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Magnetic field effects in the Anderson model of dilute magnetic alloys. I. Self-consistent solution

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We have studied the infinite-U Anderson dilute-alloy model in arbitrary magnetic fields by means of the double-time Green's-function method. Using a truncation procedure, the coupled equations are reduced to a singular integral equation for the transition matrix. The integral equation is then solved exactly by analytic methods. The impurity-electron occupation number $\langle n \rangle$ is calculated for general values of parameters, Δ, ϵ_d, and T at zero field. It is found that the local moment exhibits strong temperature dependence at temperatures above the Kondo temperature.

I. INTRODUCTION

The anomalous transport and related properties of dilute magnetic alloys have been investigated intensively in both theoretical and experimental fields since the discovery of the Kondo effect.[1] Much of the theoretical work has been done in the s-d exchange model.[2] However, in the s-d model, a local spin is assumed *a priori* to exist in the electron gas. The strong localized correlations which form the basic mechanism for the phenomena enter only in an indirect manner. In order to study the strong Coulomb interactions present on transition impurities, the extraorbital model of Anderson appears to be more appropriate as the interactions are exhibited explicitly in the Hamiltonian.[3] Moreover, the existence of a moment on the impurity site is not assumed but must emerge in a self-consistent manner from the dynamics of the problem. The same dynamics are also responsible for the resistivity anomalies observed in dilute-alloy systems. Over the years, considerable effort has been expended in studying the correlations in the Anderson model. Self-consistent calculations beyond the Hartree-Fock approximation have been performed by a few authors[4-9] for simplifying values of the parameters, ϵ_d, V, and U of the model. Nevertheless, all of these studies are confined to zero-field calculations.

In the literature, field-dependent calculations can be found mainly in the s-d model and little work has been recorded in the Anderson model. In the s-d model, there have been perturbation calculations by Abrikosov[10] and Béal-Monod and Weiner,[11] and the approximate anomalous Green's-function calculation of Kurata.[12] Their results on the magnetoresistance indicate good agreement with experiments in the limiting situations: $T > T_K$ and $H \ll H_K$. More exact calculations have been done by More and Suhl[13] using S-matrix theory and Bloomfield, Hecht, and Sievert[14] using a Green's-function method. Their results are numerical and show qualitative agreement with experiments. A parallel study based on the single-impurity Wolff model has been performed by Appelbaum and Penn[15] but only zero-field properties have been investigated.

It is our purpose in this study to calculate the properties of the Anderson model in arbitrary magnetic fields by means of the double-time Green's-function method. For simplicity, we consider only the $U \to \infty$ limit. In this limit, the impurity electrons are strongly correlated and the general Anderson's Hamiltonian can be simplified to yield a simple infinite-U model Hamiltonian.[8] Investigations with this Hamiltonian have been made[8,9] in the absence of an external field. The results yield the low-temperature anomalies analogous to those obtained in the context of the s-d model. In this paper, we present the self-consistent treatment of the field-dependent infinite-U Hamiltonian and the evaluation of the temperature variations of the local moments. Other physical properties investigated are given in a subsequent publication.

The outline of the paper is as follows. In Sec. II, the equation-of-motion technique is applied to the model Hamiltonian. An approximation scheme is then introduced to truncate the chain of Green's functions and a self-consistent integral equation for the transition matrix is derived. The equation is solved formally in Sec. III. The impurity-electron occupation number is calculated in Sec. IV for general values of parameters. A brief remark is given in Sec. V.

II. MODEL HAMILTONIAN AND GREEN'S-FUNCTION METHOD

The magnetic-field-dependent infinite-U model Hamiltonian is

$$\mathcal{H} = \sum_{k\sigma} \epsilon_{k\sigma} a_{k\sigma}^\dagger a_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} n_\sigma (1 - n_{\bar\sigma}) + V \sum_{k\sigma} (a_{k\sigma}^\dagger d_\sigma + d_\sigma^\dagger a_{k\sigma})(1 - n_{\bar\sigma}) , \qquad (2.1)$$

where

$$\epsilon_{k\sigma} = \epsilon_k - \tfrac{1}{2}\sigma g_e \mu_B h ,$$
$$\epsilon_{d\sigma} = \epsilon_d - \tfrac{1}{2}\sigma g_i \mu_B h ,$$
$$n_\sigma = d_\sigma^\dagger d_\sigma .$$

In the above, $\sigma = -\bar\sigma = \pm 1$ corresponding to spin up ↑ or down ↓, respectively. The $a_{k\sigma}^\dagger$ and $a_{k\sigma}$ are creation and annihilation operators of electrons in the conduction band with energy ϵ_k and states k and σ. n_σ is the number operator of the localized d-state electrons on the impurity with energy ϵ_d and spin σ. The energies ϵ_k and ϵ_d are measured from the Fermi level. μ_B is the Bohr magneton and h is the magnitude of the external magnetic field. g_e and g_i are the electron- and impurity-spin g factors. V is the admixture matrix element which connects the localized electron state and the conduction-electron state, and is assumed to be a real constant for simplicity. The Coulomb repulsion energy U for antiparallel spin electrons at the impurity is taken to be infinite. The exchange character of the Coulomb interaction has already been built into the Hamiltonian (2.1). Our analysis is based on the equation of motion of the retarded double-time Green's functions defined in terms of operators A and B in the usual way as[16]

$$\langle\langle A/B \rangle\rangle = -i\Theta(t)\langle\{A(t), B(0)\}\rangle , \qquad (2.2)$$

where $\langle\ \rangle$ denotes the statistical average, the curly bracket denotes an anticommutator, and $\Theta(t)$ is a step function. From the analytical property of the Green's function,

$$\langle BA \rangle = i\int_{-\infty}^{\infty} d\omega f(\omega)(\langle\langle A/B\rangle\rangle_{\omega+i\delta} - \langle\langle A/B\rangle\rangle_{\omega-i\delta}) , \qquad (2.3)$$

where $f(\omega) = (e^{\omega/T}+1)^{-1}$ is the Fermi distribution function.

By using the usual method of calculating the single-particle Green's function $G_{kk'}^\sigma$ for the conduction electrons with the mod/l Hamiltonian (2.1), we obtain a chain of equations of motion for the Green's functions:

$$(\omega - \epsilon_{k'\sigma}) G_{kk'}^\sigma(\omega) = \frac{1}{2\pi}\delta_{k'k} + V\Gamma_k^\sigma(\omega) , \qquad (2.4)$$

$$(\omega - \epsilon_{d\sigma})\Gamma_k^\sigma(\omega) = V\sum_p \Lambda_{kp}^\sigma(\omega) + V\sum_p \Xi_{kp}^\sigma(\omega) , \qquad (2.5)$$

$$(\omega - \epsilon_{p\sigma})\Lambda_{kp}^\sigma(\omega) = \frac{1}{2\pi}(1 - \langle n_{\bar\sigma}\rangle)\delta_{pk} + V\Gamma_k^\sigma(\omega) + V\sum_l \langle\langle a_{l\bar\sigma}^\dagger \tilde d_{\bar\sigma} a_{p\sigma} / a_{k\sigma}^\dagger\rangle\rangle - V\sum_l \langle\langle \tilde d_{\bar\sigma}^\dagger a_{l\bar\sigma} a_{p\sigma} / a_{k\sigma}^\dagger\rangle\rangle , \qquad (2.6)$$

$$(\omega - \epsilon_{p\bar\sigma} + \sigma g_i \mu_B h)\Xi_{kp}^\sigma(\omega) = V\sum_l \langle\langle a_{l\bar\sigma}^\dagger a_{p\bar\sigma} \tilde d_\sigma / a_{k\sigma}^\dagger\rangle\rangle - V\sum_l \langle\langle \tilde d_{\bar\sigma}^\dagger a_{p\bar\sigma} a_{l\sigma} / a_{k\sigma}^\dagger\rangle\rangle , \qquad (2.7)$$

where the Green's functions are defined as

$$G_{kk'}^\sigma(\omega) \equiv \langle\langle a_{k'\sigma} / a_{k\sigma}^\dagger\rangle\rangle ,$$
$$\Gamma_k^\sigma(\omega) \equiv \langle\langle \tilde d_\sigma / a_{k\sigma}^\dagger\rangle\rangle ,$$
$$\Xi_{kp}^\sigma(\omega) \equiv \langle\langle d_\sigma a_{p\bar\sigma} d_{\bar\sigma}^\dagger / a_{k\sigma}^\dagger\rangle\rangle ,$$
$$\Lambda_{kp}^\sigma(\omega) \equiv \langle\langle a_{p\sigma} d_{\bar\sigma} d_{\bar\sigma}^\dagger / a_{k\sigma}^\dagger\rangle\rangle ,$$
$$\tilde d_\sigma = d_\sigma(1 - n_{\bar\sigma}) .$$

The higher-order Green's functions appearing on the right-hand side of Eqs. (2.6) and (2.7) are to be decoupled. Approximations are introduced in such a way as to treat correlations on the impurity site as accurately as possible. To achieve this, the truncation is made without splitting two d operators with spin up and down, thus without breaking the correlations on the impurity site. Using this procedure, the higher-order Green's functions are approximated as

$$\langle\langle a_{l\bar\sigma}^\dagger \tilde d_{\bar\sigma} a_{p\sigma} / a_{k\sigma}^\dagger\rangle\rangle \approx \langle a_{l\bar\sigma}^\dagger \tilde d_{\bar\sigma}\rangle G_{kp}^\sigma , \qquad (2.8a)$$

$$\langle\langle \tilde d_{\bar\sigma}^\dagger a_{l\bar\sigma} a_{p\sigma} / a_{k\sigma}^\dagger\rangle\rangle \approx \langle \tilde d_{\bar\sigma}^\dagger a_{l\bar\sigma}\rangle G_{kp}^\sigma , \qquad (2.8b)$$

$$\langle\langle a_{l\bar\sigma}^\dagger a_{p\bar\sigma} \tilde d_\sigma / a_{k\sigma}^\dagger\rangle\rangle \approx \langle a_{l\bar\sigma}^\dagger a_{p\bar\sigma}\rangle \Gamma_k^\sigma , \qquad (2.8c)$$

$$\langle\langle \tilde d_{\bar\sigma}^\dagger a_{p\bar\sigma} a_{l\sigma} / a_{k\sigma}^\dagger\rangle\rangle \approx \langle \tilde d_{\bar\sigma}^\dagger a_{p\bar\sigma}\rangle G_{kl}^\sigma . \qquad (2.8d)$$

We note that the decoupling at this stage just corresponds to the Nagaoka decoupling scheme[17] in the s-d model since V^2 is proportional to J, the s-d exchange integral. An approximation of this kind has been employed by Theumann[4] and by Appelbaum and Penn.[15]

We also apply the Hermiticity condition for the averages

$$\langle a_{n\sigma}^\dagger a_{k\sigma}\rangle = \langle a_{k\sigma}^\dagger a_{n\sigma}\rangle ,$$
$$\langle a_{l\sigma}^\dagger \tilde d_\sigma\rangle = \langle \tilde d_\sigma^\dagger a_{l\sigma}\rangle , \qquad (2.9)$$

and note that now $\langle n_\sigma\rangle \ne \langle n_{\bar\sigma}\rangle$ and $\langle d_\sigma^\dagger a_{l\sigma}\rangle \ne \langle d_{\bar\sigma}^\dagger a_{l\bar\sigma}\rangle$ because of the presence of the external magnetic field.

Carrying out the above truncation procedure and using condition (2.9), we derive the single-particle Green's function for the conduction electrons, giving

$$G_{kk'}^\sigma(\omega) = \frac{1}{2\pi}\left(\frac{\delta_{k'k}}{\omega - \epsilon_{k'\sigma}} + \frac{V^2 t^\sigma(\omega)}{(\omega - \epsilon_{k'\sigma})(\omega - \epsilon_{k\sigma})}\right) , \qquad (2.10)$$

where the transition matrix $t(\omega)$ is given by

$$t^\sigma(\omega) = \frac{1 - \langle n_{\bar\sigma}\rangle - F^\sigma(\omega)}{\omega - \epsilon_{d\sigma} - \Lambda^\sigma(\omega) - K^\sigma(\omega) + \Lambda^\sigma(\omega)F^\sigma(\omega)} , \qquad (2.11)$$

and

$$\Gamma_k^\sigma(\omega)=\frac{1}{2\pi}\frac{V}{\omega-\epsilon_{k\sigma}}\,t^\sigma(\omega)\,, \tag{2.12}$$

$$\langle\langle \tilde{d}_\sigma/d_\sigma^\dagger\rangle\rangle_\omega=\frac{1}{2\pi}\,t^\sigma(\omega)\,, \tag{2.13}$$

$$\Lambda^\sigma(\omega)=\sum_p\frac{V^2}{\omega-\epsilon_{p\sigma}}\,, \tag{2.14}$$

$$K^\sigma(\omega)=\sum_{lp}\frac{V^2\langle a_{l\bar\sigma}^\dagger a_{p\bar\sigma}\rangle}{\omega-\epsilon_{p\bar\sigma}+\sigma g_i\mu_B h}\,, \tag{2.15}$$

$$F^\sigma(\omega)=\sum_p\frac{V\langle \tilde{d}_{\bar\sigma}^\dagger a_{p\bar\sigma}\rangle}{\omega-\epsilon_{p\bar\sigma}+\sigma g_i\mu_B h}\,. \tag{2.16}$$

In the above, the Green's function $\langle\langle \tilde{d}_\sigma/d_\sigma^\dagger\rangle\rangle_\omega$ has been derived in the same approximation. This function plays the role of the transition matrix for the scattering of conduction electrons off the impurity site. We note in passing that results identical to (2.10)–(2.16) can be obtained if one approaches the problem using the general Anderson's Hamiltonian and letting $U\to\infty$ in the subsequent equation for the transition matrix. At zero field, Eq. (2.11) reduces to the t matrix obtained by Brereton and Poo.[8]

Next, we introduce the following identity[16]:

$$\langle\{A,B\}\rangle=i\int_{-\infty}^{\infty}d\omega(\langle\langle A/B\rangle\rangle_{\omega+i\delta}-\langle\langle A/B\rangle\rangle_{\omega-i\delta})\,, \tag{2.17}$$

and the functional notation

$$\mathcal{P}_\omega\{\langle\langle A/B\rangle\rangle_\omega\}=i\int d\omega[f(\omega)-\tfrac{1}{2}]\times(\langle\langle A/B\rangle\rangle_{\omega+i\delta}-\langle\langle A/B\rangle\rangle_{\omega-i\delta})\,. \tag{2.18}$$

In (2.18), the form $[f(\omega)-\frac{1}{2}]$ is used because it possesses a definite symmetry, that is odd in ω.

Making use of Eqs. (2.17), (2.18), and (2.3), one can express the impurity-electron occupation number $\langle n_\sigma\rangle$ and the correlation functions F^σ and K^σ in terms of $t(\omega)$ as follows:

$$\langle n_\sigma\rangle=\tfrac{1}{2}(1-\langle n_{\bar\sigma}\rangle)+\frac{1}{2\pi}\mathcal{P}_\xi\{t^\sigma(\xi)\}\,, \tag{2.19}$$

$$F^\sigma(\omega)=\frac{1}{2\pi}\mathcal{P}_\xi\left(\frac{\Lambda^{\bar\sigma}(\xi)-\Lambda^{\bar\sigma}(\omega+\sigma g_i\mu_B h)}{\omega-\xi+\sigma g_i\mu_B h}\,t^{\bar\sigma}(\xi)\right)\,, \tag{2.20}$$

$$K^\sigma(\omega)=\frac{1}{2\pi}\mathcal{P}_\xi\left(\frac{\Lambda^{\bar\sigma}(\xi)-\Lambda^{\bar\sigma}(\omega+\sigma g_i\mu_B h)}{\omega-\xi+\sigma g_i\mu_B h}[1+\Lambda^{\bar\sigma}(\xi)t^{\bar\sigma}(\xi)]\right)+\tfrac{1}{2}\Lambda^{\bar\sigma}(\omega+\sigma g_i\mu_B h)\,. \tag{2.21}$$

The expressions for F^σ and K^σ appear quite complex. To simplify them, we specialize to the case of equal g factors, that is $g_e=g_i=g$. In this case,

$$\Lambda^{\bar\sigma}(\omega+2\sigma H)=\Lambda^\sigma(\omega) \tag{2.22}$$

and

$$\Lambda^{\bar\sigma}(\omega+\sigma H)=\Lambda(\omega)=\sum_p\frac{V^2}{\omega-\epsilon_p}\,, \tag{2.23}$$

where

$$H=\tfrac{1}{2}g\mu_B h\,. \tag{2.24}$$

Substituting Eqs. (2.20)–(2.24) into (2.11) and making a change of variable from ω to $\omega-\sigma H$, we obtain the following integral equation for t-matrix:

$$t^\sigma(\omega-\sigma H)=\frac{1-\langle n_{\bar\sigma}\rangle-\frac{1}{2\pi}\mathcal{P}_{\xi+\sigma H}\left\{\frac{\Lambda(\xi)-\Lambda(\omega)}{\omega-\xi}\,t^{\bar\sigma}(\xi+\sigma H)\right\}}{\omega-\epsilon_d-\frac{3}{2}\Lambda(\omega)-\frac{1}{2\pi}\mathcal{P}_{\xi+\sigma H}\left\{\frac{\Lambda(\xi)-\Lambda(\omega)}{\omega-\xi}\right\}-\frac{1}{2\pi}\mathcal{P}_{\xi+\sigma H}\left\{\frac{[\Lambda(\xi)-\Lambda(\omega)]^2}{\omega-\xi}\,t^{\bar\sigma}(\xi+\sigma H)\right\}}\,. \tag{2.25}$$

To proceed with the calculation, one has to evaluate the function $\Lambda(\omega)$ which depends on the density of states of the host. One can choose either a constant square band or a Lorentzian-type density of states. In either case, a cutoff parameter has to be introduced. This requires particular care when the magnetic field is present. If the resulting cutoff is field dependent, it will lead to spurious contributions to physical quantities from the band edge.[18] We have avoided this complication by making a change of variable from ω to $\omega-\sigma H$ in (2.25). As a result, the explicit field dependence of $\Lambda^\sigma(\omega)$ is removed. We can now introduce the cutoff to the function $\Lambda(\omega)$ which is no longer field dependent.

III. SOLUTION OF INTEGRAL EQUATIONS

For simplicity, we assume a constant density of states and approximate $\Lambda(\omega)$ by

$$\Lambda(\omega\pm i\delta)=\mp i\Delta \quad \text{for } |\omega|<D\,,$$
$$=0 \quad \text{otherwise}, \tag{3.1}$$

where Δ is the width of the localized d level, given by

$$\Delta=\pi\rho_0 V^2\,, \tag{3.2}$$

ρ_0 being the constant density of states assumed and D the half bandwidth of the conduction band. In this case, the equation of $t(\omega)$ (2.25) can be simplified to give

$$t^{\sigma}(\omega-\sigma H+i\delta)=\frac{1-\langle n_{\bar\sigma}\rangle-\dfrac{\Delta}{\pi}\displaystyle\int_{-D}^{D}d\xi\,\frac{f(\xi+\sigma H)-\frac12}{\omega-\xi+i\delta}\,t^{\bar\sigma}(\xi+\sigma H-i\delta)}{\omega-\epsilon_d+i\frac32\Delta-\dfrac{\Delta}{\pi}\displaystyle\int_{-D}^{D}d\xi\,\frac{f(\xi+\sigma H)-\frac12}{\omega-\xi+i\delta}-i\,\frac{2\Delta^2}{\pi}\int_{-D}^{D}d\xi\,\frac{f(\xi+\sigma H)-\frac12}{\omega-\xi+i\delta}\,t^{\bar\sigma}(\xi+\sigma H-i\delta)}\ . \tag{3.3}$$

This equation is similar to Eq. (3.3) obtained by Appelbaum and Penn[15] if one makes the correspondence $\Delta\to d$ and $\epsilon_d\to V$. Inspection of this equation reveals that essentially there are four sets of integral equations for $t^{\dagger}(\omega-H\pm i\delta)$ and $t^{\downarrow}(\omega+H\pm i\delta)$, where $t^{\sigma}(\omega-\sigma H-i\delta)=[t^{\sigma}(\omega-\sigma H+i\delta)]^*$. Nevertheless, these equations separate such that $t^{\dagger}(\omega-H+i\delta)$ couples with only $t^{\downarrow}(\omega+H-i\delta)$ and $t^{\dagger}(\omega-H-i\delta)$ with $t^{\downarrow}(\omega+H+i\delta)$.

To solve (3.3), we define the following auxiliary functions related to the t matrix

$$\psi^{\sigma}(\omega-\sigma H\pm i\delta)=1\mp i\,2\Delta t^{\sigma}(\omega-\sigma H\pm i\delta)\ . \tag{3.4}$$

Then, in terms of ψ^{σ}, two simultaneous equations are derived as

$$\psi^{\dagger}(\omega-H+i\delta)=\frac{d^{\downarrow}-ie(\omega)+X_1(\omega+i\delta)}{1-ie(\omega)+\phi_1(\omega+i\delta)}\ , \tag{3.5}$$

$$\psi^{\downarrow}(\omega+H-i\delta)=\frac{d^{\dagger}+ie(\omega)+X_2(\omega-i\delta)}{1+ie(\omega)+\phi_2(\omega-i\delta)}\ , \tag{3.6}$$

where

$$X_1(z)=\frac{2i}{3\pi}\int_{-D}^{D}d\xi\,\frac{f(\xi+H)-\frac12}{z-\xi}\ , \tag{3.7}$$

$$X_2(z)=-\frac{2i}{3\pi}\int_{-D}^{D}d\xi\,\frac{f(\xi-H)-\frac12}{z-\xi}\ , \tag{3.8}$$

$$\phi_1(z)=\frac{2i}{3\pi}\int_{-D}^{D}d\xi\,\frac{f(\xi+H)-\frac12}{z-\xi}\,\psi^{\downarrow}(\xi+H-i\delta)\ , \tag{3.9}$$

$$\phi_2(z)=-\frac{2i}{3\pi}\int_{-D}^{D}d\xi\,\frac{f(\xi-H)-\frac12}{z-\xi}\,\psi^{\dagger}(\xi-H+i\delta), \tag{3.10}$$

$$e(\omega)=(2/3\Delta)(\omega-\epsilon_d)\ , \tag{3.11}$$

$$d^{\sigma}=\tfrac13(4\langle n_\sigma\rangle-1)\ . \tag{3.12}$$

The functions $X_1(z)$, $X_2(z)$, $\phi_1(z)$, and $\phi_2(z)$ are "sectionally holomorphic," that is, they are analytic on the upper and lower half-plane, but they have a cut on the real axis for $-D<\omega<D$. The notations $+i\delta$ and $-i\delta$ are used to indicate the values of these functions on the real axis, depending on whether this cut is approached from above or below. By inspecting the discontinuity of these functions across the real axis, one gets, for $|\omega\pm H|<D$,

$$X_1(\omega+i\delta)-X_1(\omega-i\delta)=\tfrac43[f(\omega+H)-\tfrac12]\ , \tag{3.13}$$

$$X_2(\omega+i\delta)-X_2(\omega-i\delta)=-\tfrac43[f(\omega-H)-\tfrac12], \tag{3.14}$$

$$\phi_1(\omega+i\delta)-\phi_1(\omega-i\delta)=[X_1(\omega+i\delta)-X_1(\omega-i\delta)]\times\psi^{\downarrow}(\omega+H-i\delta)\ , \tag{3.15}$$

$$\phi_2(\omega+i\delta)-\phi_2(\omega-i\delta)=[X_2(\omega+i\delta)-X_2(\omega-i\delta)]\times\psi^{\dagger}(\omega-H+i\delta)\ . \tag{3.16}$$

Substituting Eqs. (3.15) and (3.16) into (3.5) and (3.6), one gets,

$$\frac{\phi_1(\omega+i\delta)-\phi_1(\omega-i\delta)}{X_1(\omega+i\delta)-X_1(\omega-i\delta)}=\frac{d^{\dagger}+ie(\omega)+X_2(\omega-i\delta)}{1+ie(\omega)+\phi_2(\omega-i\delta)}\ , \tag{3.17}$$

$$\frac{\phi_2(\omega+i\delta)-\phi_2(\omega-i\delta)}{X_2(\omega+i\delta)-X_2(\omega-i\delta)}=\frac{d^{\downarrow}-ie(\omega)+X_1(\omega+i\delta)}{1-ie(\omega)+\phi_1(\omega+i\delta)}\ . \tag{3.18}$$

Combining (3.17) and (3.18), we can show that the function $\Omega(z)$ defined as

$$\Omega(z)\equiv\phi_1(z)\phi_2(z)-X_1(z)X_2(z)+[1+ie(z)]\phi_1(z)+[1-ie(z)]\phi_2(z)-[d^{\dagger}+ie(z)]X_1(z)-[d^{\downarrow}-ie(z)]X_2(z) \tag{3.19}$$

is continuous across the cut $(-D, D)$ and hence is analytic on the whole z plane. Examination of the asymptotic form of this function shows that (3.19) is a constant, denoted as C, giving

$$\Omega(z)=C \tag{3.20}$$

where

$$C=\lim_{z\to\infty}\frac{2iz}{3\Delta}[\phi_1(z)-\phi_2(z)-X_1(z)+X_2(z)]=\frac{8i}{9\pi}\left(\int_{-D}^{D}d\xi\,[f(\xi-H)-\tfrac12]t^{\dagger}(\xi-H+i\delta)-\int_{-D}^{D}d\xi\,[f(\xi+H)-\tfrac12]t^{\downarrow}(\xi+H-i\delta)\right)\ . \tag{3.21}$$

Solving for $\phi_1(z)$ using (3.17)–(3.21), we get

$$\frac{\phi_{1+}+1-ie}{\phi_{1-}+1-ie}=\frac{1+e^2+C+(d^{\dagger}+ie)X_{1+}+(d^{\downarrow}-ie)X_{2-}+X_{1+}X_{2-}}{1+e^2+C+(d^{\dagger}+ie)X_{1-}+(d^{\downarrow}-ie)X_{2-}+X_{1-}X_{2-}}\equiv H_1(\omega) \tag{3.22}$$

where $\phi_{1\pm}\equiv\phi_1(\omega\pm i\delta)$, $X_{1\pm}\equiv X_1(\omega\pm i\delta)$, and $e\equiv e(\omega)$. The function $H_1(\omega)$ is a complex function of real variable ω. It can be shown easily that when $\omega\to\pm D$, $\ln H_1(\pm D)=0$ and the phase of $H_1(\omega)$ is always between $\pm\frac12\pi$. Therefore, the fundamental solution of $\phi_1(z)$ is given by[19]

$$\phi_1(z)+1-ie(z)=[1-ie(z)+\eta_1]\,e^{-Q_1(z)} \tag{3.23}$$

$$Q_1(z)=(2\pi i)^{-1}\int_{-D}^{D}\frac{\ln H_1(\xi)}{z-\xi}\,d\xi\ . \tag{3.24}$$

The constant η_1 is determined by expanding both sides of (3.23) in a Taylor-Laurent series, giving

$$\eta_1 = -(3\pi\Delta)^{-1}\int_{-D}^{D} \ln H_1(\xi)\, d\xi \ . \qquad (3.25)$$

Likewise, using (3.17)–(3.21), one can solve for $\phi_2(z)$ to give

$$\frac{\phi_{2+}+1+ie}{\phi_{2-}+1+ie} = \frac{1+e^2+C+(d^{\dagger}+ie)X_{1+}+(d^{\dagger}-ie)X_{2+}+X_{1+}X_{2+}}{1+e^2+C+(d^{\dagger}+ie)X_{1+}+(d^{\dagger}-ie)X_{2-}+X_{1+}X_{2-}} \equiv H_2(\omega) \ . \qquad (3.26)$$

The solution to (3.26) is

$$\phi_2(z)+1+ie(z) = [1+ie(z)+\eta_2]\, e^{-Q_2(z)} \qquad (3.27)$$

with

$$Q_2(z) = (2\pi i)^{-1}\int_{-D}^{D} \frac{\ln H_2(\xi)}{z-\xi}\, d\xi \qquad (3.28)$$

and

$$\eta_2 = (3\pi\Delta)^{-1}\int_{-D}^{D} \ln H_2(\xi)\, d\xi \ . \qquad (3.29)$$

In order to determine C and $\langle n_{\uparrow,\downarrow}\rangle$ self-consistently, we examine the asymptotic form of the functions ϕ_1, ϕ_2, X_1, and X_2. Carrying out the asymptotic expansion of (3.23) and (3.27) in Taylor-Laurent series and equating equal powers of z, we find

$$\lim_{z\to\infty} \frac{z}{\Delta}\, \phi_1(z) = \frac{M_1}{3\pi} + \frac{iM_0}{2\pi} - \frac{\epsilon_d M_0}{3\pi\Delta} - \frac{iM_0^2}{12\pi^2}\, , \qquad (3.30)$$

$$\lim_{z\to\infty} \frac{z}{\Delta}\, \phi_2(z) = -\frac{N_1}{3\pi} + \frac{iN_0}{2\pi} + \frac{\epsilon_d N_0}{3\pi\Delta} + \frac{iN_0^2}{12\pi^2}\, , \qquad (3.31)$$

where

$$M_r = \Delta^{-r-1}\int_{-D}^{D} \xi^r \ln H_1(\xi)\, d\xi \ , \qquad (3.32)$$

$$N_r = \Delta^{-r-1}\int_{-D}^{D} \xi^r \ln H_2(\xi)\, d\xi \ . \qquad (3.33)$$

It can be shown easily that

$$\lim_{z\to\infty} z[X_1(z) - X_2(z)] = \frac{2i}{3\pi}\int_{-D}^{D} d\xi\, [f(\xi+H) + f(\xi-H) - 1] = 0 \ . \qquad (3.34)$$

This is an exact result. Substituting (3.30)–(3.34) into (3.21), we obtain an implicit transcendental equation for C and $\langle n_{\uparrow,\downarrow}\rangle$, giving

$$C = \frac{2i}{9\pi}(M_1+N_1) - \frac{1}{3\pi}(M_0-N_0) - \frac{2i\epsilon_d}{9\pi\Delta}(M_0+N_0) + \frac{1}{18\pi^2}(M_0^2+N_0^2) \ . \qquad (3.35)$$

We need two more such equations in order to determine the three unknowns C and $\langle n_{\uparrow,\downarrow}\rangle$. These can be obtained from the equation for $\langle n_\sigma\rangle$, (2.19). For $\sigma=\uparrow$, (2.19) can be written as

$$\langle n_\uparrow\rangle = \tfrac{1}{2}(1-\langle n_\downarrow\rangle) - \pi^{-1}\int_{-D}^{D} d\xi\, [f(\xi)-\tfrac{1}{2}]\, \mathrm{Im}\, t^{\uparrow}(\xi+i\delta) \ . \qquad (3.36)$$

By a change of variables from ξ to $\xi - H$, (3.36) becomes

$$\langle n_\uparrow\rangle = \tfrac{1}{2}(1-\langle n_\downarrow\rangle) - \pi^{-1}\int_{-D}^{D} d\xi\, [f(\xi-H)-\tfrac{1}{2}] \times \mathrm{Im}\, t^{\uparrow}(\xi-H+i\delta) - \tfrac{1}{2}H\, \mathrm{Im}\, t^{\uparrow}(-D+i\delta) - \tfrac{1}{2}H\, \mathrm{Im}\, t^{\uparrow}(D+i\delta) \quad (D\gg H) \ . \qquad (3.37)$$

Similar equation can be obtained for $\sigma=\downarrow$, giving

$$\langle n_\downarrow\rangle = \tfrac{1}{2}(1-\langle n_\uparrow\rangle) + \pi^{-1}\int_{-D}^{D} d\xi\, [f(\xi+H)-\tfrac{1}{2}] \times \mathrm{Im}\, t^{\downarrow}(\xi+H-i\delta) + \tfrac{1}{2}H\, \mathrm{Im}\, t^{\downarrow}(-D-i\delta) + \tfrac{1}{2}H\, \mathrm{Im}\, t^{\downarrow}(D-i\delta) \quad (D\gg H) \ . \qquad (3.38)$$

The functions $\mathrm{Im}\, t^\sigma(\pm D \pm i\delta)$ describe the density of states of the impurity level at the host band edge. By physical considerations, that region cannot be of any importance as the density of states should go to zero there. Hence, for $D/\Delta \gg 1$, these functions can be neglected without affecting the physical results of $\langle n_\uparrow\rangle$ and $\langle n_\downarrow\rangle$.[18] Carrying out the asymptotic expansion of (3.9) and (3.10), and combining these results with Eqs. (3.4), (3.30), (3.31), (3.37), and (3.38), we derive the following equations for $\langle n_\uparrow\rangle$ and $\langle n_\downarrow\rangle$:

$$\langle n_\uparrow\rangle = \tfrac{1}{2}(1-\langle n_\downarrow\rangle) + \frac{H}{2\pi\Delta} - \frac{\mathrm{Im} N_1}{4\pi} + \frac{3\,\mathrm{Re} N_0}{8\pi} + \frac{\epsilon_d\, \mathrm{Im} N_0}{4\pi\Delta} + \frac{1}{16\pi^2}[(\mathrm{Re} N_0)^2 - (\mathrm{Im} N_0)^2] \ , \qquad (3.39)$$

$$\langle n_\downarrow\rangle = \tfrac{1}{2}(1-\langle n_\uparrow\rangle) - \frac{H}{2\pi\Delta} - \frac{\mathrm{Im}\, M_1}{4\pi} - \frac{3\,\mathrm{Re} M_0}{8\pi} + \frac{\epsilon_d\, \mathrm{Im} M_0}{4\pi\Delta} + \frac{1}{16\pi^2}[(\mathrm{Re} M_0)^2 - (\mathrm{Im} M_0)^2] \ . \qquad (3.40)$$

Also, a simple auxiliary result can be deduced from Eqs. (3.21) and (3.36) to give

$$\mathrm{Re}\, C = \tfrac{4}{3}(\langle n_\uparrow\rangle + \langle n_\downarrow\rangle - \tfrac{2}{3}) \ . \qquad (3.41)$$

Equations (3.35), (3.39), and (3.40) form three independent transcendental equations from which $\langle n_\uparrow\rangle$, $\langle n_\downarrow\rangle$, and C can be determined. The formal solution to the integral Eq. (3.3) is thus completed.

The solutions for ψ^σ give

$$\psi^{\uparrow}(\omega - H + i\delta) = \frac{d^{\dagger} - ie(\omega) + X_1(\omega+i\delta)}{1 - ie(\omega) - M_0/3\pi}\, e^{Q_1(\omega+i\delta)}\, , \qquad (3.42)$$

$$\psi^{\downarrow}(\omega + H - i\delta) = \frac{d^{\dagger} + ie(\omega) + X_2(\omega-i\delta)}{1 + ie(\omega) + N_0/3\pi}\, e^{Q_2(\omega-i\delta)} \ . \qquad (3.43)$$

However, it is instructive to express the solutions in a somewhat different form. From Eqs. (3.17) and (3.20), we get

$$(\phi_{1+}+1-ie)(\phi_{2-}+1+ie)=1+e^2+C+(d'+ie)X_{1+}+(d'-ie)X_{2-}+X_{1+}X_{2-}\equiv H_1^D(\omega)\ . \quad (3.44)$$

Substituting (3.23) and (3.27) into (3.44) and taking the square root on both sides, we obtain the condition

$$(1-ie-M_0/3\pi)^{1/2}(1+ie+N_0/3\pi)^{1/2}[H_1^D(\omega)]^{-1/2}\times e^{-(Q_{1+}+Q_{2-})/2}=1\ . \quad (3.45)$$

Combining Eqs. (3.24), (3.28), and (3.45), we can express the solutions of ψ^σ as

$$\psi^{\dagger}(\omega-H+i\delta)=\left(\frac{1+ie+N_0/3\pi}{1-ie-M_0/3\pi}\right)^{1/2}\frac{B_1(\omega)-iA_1(\omega)}{[H_1^D(\omega)]^{1/2}}\times\left(\frac{H_1^{-1}(\omega)}{H_2(\omega)}\right)^{1/4}e^{Q_3(\omega)}\ , \quad (3.46)$$

$$\psi^{\dagger}(\omega+H-i\delta)=\left(\frac{1-ie-M_0/3\pi}{1+ie+N_0/3\pi}\right)^{1/2}\frac{B_2(\omega)+iA_2(\omega)}{[H_1^D(\omega)]^{1/2}}\times\left(\frac{H_1^{-1}(\omega)}{H_2(\omega)}\right)^{-1/4}e^{-Q_3(\omega)}\ , \quad (3.47)$$

where the functions $X_{1\pm}$ and $X_{2\pm}$ have been evaluated in terms of digamma function Ψ and

$$Q_3(\omega)=\frac{i}{4\pi}P\int_{-D}^{D}d\xi\ \frac{\ln[H_1^{-1}H_2(\xi)]}{\omega-\xi}\ , \quad (3.48)$$

$$B_1(\omega)=d'-\tfrac{1}{3}\tanh\frac{\omega+H}{2T}\ , \quad (3.49)$$

$$B_2(\omega)=d'-\tfrac{1}{3}\tanh\frac{\omega-H}{2T}\ , \quad (3.50)$$

$$A_1(\omega)=\frac{2}{3\pi}\left[\frac{\pi\omega}{\Delta}-\frac{\pi\epsilon_d}{\Delta}+\mathrm{Re}\Psi\left(\frac{1}{2}-\frac{i(\omega+H)}{2\pi T}\right)-\frac{1}{2}\ln\left|\frac{D^2-\omega^2}{(2\pi T)^2}\right|\right]\ , \quad (3.51)$$

$$A_2(\omega)=\frac{2}{3\pi}\left[\frac{\pi\omega}{\Delta}-\frac{\pi\epsilon_d}{\Delta}+\mathrm{Re}\Psi\left(\frac{1}{2}+\frac{i(\omega-H)}{2\pi T}\right)-\frac{1}{2}\ln\left|\frac{D^2-\omega^2}{(2\pi T)^2}\right|\right]\ . \quad (3.52)$$

It is desirable to define self-consistently two characteristic quantities of our system: the Kondo temperature T_K and the corresponding magnetic field H_K. T_K is defined as the temperature when $H\to 0$ and $A_1(0)=0$, whereas H_K is given as the field when $T\to 0$ and $A_1(0)=0$. This gives

$$H_K/D=\pi T_K/2\alpha D=e^{\pi\epsilon_d/\Delta} \quad (3.53)$$

where $\ln\alpha$ is the Euler's constant. For reasons of physical interest, ϵ_d should lie below the Fermi level, that is, $-D<\epsilon_d<0$. Moreover, T_K/D and hence H_K/D should be small, then $|\epsilon_d|/\Delta\gg 1$. Equations (3.51) and (3.52) can then be expressed in terms of T_K, giving

$$A_1(\omega)=\frac{2}{3\pi}\left[\frac{\pi\omega}{\Delta}+\ln\left(\frac{T}{T_K}\frac{D}{(D^2-\omega^2)^{1/2}}\right)+\phi\left(\frac{\omega+H}{2\pi T}\right)\right]\ , \quad (3.54)$$

$$A_2(\omega)=\frac{2}{3\pi}\left[\frac{\pi\omega}{\Delta}+\ln\left(\frac{T}{T_K}\frac{D}{(D^2-\omega^2)^{1/2}}\right)+\phi\left(\frac{\omega-H}{2\pi T}\right)\right]\ , \quad (3.55)$$

where

$$\phi(y)=\mathrm{Re}[\Psi(\tfrac{1}{2}\mp iy)-\Psi(\tfrac{1}{2})]\ . \quad (3.56)$$

IV. LOCAL MOMENT

In this section, the impurity-electron occupation number $\langle n\rangle$ is calculated for the special case $H=0$. In this case, $\mathrm{Re}N_r=-\mathrm{Re}M_r$, $\mathrm{Im}N_r=\mathrm{Im}M_r$ and $\mathrm{Im}C=0$, Eqs. (3.39) and (3.40) become identical, yielding

$$\langle n\rangle=\frac{1}{3}-\frac{\mathrm{Im}M_1}{6\pi}-\frac{\mathrm{Re}M_0}{4\pi}+\frac{\epsilon_d\,\mathrm{Im}M_0}{6\pi\Delta}+\frac{1}{24\pi^2}[(\mathrm{Re}M_0)^2-(\mathrm{Im}M_0)^2]\ . \quad (4.1)$$

The moments M_r and related functions can be simplified to give

$$M_r=-\Delta^{-r-1}\int_{-D}^{D}\omega^r\ln H(\omega)\,d\omega\ , \quad (4.2)$$

$$H(\omega)=\frac{1+C+(e+iX_-)^2}{1+e^2+C+(d+ie)X_+-(d-ie)X_--X_+X_-}\ , \quad (4.3)$$

$$X_\pm=-\frac{i}{3\pi}\ln\left|\frac{\pi^2T^2+\omega^2}{D^2-\omega^2}\right|\mp\tfrac{1}{3}\tanh\frac{\omega}{2T}\ , \quad (4.4)$$

$$d=\tfrac{1}{3}(\langle n\rangle-1)\ , \quad (4.5)$$

$$C=\mathrm{Re}C=\tfrac{8}{9}(3\langle n\rangle-1)\ . \quad (4.6)$$

Equation (4.1) forms a self-consistent equation for $\langle n\rangle$ since the moments M_0 and M_1 depend on $\langle n\rangle$ via the dependence of $H(\omega)$ on $\langle n\rangle$. The equation was solved numerically using a standard fixed-point iteration method and the moments evaluated by Romberg integration techniques.[20] The interval $(-D, D)$ is divided into many subintervals so that each subinterval can be integrated to the desired accuracy. The final result of $\langle n\rangle$ is ensured to attain the absolute accuracy of 10^{-4}.

In this calculation, we aim to detect firstly the variation of $\langle n\rangle$ with the parameter $\Delta/|\epsilon_d|$ for a fixed temperature and secondly the temperature variation of $\langle n\rangle$ for a fixed ratio $\Delta/|\epsilon_d|$ which can be expressed in terms of T_K via Eq. (3.53). For the ratio $\Delta/|\epsilon_d|$, we fix ϵ_d and vary Δ since physically, ϵ_d is determined once a particular alloy is selected.

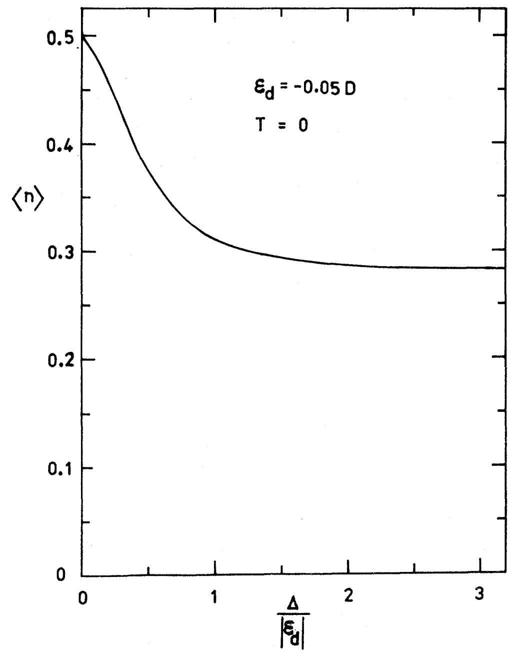

FIG. 1. Variation of $\langle n\rangle$ as a function of $\Delta/|\epsilon_d|$ for $\epsilon_d=-0.05D$ and $T=0$, in a linear plot.

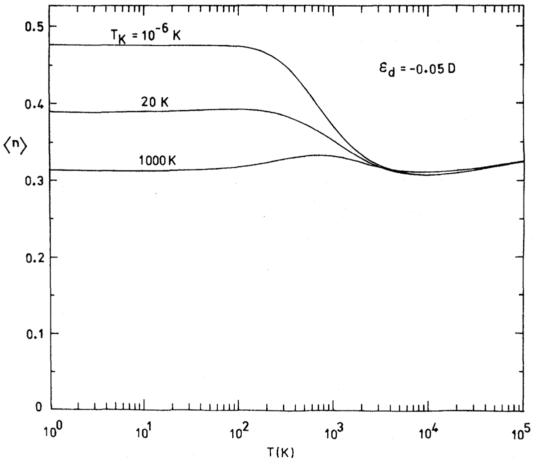

FIG. 3. Variation of $\langle n\rangle$ as a function of temperature for $\epsilon_d=-0.05D$ and three values of T_K.

We choose $D=2\times 10^4$ K and $\epsilon_d=-0.05D$ in our computation. The variation of $\langle n\rangle$ with $\Delta/|\epsilon_d|$ at $T=0$ is shown in Fig. 1 in a linear plot. The curve of $\langle n\rangle$ exhibits a fast initial drop and then levels off gradually when $\Delta/|\epsilon_d|$ becomes large. To amplify the rapid varying portion, the same curve is plotted in a semilogarithmic scale in Fig. 2. It can be seen clearly that in the region (0.1, 1) of $\Delta/|\epsilon_d|$, $\langle n\rangle$ changes by about 40% of its initial value. When $\Delta\to 0$, the value of n tends to $\frac{1}{2}$. This value is expected when the impurity state becomes completely localized, free of s-d interaction and thermal fluctuation. In Fig. 2, we also exhibit curves for two finite temperatures, one at $T=600$ K and the other at $T=1000$ K. The value of $\langle n\rangle$ reduces appreciably at low $\Delta/|\epsilon_d|$. As a result, the variation becomes rather gentle at high temperatures.

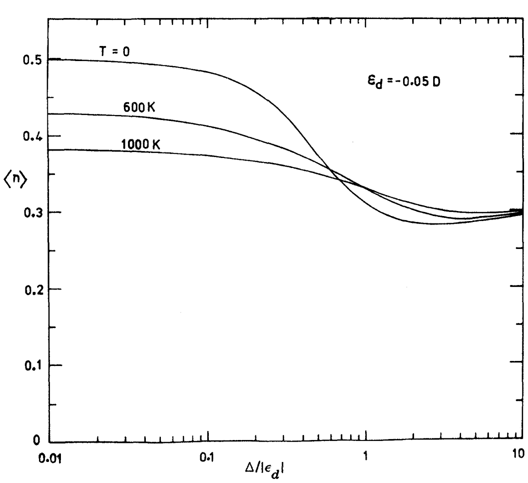

FIG. 2. Variation of $\langle n\rangle$ as a function of $\Delta/|\epsilon_d|$ for $\epsilon_d=-0.05D$ and three values of temperatures, in a semilogarithmic plot.

The temperature variation of $\langle n\rangle$ is shown in Fig. 3 for several values of the Kondo temperature. For low T_K, $\langle n\rangle$ shows no significant temperature dependence below and around T_K. This feature confirms the result of the previous calculation.[8] However, strong temperature dependence is observed at $T>T_K$ for $T_K<\epsilon_d$ and the variation is rather rapid. The value of $\langle n\rangle$ decreases sharply in a logarithmic manner, before receding to a sinusoidal tail. With increasing T_K, the variation becomes gentler and eventually at high T_K, it reduces to small oscillations at high temperatures.

The region where $\langle n\rangle$ exhibits strong temperature variations depends sensitively on the choice of ϵ_d, the position of the impurity level. We have attempted the computation for various values of ϵ_d. The results indicate that when ϵ_d is shifted nearer to the bottom of the band, the region will move to higher temperature. On the other hand, when ϵ_d is shifted towards the Fermi level, then, the region will correspondingly appear at lower temperature which may lie below or around T_K provided T_K is not too low.

The temperature dependence of the local moment is obviously related to the thermal depopulation of the extra orbital. It will inevitably affect the impurity susceptibility, electrical resistivity, and other related properties.[21] Nevertheless, for systems having low Kondo temperatures, it is quite safe to conclude that the value of $\langle n\rangle$ will not be affected by thermal fluctuations at temperatures below and around T_K.

V. REMARKS

We have, in Sec. III, solved analytically the integral equation for the t matrix. The solution gives rise to three nonlinear transcendental integral equations for three variables $\langle n_\uparrow \rangle$, $\langle n_\downarrow \rangle$, and Im$C$. One has to solve these equations in order to calculate physical quantities in a self-consistent manner. Straightforward computation is very difficult as we have as many as five parameters to vary. In a subsequent paper, we have simplified the problem by introducing an auxiliary condition which connects the variables $\langle n_\uparrow \rangle$ and $\langle n_\downarrow \rangle$ to $\langle n \rangle$, the zero-field occupation number. In this way, we are able to reduce the three integral equations to two, thus greatly simplifying the numerical computation. The calculation of $\langle n \rangle$ in Sec. IV is therefore essential. It serves to pave the way for the eventual evaluations of physical quantities such as the impurity magnetization, the magnetoresistivity, and the Hall coefficient.

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[21]The zero-field impurity susceptibility and electrical resistivity are related to $\langle n \rangle$ as (see Ref. 8) $\chi_{dd} = A\langle n \rangle / T$ and $\Delta\rho = B[\tau(\epsilon_F, \langle n \rangle)]^{-1}$.