alternately + and −, on a line of length β. Their interaction is the two-dimensional Coulomb force

$$\frac{V(x-x')}{T} = \pm 2(1-\epsilon)\ln\left(\frac{x_n - x_{n'}}{\tau}\right)$$
$$= \infty \quad (|x_n - x_{n'}| < \tau). \tag{16}$$

The chemical potential is given by

$$e^{-\mu} = J; \tag{17}$$

and the free energy $f(T)$ per unit length determines the ground-state energy according to

$$F(i\beta) \sim e^{+\beta\omega_0} \sim e^{-\beta f(T)/T}. \tag{18}$$

In a subsequent Letter we will show that the point $\epsilon = 0$ (for small J) is a critical point of this system, separating the region where the charged pairs are all associated from that where some are ionized, the latter being the region of zero net spin. It is fascinating that the simple-appearing Kondo system is isomorphous with one which certainly has at least one critical point and possible more. (It is a commonplace that one-dimensional systems with long-range interactions often have critical points.)

We thank J. J. Hopfield and P. Nozières for discussions and use of their work before publication.

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THEORY OF ITINERANT FERROMAGNETS EXHIBITING LOCALIZED-MOMENT BEHAVIOR ABOVE THE CURIE POINT*

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By using a functional integral formulation of the theory of itinerant ferromagnets above the Curie point, we show that for strong Coulomb interaction U, there are localized moments exhibiting a characteristic Curie-law susceptibility with the correct free spin-$\frac{1}{2}$ limiting value of the Curie constant. For weak U the same formulation gives a Pauli-like susceptibility, again with the proper limit, while for intermediate values the theory gives a smooth interpolation between the extreme cases.

The presence of local-moment aspects in band ferromagnetism has long been a baffling problem. The most striking example of this is iron. The high-temperature susceptibility, neutron scattering, alloy experiments, etc., all point to the presence of localized moments, while transport properties show unambiguously the itinerant character of the d electrons.[1] We report here on the first results of a new theoretical approach to such systems. The theory is based on an exact transformation of Stratonovich[2] and Hubbard[3] which eliminates the two-body interaction in favor of a Gaussian average over fluctuating one-body potentials. We concentrate here on the paramagnetic phase, leaving cooperative effects for future publication.

Since there is little short-range order at high temperatures, we expect the problem to be equivalent to an aggregation of one-center problems. The one-center problem can be represented by an Anderson model[4] of an "impurity" atom immersed in an effective band. While orbital degeneracy (Hund's rule) is important in practice, most of the essential features are already contained in the nondegenerate orbital model treated here.

The Hamiltonian is $H_0 + H_1$, where if $\sigma \equiv \pm 1$,

$$H_0 = \sum_{k,\sigma} \epsilon_{k\sigma} n_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} n_{d\sigma} + \sum_{k,\sigma} [V_k c_{k\sigma}^{\dagger} c_{d\sigma} + \text{H.c.}], \tag{1a}$$

$$H_1 = U n_{d\uparrow} n_{d\downarrow} = -\tfrac{1}{2} U (n_{d\uparrow} - n_{d\downarrow})^2 + \tfrac{1}{2} U (n_{d\uparrow} + n_{d\downarrow}). \tag{1b}$$

In Eq. (1b) we have used $n_{d\sigma}{}^2 = n_{d\sigma}$. The second term of H_1 can be absorbed into H_0 by defining $\bar{\epsilon}_{d\sigma} = \epsilon_{d\sigma} + \frac{1}{2}U$. Following Hubbard, Mühlschlegel[5] has shown that the partition function can be written as the Gaussian functional average over an effective "magnetic" field $\xi(\tau)$ of the partition function $Z(\xi)$ for a one-body Hamiltonian:

$$Z = \int \mathfrak{D}\xi(\tau) \exp[-\pi \int_0^1 \xi^2(\tau) d\tau] Z(\xi), \tag{2a}$$

$$Z(\xi) = \mathrm{Tr}\{T \exp \int_0^1 [-\beta H_{0\tau} + c\xi(\tau)(n_{d\uparrow\tau} - n_{d\downarrow\tau})] d\tau\}, \tag{2b}$$

where $c \equiv (2\pi\beta U)^{1/2}$, and T is the ordering symbol for the fictitious "imaginary time" τ.[6]

To evaluate Eq. (2), it is convenient to Fourier analyze $\xi(\tau)$:

$$\xi(\tau) = \sum_{\nu=-\infty}^{\infty} \xi_\nu e^{i\Omega_\nu \tau}, \quad \Omega_\nu = 2\pi\nu, \quad \xi_\nu = \xi_{-\nu}{}^*. \tag{3}$$

By introducing a dimensionless coupling constant, λ, multiplying c, it follows that

$$\frac{\partial \ln Z(\xi)}{\partial \lambda} = \langle \sum_\sigma \int_0^1 d\tau \; c\xi(\tau) \sigma n_{\sigma\tau} \rangle$$

$$= - \sum_{\sigma,\nu,n} v_\nu{}^\sigma G_{nn+\nu}{}^\sigma, \tag{4}$$

where $v_\nu{}^\sigma = -\sigma c \xi_\nu$. $G_{nn'}{}^\sigma$ is the one-particle Green's function which satisfies the Dyson equation:

$$G_{nn'}{}^\sigma = G_n{}^{0\sigma}\delta_{nn'} + \sum_m G_n{}^{0\sigma} v_{n-m} G_{mn'}, \tag{5a}$$

where $G_n{}^{0\sigma}$ is the zero-order one-electron Green's function in the presence of the τ-averaged potential $-\sigma c \xi_0$,

$$G_n{}^{0\sigma} = (i\omega_n - \beta\bar{\epsilon}_{d\sigma} + \sigma c\xi_0 + i\beta\Gamma \, \mathrm{sgn}\omega_n)^{-1},$$

$$\omega_n = (2n+1)\pi. \tag{5b}$$

Γ is the virtual level width $\pi N(0)|V|^2$.

Using the Fredholm solution of Eq. (5a) and the relations

$$\mathrm{Tr}N = -\partial D/\partial\lambda, \quad D = e^{\mathrm{Tr}\ln(1-K)}$$

for the Fredholm numerator and denominator, it is straightforward to show that an exact expression for Z is

$$Z = \int_{-\infty}^{\infty} d\xi_0 \prod_{\nu>0} 2\int d^2\xi_\nu \exp\{-\pi \sum_{\nu'=-\infty}^{\infty} |\xi_{\nu'}|^2 + \sum_\sigma \mathrm{Tr}\ln(1-K^\sigma)\} Z_0(\xi_0), \tag{6}$$

where $\int d^2\xi_\nu$ denotes an integral over the complex ξ_ν plane.[7] The Tr ln term takes account of the fluctuating parts of the effective field, i.e., the ξ_ν's for $\nu \neq 0$. K^σ is a matrix in the frequency variables, and is defined by

$$K_{mn}{}^\sigma = v_{m-n}{}^\sigma G_n{}^{0\sigma}, \quad K_{nn}{}^\sigma \equiv 0. \tag{7}$$

Clearly K describes the scattering of the virtual-level electron by the fluctuating field $[\xi(\tau) - \xi_0]$, with the τ-averaged effects included in zero order. The nth term in the power series expansion of the Tr ln term can be represented by a single closed-loop diagram with n v^σ lines attached.

$Z_0(\xi_0)$ in Eq. (6) is the value that $Z(\xi)$ [Eq. (2b)] takes on if $\xi(\tau)$ is replaced by its τ average ξ_0. Explicitly, for the symmetric case, $\epsilon_d + \frac{1}{2}U = 0$, and for large $\beta\Gamma$,

$$\ln\left[\frac{Z_0(\xi_0)}{A}\right] = \frac{2c\xi_0}{\pi} \tan^{-1}\left(\frac{c\xi_0}{\beta\Gamma}\right) - \frac{\beta\Gamma}{\pi} \ln\left[1 + \left(\frac{c\xi_0}{\beta\Gamma}\right)^2\right], \tag{8}$$

where A is the partition function for H_0 with $\epsilon_{d\sigma}$ replaced by $\bar{\epsilon}_{d\sigma}$. In Fig. 1 we plot $(\pi\xi_0{}^2 - \ln Z_0)/\beta$, which is the effective free energy for a τ-independent field ξ_0, for several values of $U/\pi\Gamma$.[8]

When calculating the partition function, it is useful to distinguish four separate regimes of the parameters $\beta\Gamma$ and $U/\pi\Gamma$: (1) $U/\pi\Gamma \ll 1$. This corresponds to a nonmagnetic impurity with weak exchange effects. (2) $U/\pi\Gamma \gg 1$ and $T \gg T_K$, where T_K is a Kondo-like temperature of order $(U/k_B)e^{-\pi U/8\Gamma}$. This corresponds to a strongly localized moment above the Kondo regime. (3) $U/\pi\Gamma \gg 1$ and $T \lesssim T_K$. This is the Kondo regime where the localized moment tends to be averaged to zero. (4) $U/\pi\Gamma \sim 1$. This is an intermediate regime which is characterized by large fluctuations in the size and direction of the localized moment.[9]

In case (1) only small-amplitude fluctuations ξ_ν

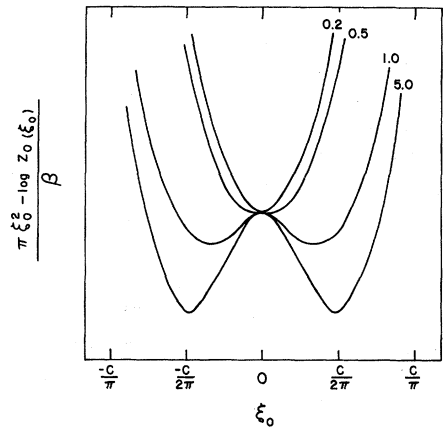

FIG. 1. Effective free energy for a τ-independent field ξ_0. The curves are labeled by $U/\pi\Gamma$.

contribute appreciably to Z, so that the expansion of Tr ln(1−K) to order $|\xi_\nu|^2$ suffices in this case (the linear terms vanish). On performing the $d^2\xi_\nu$ integrations one finds

$$Z=\int_{-\infty}^{\infty}d\xi_0 e^{-\pi\xi_0^2}Z_0(\xi_0)\prod_{\nu>0}\left[1-\frac{c^2}{\pi}\varphi_\nu(\xi_0)\right], \quad (9a)$$

where the "polarization bubble" is, for $\nu>0$,

$$\varphi_\nu=-\sum_n G_n{}^{0\sigma}G_{n+\nu}{}^{0\sigma}$$

$$=\frac{\beta\Gamma}{\pi\Omega_\nu(\Omega_\nu+2\beta\Gamma)}\ln\left[1+\frac{\Omega_\nu(\Omega_\nu+2\beta\Gamma)}{\beta^2\Gamma^2+c^2\xi_0{}^2}\right], \quad (9b)$$

and $\varphi_\nu=\varphi_{-\nu}$. For $|\Omega_\nu/\beta\Gamma|\ll 1$, φ_ν becomes

$$\varphi_\nu\simeq\frac{1}{\pi\beta\Gamma}R\left[1-\frac{|\Omega_\nu|}{\beta\Gamma}R+\cdots\right], \quad (10)$$

where $R=[1+(c\xi_0/\beta\Gamma^2]^{-1}$.[10] In this small-($U/\pi\Gamma$) limit one can also expand $\ln Z_0$ to order $\xi_0{}^2$, as one can see from Fig. 1 since the effective free energy has a single minimum at the origin and large positive curvature in this case. This procedure is exact in this limit and is equivalent to the random-phase approximation including both bubble and ladder diagrams with correct spin counting.

One can see from Fig. 1 that in case (2) the dominant contributions to the partition function will come from values of ξ_0 near the two minima. By inspection of Eq. (9) it is clear that for ξ_0 near the minima the $\nu>0$ contribution is small, thereby justifying the Gaussian approximation for the ξ_ν integrals in this ξ_0 neighborhood. For ξ_0 far from the minima, a careful treatment of the $\nu\neq 0$ terms shows that the entire ξ_0 integrand in Eq. (6) is negligible. Therefore Eq. (9a) gives an accurate value of Z so long as the integral is carried out only near the minima in effective free energy.

In case (3) the small energy arising from scattering from the vicinity of one minimum to the other must be carefully included. Fluctuations about a given minimum are correctly included in Eq. (9); however, the infrequent hopping from minimum to minimum must be treated separately.[11]

In case (4) a number of low-frequency ξ_ν's give appreciable non-Gaussian contributions to Z. This problem is presently under study.

To obtain the static magnetic susceptibility of this system, we use the relation $\chi=(1/\beta)[\partial^2\ln Z/\partial h^2]_{h=0}$ where h is a magnetic field applied in the z direction. Since the Zeeman energy enters additively in H with $c\xi_0/\beta$, one can shift the origin of ξ_0 by $\beta\mu_B h/c$ so that, aside from A, the Zeeman energy appears only in the Gaussian factor in Eq. (6). It follows that

$$\chi=\frac{2\mu_B{}^2}{\pi\Gamma}+\frac{\mu_B{}^2}{U}[2\pi\langle\xi_0{}^2\rangle-1]+\chi_{\text{band}}, \quad (11)$$

where $\langle\xi_0{}^2\rangle$ is given by inserting $\xi_0{}^2$ into the integrand of Eq. (6) and dividing by Z.

The numerical results for the susceptibility as a function of temperature are shown in Fig. 2. It is interesting to note that for $U/\pi\Gamma\gg 1$, the susceptibility is Curie-like over a wide temperature range. For large $U/\pi\Gamma$, the susceptibility approaches the Curie law appropriate for a free spin-$\frac{1}{2}$ moment. For $U/\pi\Gamma\ll 1$, χ is essentially temperature independent, corresponding to a weakly-enhanced Pauli susceptibility.

In regimes (1) and (2) the curves in Fig. 2 were calculated from Eq. (9) as discussed above. In regime (4), $U/\pi\Gamma\sim 1$, the curves in the figure were calculated using the exact expression [Eq. (8)] for Z_0 but neglecting the Tr ln term of Eq. (6). This approximation corresponds to neglecting finite frequency fluctuations of the effective field. Work is currently proceeding to include the contribution of terms for finite ν in regime (4).

The coupling between moments, which is a two-center problem in first approximation, is currently under study. Extension to degenerate orbitals will be undertaken in the near future.

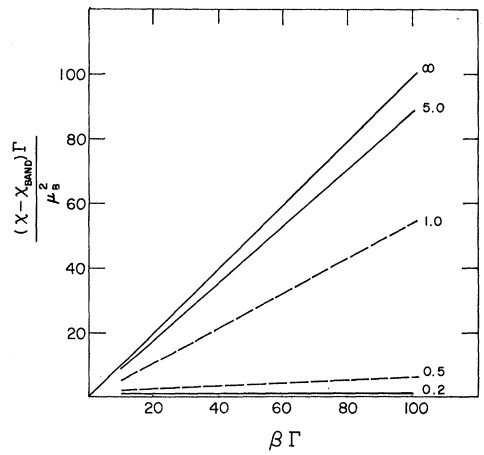

FIG. 2. Plots of the dimensionless quantities $(\chi-\chi_{\text{band}})\Gamma/\mu_B{}^2$ vs $\beta\Gamma$. The full lines are calculated directly from Eqs. (9a) and (11); the dashed lines are calculated by neglecting Tr ln(1−K) in Eq. (6) as explained in the text. The asymptote for large $U/\pi\Gamma$ is the correct Curie law for a free spin $\frac{1}{2}$. For small $U/\pi\Gamma$, the correct exchange-enhanced Pauli susceptibility is obtained.

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[6]There are other ways of writing Z in functional average form as Mühlschlegel (Ref. 5) has shown. Independently, D. R. Hamann, this issue [Phys. Rev. Letters 23, 95 (1969)] has employed two random fields to study the Kondo problem.

[7]In polar coordinates, $d^2\xi_\nu = \frac{1}{2}dR_\nu{}^2 d\theta_\nu$.

[8]An alternative scheme for the evaluation of Eq. (2) is to perform a coupling-constant integral over the strength of V_k as Mühlschlegel (Ref. 5) has done. Unfortunately, in the full ferromagnetism problem as opposed to the one-center approximation, this procedure has the serious drawback of requiring one to integrate through the insulator-metal transition.

[9]Large-amplitude localized spin fluctuations have been discussed from other points of view by A. D. Caplin and C. Rizzuto [Phys. Rev. Letters 21, 746 (1968)]; P. Lederer and D. L. Mills [Phys. Rev. Letters 20, 1036 (1968)]; N. Rivier and M. J. Zuckerman [Phys. Rev. Letters 21, 904 (1968)]; and M. Levine and H. Suhl [Phys. Rev. 171, 567 (1968)].

[10]We note that the terms 1 and $-|\Omega_\nu|R/\beta\Gamma$ in Eq. (10) correspond to the adiabatic and transient terms, respectively, in the Nozières–de Dominicis [P. Nozières and C. de Dominicis, Phys. Rev. 178, 1097 (1969)] solution of the x-ray intensity problem as employed in the magnetic impurity problem by P. W. Anderson and G. Yuval [Phys. Rev. Letters 23, 89 (1969) (this issue)] and by Hamann (Ref. 6).

[11]Hamann, Ref. 6.

FLUCTUATION THEORY OF DILUTE MAGNETIC ALLOYS

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A simple explanation of the Kondo effect is shown to follow from a functional integral form of Anderson's dilute-alloy model.

This Letter describes a new approach to the theory of dilute magnetic alloys. The nonperturbational energy lowering associated with the Kondo effect[1] is shown to be a simple consequence of the statistics of fluctuations on the impurity site.

This theory uses a transformation due to Hubbard to replace the two-particle interaction by a Gaussian average over fluctuating one-particle potentials.[2] To apply Hubbard's transformation, Anderson's dilute-alloy Hamiltonian[3] must be written in the form

$$\mathcal{H}_0 = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \sum_\sigma \epsilon_{d\sigma} + V \sum_{k\sigma} [C_{k\sigma}{}^\dagger C_{d\sigma} + C_{d\sigma}{}^\dagger C_{k\sigma}], \tag{1}$$

$$\mathcal{H}_1 = \tfrac{1}{4} U[(n_d)^2 - (S_{dz})^2], \tag{2}$$

where

$$n_d = n_{d\uparrow} + n_{d\downarrow}, \tag{3}$$

$$S_{dz} = n_{d\uparrow} - n_{d\downarrow}. \tag{4}$$

Straightforward application of Hubbard's method gives the partition function Z as the double functional integral

$$Z = Z_0 \int \delta x \, \delta y \langle T_\tau \exp\{-\int_0^\beta d\tau [\pi x^2/\beta + \pi y^2/\beta + \tilde{\mathcal{H}}_1]\}\rangle, \tag{5}$$

where

$$\tilde{\mathcal{H}}_1 = (\pi U/\beta)^{1/2}[x(\tau) S_{dz}(\tau) + i y(\tau) n_d(\tau)]. \tag{6}$$