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Magnetic susceptibility in the Anderson model

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An expression for the partition function for the Anderson model obtained via the functional-integral technique is used to calculate the magnetic susceptibility. The result indicates the appearance of a characteristic temperature in the strong-coupling regime, and is free of divergences at low temperatures.

The functional-integral method has been extensively[1,2] applied to the study of magnetic susceptibility of the Anderson model for very dilute magnetic alloys. In this paper we would like to report the result of a calculation using a new[3] approximation wherein we overcome divergence difficulties present in previous works. In particular we obtain the following results: (1) The zero-external-magnetic-field susceptibility simulates that of an antiferromagnet in the strong-coupling regime and of a simple paramagnet in the weak-coupling regime; (2) the magnetic susceptibility is expressed as an infinite series which converges rapidly in the high-β^{-1} temperature region and is weakly convergent in the very-low temperature limit. The asymptotic ($\beta\to\infty$) form of the latter is proposed; (3) the magnetic field dependence of the magnetization and the susceptibility shows close similarity to the s-d coupling-model self-consistent calculations.[4] It should be noted that all our calculations are based on the so-called symmetric case of the Anderson model, wherein the impurity d-energy level is virtually bound at $\frac{1}{2}U$ below the Fermi level, U being the Coulomb repulsion at the impurity site.

Starting with the Anderson Hamiltonian for the nondegenerate orbital model

$$H=\sum_{k,\sigma}\epsilon_{k\sigma}n_{k\sigma}+\sum_{\sigma}\epsilon_{d\sigma}n_{d\sigma}+\sum_{k,\sigma}(V_{kd}C^{\dagger}_{k\sigma}C_{d\sigma}+\text{H. c.})+Un_{d\uparrow}n_{d\downarrow}, \tag{1}$$

and writing the Coulomb two-particle interaction term as

$$Un_{d\uparrow}n_{d\downarrow}=(U^{1/2}C^{\dagger}_{d\uparrow}D^{\dagger}_{d\downarrow})(U^{1/2}C_{d\downarrow}C_{d\uparrow}) \tag{2}$$

we use a Stratonovich-Hubbard transformation formula

$$e^{-b^{*}b}=\int_{-\infty}^{\infty}d\,\text{Re}\,\zeta\int_{-\infty}^{\infty}d\,\text{Im}\,\zeta\times\exp[-\pi|\zeta|^{2}+i\pi^{1/2}(b^{*}\zeta+b\zeta^{*})] \tag{3}$$

in order to obtain the exact formal expression for the grand-canonical-partition function (GCPF) of the Anderson model[3]:

$$Z=\int\mathfrak{D}\zeta(\tau)\exp\left(-\int_{0}^{1}\pi|\zeta(\tau)|^{2}d\tau\right)Z[\zeta],$$
$$Z[\zeta]=Z_{0}\langle T_{\tau}\exp\{i(\pi\beta U)^{1/2}[\zeta(\tau)C^{\dagger}_{d\uparrow\tau}C^{\dagger}_{d\downarrow\tau}+\text{H. c.}]\}\rangle. \tag{4}$$

The integrand $Z[\zeta]$ represents a partition functional of "free particles" moving in an external random-pairing field $\zeta(\tau)$, which acts at the impurity site and determines a temporary existence of a quasi-bound state between the impurity and the conduction electrons. Z_0 is the partition function for the "pure" paramagnetic contribution of the impurity electrons, this quantity having been calculated by Keiter and Kimball.[5]

Using nonequilibrium- Green's-function techniques one finds, after Fourier analyzing, that

$$Z[\zeta]=Z_{0}\exp[\text{Tr}\ln(1+P)], \tag{5}$$

where P is a matrix in the discrete frequency variables:

$$(P)_{mn}=-\alpha^{2}\sum_{q}(\zeta_{m-n}G^{\uparrow *}_{q})(\zeta^{*}_{n-q}G^{\downarrow}_{n}),\quad \alpha=(\pi\beta U)^{1/2}. \tag{6}$$

G^{σ}_{n} is the free ($U=0$) d-level Green's function given by

$$G^{\sigma}_{n}=(i\omega_{n}-\beta\epsilon_{d\sigma}+i\beta\Delta\,\text{sgn}\omega_{n})^{-1},\quad \omega_{n}=(2n+1)\pi. \tag{7}$$

In Eq. (7) $\epsilon_{d\uparrow,\downarrow}=-\frac{1}{2}U\mp h$ and $\Delta=\pi N(0)|V_{kd}|^{2}_{\text{av}}$ are the energy and the width of the d level, where $N(0)$ represents the density of states of the conduction electrons at the Fermi level. The Planck and Boltzmann constants $\hbar$ and k_b and the magnetic moment of the impurity electrons $\frac{1}{2}g_d\mu_B$ are put equal to 1.

Assuming statistical independence of the different Fourier components of the random field ζ, and retaining only the diagonal matrix element of P in Eq. (5), the integrations over the infinity values of the random variables ζ_ν were accomplished.[3] The exact analytical integrations enabled us to obtain the following expression for Z:

$$Z_{D}=Z_{0}\prod_{\nu=-\infty}^{\infty}(1+\beta U\Phi_{\nu}), \tag{8}$$

where Z_D represents the complete GCPF of the Anderson Hamiltonian obtained in the "diagonal approximation,"[3] normalized by the band-electrons part Z_B. The polarization bubble Φ_ν defined as

$$\Phi_\nu = -\sum_n G_n^{\uparrow *} G_{n+\nu}^{\downarrow} \tag{9}$$

was explicitly calculated in terms of physical parameters,[3] and represents the interaction between a free ($U=0$) particle and a hole having an opposite spin. Equation (9) for Φ_ν recalls another polarization bubble introduced by Wang *et al.*[1] in their RPA approximation and explicitly calculated by Keiter,[2] but in fact these two quantities have different components. In our case Φ_ν exhibits an antiparallel spin interaction in contradiction with the parallel obtained in the RPA. The latter is artificially introduced in the RPA and gives a nonphysical divergence in the GCPF, a divergence which, as explained by Keiter,[2] can be overlooked by a complicated renormalization scheme, or directly by using a two-variable functional-integral scheme, as pointed out by Amit and Keiter.[2] Our explicit result for Φ_ν is

$$\Phi_{\nu\geq 0} = \frac{1}{(2\pi)^2} \sum_{\sigma=\uparrow,\downarrow} \left(\frac{1}{\nu + i\beta\epsilon_d/\pi + \beta\Delta/\pi} [\Psi(a+\nu+i\beta\epsilon_{d\sigma}/2\pi) - \Psi(a+i\beta\epsilon_{d\sigma}/2\pi)] + \frac{-1}{\nu + i\beta\epsilon_d/\pi} [\Psi(a+\nu+i\beta\epsilon_{d\sigma}/2\pi) - \Psi(a-i\beta\epsilon_{d\sigma}/2\pi)] \right), \tag{10}$$

where $a=\frac{1}{2}+\beta\Delta/2\pi$ and $\Psi(z)$ is the digamma (psi) function.[6]

Using the formula $\chi_D = \beta^{-1}(\partial^2 \ln Z_D/\partial h^2)_{h=0}$, the zero-magnetic-field susceptibility is given by

$$\chi_D = \chi_{\text{par}} + \chi_{\nu=0} + \sum_{\nu=1}^{\infty} \chi_\nu . \tag{11}$$

$$\chi_0 = \frac{\beta}{4\pi^2} \frac{\text{Im}\Psi^{(2)}(z)}{\frac{1}{2}\pi - \text{Im}\Psi(z)}, \qquad \chi_{\nu>0} = \frac{\beta^2 U}{4\pi^4} \text{Re}\left(\frac{A_\nu}{1-(\beta U/2\pi^2)C_\nu} \right), \tag{12}$$

where

$$A_\nu = \frac{(\beta\Delta/\pi)\Psi^{(2)}(z^*+\nu)}{(\nu - i\beta U/2\pi)(\nu + \beta\Delta/\pi - i\beta U/2\pi)} + \frac{\Psi^{(2)}(z^*)}{\nu+\beta\Delta/\pi - i\beta U/2\pi} - \frac{\Psi^{(2)}(z)}{\nu - i\beta U/2\pi} .$$

C_ν has the same expression as A_ν, with the functions $\Psi^{(2)}$ replaced by Ψ.

$$\chi_{\text{par}} = (\beta/\pi^2)\,\text{Re}\Psi^{(1)}(z) . \tag{12a}$$

In Eqs. (12) $z=\frac{1}{2}+\beta\Delta/2\pi + i\beta U/4\pi$ and $\Psi(z)$, $\Psi^{(1)}(z)$, and $\Psi^{(2)}(z)$ are the first three logarithmic derivations of the Euler γ function.[6] In writing Eq. (11) we used the fact that $\Phi_{-\nu}=\Phi_\nu^*$. χ_{par} is the "pure" paramagnetic contribution of the impurity, arising from Z_0, where the "localized" magnetic part of the susceptibility is given by the infinite series and the χ_0 term of Eq. (11).

Our "static approximation" χ_{st} is the sum of χ_{par} and χ_0. In the $\Delta=0$ limit, χ_{st} equals $\beta(1+e^{-\beta U/2})^{-1}$, a result which recovers Curie behavior for sufficiently low temperatures ($\beta U \gg 1$). The remaining series gives, in the $\Delta=0$ limit, a small contribution which goes exponentially to zero for $\beta U \gg 1$.

In the strong-coupling limit $y=U/2\Delta \gg 1$ the Anderson model was shown to be equivalent to the antiferromagnetic s-d coupling model.[7] This limit corresponds to $N(0)J \ll 1$ in the s-d model, J being the s-d coupling constant. [The exact correspondence for $y \gg 1$ is $N(0)J = 4/\pi y$.] The s-d model is nonanalytic[8] in the $T\to 0$ °K, $J \to 0$ limits. Our result also possesses this property, since for $T\to 0$ °K only $\Delta=0$ (infinite y) gives divergent susceptibility (of Curie type), while $T \to 0$ °K, $y\to\infty$ ($\Delta \neq 0$) gives finite susceptibility, a result which tends to zero as y^{-1}. This should be contrasted with Wilson's low-temperature theory of the spin $\frac{1}{2}$ Kondo Hamiltonian.[9] His results, obtained within renormalization-group method and scaling considerations, exhibits a finite zero-temperature susceptibility which tends to infinity when $N(0)J\to 0$.

Our result points that for every finite Δ and U at low enough temperatures the system behaves paramagnetically.[10] In the weak-coupling regime ($y<1$) Pauli-like paramagnetic behavior is exhibited for all temperatures.

The numerical results for χ_D, for various values of $y=U/2\Delta$, are illustrated in Fig. 1. Results of previous works are also illustrated; it should be noted that these results are calculated only in the limit $\beta\Delta \gg 1$. Figure 1 illustrates the antiferromagneticlike behavior of the system for $y \gg 1$; the susceptibility shows a distinct peak at some temperature T_0. For $T>T_0$ the behavior is Curie-like, while for $T<T_0$ the susceptibility drops sharply to a Pauli-like behavior. The abrupt decrease of the zero-magnetic-field susceptibility recalls the "disappearance" of the localized magnetic moment associated with the impurity site. This disappearance is connected with the screening of the impurity spin due to the spins of the conduction electrons, which occurs well below the Kondo temperature T_K.[1] The results obtained within the s-d coupling

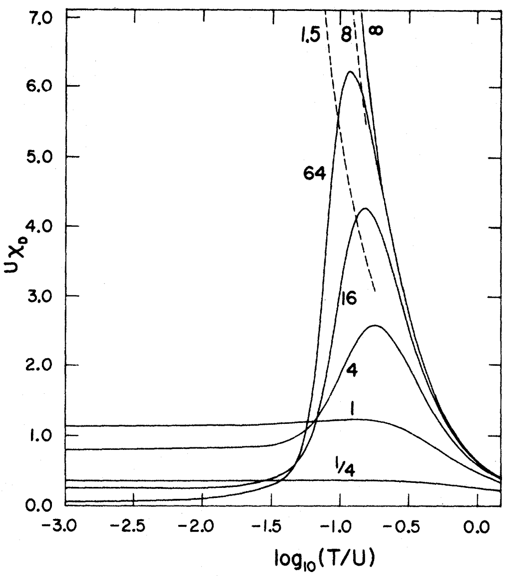

FIG. 1 Dimensionless susceptibility $U\chi_D$ as a function of the dimensionless temperature T/U in logarithmic scale for various values of $y = U/2\Delta$. The dashed lines illustrate the high-temperature extrapolation of the results of Ref. 1.

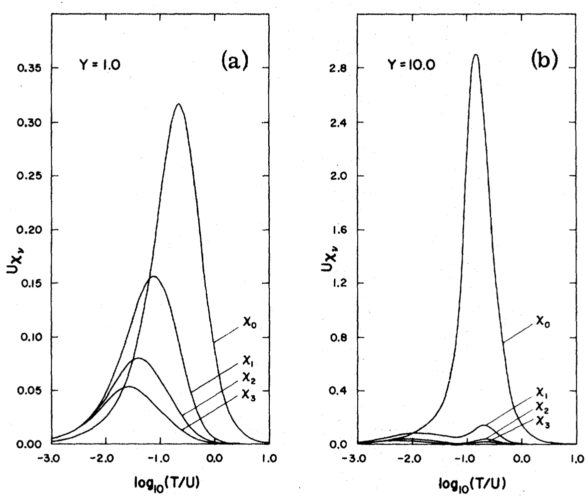

FIG. 3 (a) Temperature dependence of the $U\chi_\nu$ terms in the susceptibility series for $y = U/2\Delta = 1$; (b) the corresponding curves for $y = 10$.

calculations for the spin $\frac{1}{2}$, and reviewed recently by Brenig and Zittartz,[11] point to a complete (or over complete) screening, but they still give a divergent susceptibility (or a negative one!) in the limit $T \to 0$ °K. In our case the Curie "constant" $(T\chi)$ goes to zero (when $T \to 0$ °K) as T, a fact that ensures a Pauli-like behavior of the susceptibility at very low temperatures. However, we do not identify T_0 with T_K for the following reasons: (1) T_0 appears to be too high, e.g., for $N(0)J \simeq 0.1$ ($y \simeq 10$) and $U = 0.1$ eV, $T_K \simeq 1$ °K, while $T_0 \simeq 100$ °K. This is related to the second reason (2), T_0 shifts very slowly (logarithmically) to lower temperatures with increasing y. Numerically for $y \gg 1$, it is found that $U/T_0 \simeq 4.3 \log_{10} y - 0.98$.

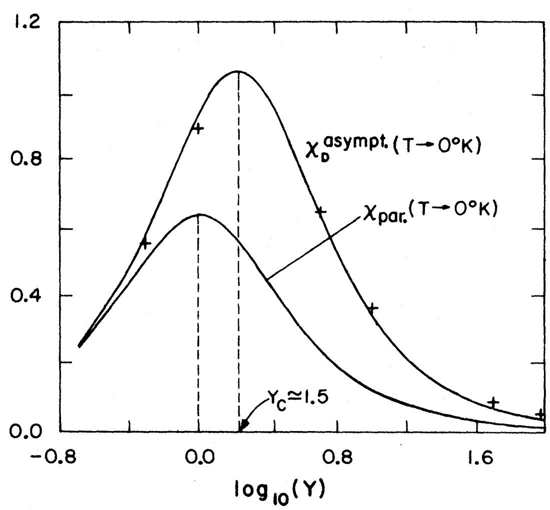

FIG. 2. $T \to 0$ °K limit of the dimensionless susceptibilities $U\chi_D^{\text{asympt}}$ of Eq. (13) and $U\chi_{\text{par}}$ of Eq. (13a) vs $\log_{10}(y)$. The crosses signify the numerical results.

The series in Eq. (11) converges slowly for low temperatures for all values of y. We obtain for the asymptotic value (for $T \to 0$ °K)

$$\chi_D^{\text{asympt}}(T \to 0\ ^\circ\text{K}) = \frac{4}{\pi U}\frac{y}{ry^2+1}, \quad r \simeq 1 - \frac{2}{\pi}. \qquad (13)$$

This shows that the series simply renormalize the $y \gg 1$ regime of the "pure" paramagnetic result [Eq. (12a)]:

$$\chi_{\text{par}}(T \to 0\ ^\circ\text{K}) = \frac{4}{\pi U}\frac{y}{y^2+1}. \qquad (13a)$$

These results are illustrated in Fig. 2. Because the terms of the series change their character (see below) at y_c, the numerical results—crosses in Fig. 2—fall below the χ_D^{asympt} curve for $y < y_c$, and above it for $y > y_c$. In Fig. 3 this character change of the various χ_ν's $(\nu > 0)$ as a function of temperature is illustrated, e.g., compare Fig. 3(a) with Fig. 3(b). The χ_ν $(\nu \neq 0)$ for $y > y_c$ are oscillatory in character and attain negative values, while for $y < y_c$ all the terms are positive throughout the low-temperature region. We expect that the oscillatory nature referred to above precludes perturbative treatment in this low-temperature range. Figure 3(b) and Eq. (11) illustrate that χ_D, for $y > y_c$, is qualitatively given by $\chi_{st} = \chi_{\text{par}} + \chi_0$.

We now turn to the calculation of the external-magnetic-field (h) dependence of susceptibility and magnetization. The calculations are performed in the static approximation which, as mentioned above,

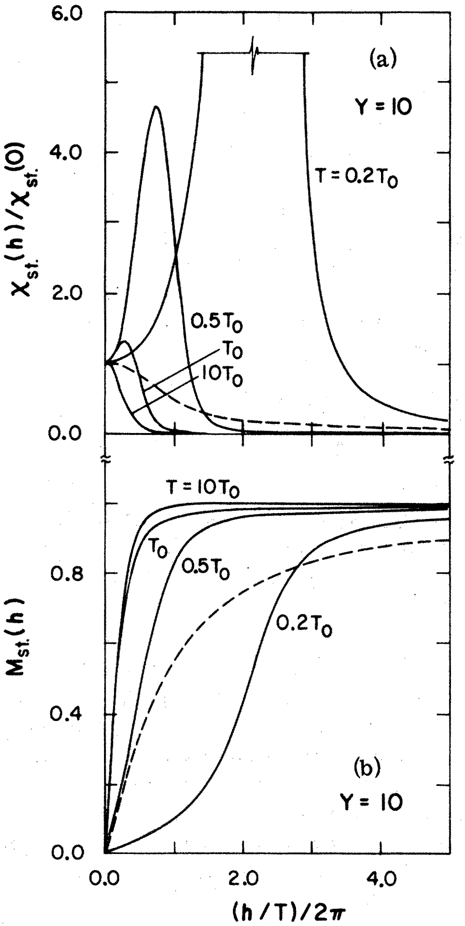

FIG. 4. (a) Magnetic field dependence of the $y=10$ susceptibility for different temperatures scaled with T_0. The dashed line represents the curve for $y=0.5$, which is typical for all temperatures; (b) the corresponding curves for the magnetization.

should give good qualitative results. Figure 4(a) exhibits the results for the susceptibility in units of $\chi_{st}(h=0)$. For $y=10$, at $T<T_0$,[12] the curves show large maxima. For $T>T_0$ the curve for the same y (=10) decreases monotonically with h. The curves for $y<1$ are monotonically decreasing functions of h for all temperatures. This is illustrated by the dashed line for which $y=0.5$. The respective curves of the magnetization $M_{st}(h)$ are given in Fig. 4(b):

$$M_{st}(h)=\frac{2}{\pi}\left(\mathrm{Im}\Psi(z+ib)-\mathrm{Im}\Psi(z-ib)-\frac{\mathrm{Re}\Psi^{(1)}(z+ib)-\mathrm{Re}\Psi^{(1)}(z-ib)}{2[\pi-\mathrm{Im}\Psi(z+ib)-\mathrm{Im}\Psi(z-ib)]}\right), \quad (14)$$

where b is $h/2\pi T$. Figures 4(a) and 4(b) are very similar to the corresponding curves obtained for the s-d coupling model by self-consistent calculations.[4] It should be noted that the above s-d curves were plotted with the temperatures scaled with the Kondo temperature for the case $N(0)J\simeq 0.125$, i.e., $y\simeq 10$.

In conclusion, we find that the Anderson Hamiltonian in the strong-coupling regime ($y\gg 1$) leads to a characteristic temperature (T_0), which signifies the transition from a Curie to a Pauli paramagnetic behavior of the susceptibility. This temperature T_0 has a weak dependence on $y=U/2\Delta$, contrary to the very strong dependence of the Kondo temperature on $N(0)J$, which equals $4/\pi y$ in this regime. Our results are free of divergences when $T\to 0$ °K.

The decoupling scheme we use in the functional integral emphasizes a virtual bound state of antiparallel spins. The importance of this state was previously considered in the s-d coupling model[8,13] and in the Anderson model.[14] We believe that the decoupling scheme used above is particularly suited for the problem of magnetic impurities in superconductors.

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