M_i for the simplest case for valence fluctuations between two magnetic configurations ($J_0 = \frac{1}{2}$) is represented in Fig. 5(a). The intermediate values of M_i take place at fields of order $\Gamma/2$ or $\Delta - \epsilon_F$ for $\Delta - \epsilon_F \sim \Gamma$ or $\Delta - \epsilon_F \gg \Gamma$, respectively.

In the latter case the change in M_i is associated with a change in the number of $4f$ electrons as illustrated in Fig. 5(b) in which we show the variation of n with magnetic field.

For $J_0 \gg 1$, the number of $4f$ electrons, impurity energy and impurity magnetization can be calculated analytically for any magnetic field using Eqs. (5.29) and (5.30). The results are

$$n_f = \frac{1}{\pi} \left[\Phi \left[\frac{\epsilon_F - \Delta + H/2}{\Gamma} \right] - \Phi \left[\frac{D - \Delta}{\Gamma} \right] \right] + n, \quad J_0 \gg 1 \tag{5.46}$$

$$E_i = \Delta n_f + \frac{\Gamma}{2\pi} \ln \left[\frac{\Gamma^2 + (E_F - \Delta + H/2)^2}{\Gamma^2 + (D - \Delta)^2} \right] + E_{J_0}, \quad J_0 \gg 1 \tag{5.47}$$

$$M_i = J_0 + \tfrac{1}{2}(n_f - n), \quad J_0 \gg 1 \tag{5.48}$$

where Φ is the arctangent function. In this limit $T_k \to 0$ [see Eqs. (5.45), (5.44), and (5.7)] and the Kondo effect disappears. Then for $\Delta - \epsilon_F \ll \Gamma$, $M_i = J_0 + \frac{1}{2}$ for any nonzero magnetic field. M_i is given directly by the number of $4f$ electrons.

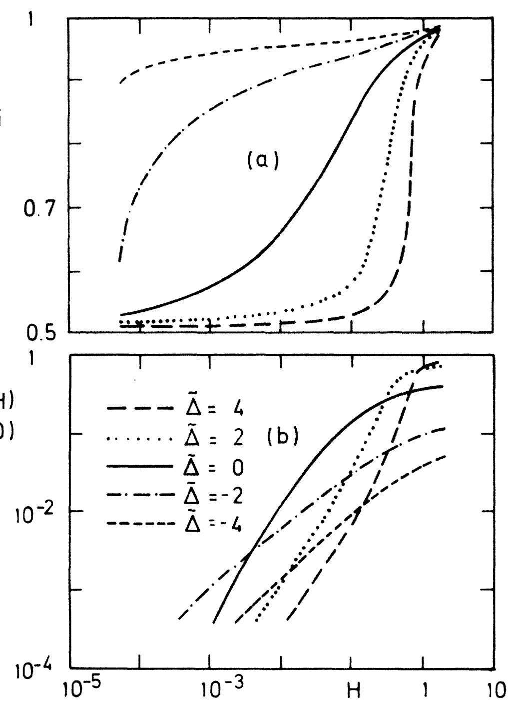

FIG. 5. (a) Impurity magnetization and (b) change of valence as functions of magnetic field for $J_0 = \frac{1}{2}$, $\Gamma = 0.1$, and different values of $\tilde{\Delta} = [\Delta - Q(H=0)]/\Gamma$.

VI. CONCLUSIONS AND DISCUSSION

We have studied the Bethe ansatz integrability of a general isotropic impurity model for valence fluctuations which hybridizes two $4f$ configurations of angular momentum J_0 and $J_1 \geq J_0$ by means of the promotion of an electron or a hole of angular momentum j_e to a conduction band.

The first Bethe ansatz solved model for valence fluctuations, the nondegenerate Anderson Hamiltonian,[4] in the limit of infinite $4f$ intra-atomic Coulomb repulsion corresponds to $J_0 = 0$ and $j_e = \frac{1}{2}$ (implying $J_1 = \frac{1}{2}$) in the model studied here. Its exact solution has been generalized for any j_e keeping $J_0 = 0$.[5,6]

In this work we have generalized the Bethe ansatz solution of the nondegenerate Anderson model for any J_0 keeping $j_e = \frac{1}{2}$ and we have shown that excluding the simplest case $j_e = 0$, the above-mentioned particular cases exhaust the values of total angular momenta for which the general model is Bethe ansatz solvable in the intermediate valence regime. In the exchange limit, the Bethe hypothesis is always valid, but the resulting eigenvalue problem (3.11) is not solvable either for $J_0 J_1 > 0$, $j_e > \frac{1}{2}$ by means of the quantum inverse scattering method or second Bethe ansatz, using the simplest parametrization of the matrices $\hat{R}$ and $\hat{S}$ [Eqs. (4.11) and (4.13)]. One could solve the eigenvalue equations (3.11), which only involve angular momenta variables by numerical or approximate methods.

Our solution for $j_e = \frac{1}{2}$ and any J_0 include a family of models for valence fluctuations between two magnetic configurations. The simplest one ($J_0 = \frac{1}{2}$, $J_1 = 1$), though does not realistically describe the $4f^{12}$ and $4f^{13}$ configurations, explains qualitatively the main properties of Tm systems.[16–21]

For $J_0 \neq 0$, contrary to the result for the other Bethe ansatz solved models for valence fluctuations,[4–7] the ground state is magnetic leading to a divergent magnetic susceptibility for vanishing temperature.

If the configuration of total angular momentum

$J_1 = J_0 + \frac{1}{2}$ is energetically favored the model reduces to a spin-J_1 Kondo model, while in the opposite limit it is equivalent to an s-d exchange model with ferromagnetic coupling between the spins of the conduction electrons and a localized spin of magnitude J_0.

In the intermediate valence regime, the variation of the number of $4f$ electrons and the impurity energy with the $4f$ level is qualitatively similar to that of the nondegenerate Anderson model. The impurity magnetization M_i is J_0 for vanishing magnetic fields. For high fields $M_i = J_0 + \frac{1}{2}$.

Among these models, that with $J_0 = 0$ (nondegenerate Anderson model) has long ago been recognized to describe qualitatively the properties of intermediate valence systems fluctuating between one magnetic and one nonmagnetic configurations. In the same way, though these models do not contain the angular momenta that correspond to real rare-earth ions, many of the properties of intermediate valence Tm, Pr, and also some U systems can be understood qualitatively in terms of the models with $J_0 J_1 > 0$, $j_e = \frac{1}{2}$.

Note added: After submission of this paper we received a copy of a paper by P. Schlottmann (unpublished) with some of the result of Chap. V and thermodynamic equations for $j_e = \frac{1}{2}$.

ACKNOWLEDGMENTS

One of us (C.A.B) gratefully acknowledges partial support by the John Simon Guggenheim Foundation (New York, NY); another (C.R.P.), partial support by Consejo Nacional de Investigaciones Cientificas y Técnicas (CONICET) Argentina.

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