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Magnetization of a Magnetic Impurity in Metal*

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A diagrammatic Green's-function method is developed for the calculation of the magnetization of a magnetic impurity in metal. The validity of the approach is within Abrikosov and Suhl's limit. Therefore, the result in this paper should be regarded as an improvement over that obtained by Giovanini *et al.* insofar as the temperature range is concerned.

The magnetization of a dilute magnetic alloy was first calculated in the *s-d* exchange model by Giovanini *et al.*[1] to second order in perturbation theory for general values of the magnetic field. Since then, very little progress has been made on this subject. Recently Osaka[2] calculated the magnetic susceptibility by using Suhl's approach. The present author[3] and Brenig *et al.*[4] made calculations on the susceptibility by using diagrammatic methods. The results these authors obtained are identical at temperatures $T=0$, $T=T_K$, the Kondo temperature, and at $T\gg T_K$; therefore they cannot be materially different. One essential feature of these results is that the dressed Curie constant vanishes for the impurity with spin $S=\frac{1}{2}$ at $T=0$. This property is entirely due to the impurity spin fluctuation according to our formulation.[3,4] On the other hand, Anderson, Yuval, and Hamann recently made a much more rigorous formalism for the *s-d* exchange problem.[5,6] However, this approach is exact only for $T\ll T_K$, and the equations they obtained are too complicated, at least for the present, to obtain temperature-dependent measurable quantities. In this paper we will extend our previous method[3] to calculate the magnetization of a magnetic impurity in an arbitrary magnetic field.

In Ref. 3, the diagrams we have used to evaluate the zero-field magnetic susceptibility are obtained by differentiating the free-energy graphs twice with respect to the external magnetic field B. This selection of free-energy diagrams gives Suhl's equation when functionally differentiated with respect to the conduction-electron Green's function. In our present magnetization computation, the external magnetic field comes into the calculation through the conduction-electron propagator $G(\omega)$ and the pseudofermion Green's function $g(\omega)$.[3,7] Then the shift of the magnetization due to the *s-d* exchange interaction is given by $\Delta M=-\partial\Delta F/\partial B$, and

$$\frac{\partial\Delta F}{\partial B}=\frac{\delta\Delta F}{\delta G}\,\frac{\partial G}{\partial B}+\frac{\delta\Delta F}{\delta g}\,\frac{\partial g}{\partial B}\ ,$$

where $\delta\Delta F/\delta G$ and $\delta\Delta F/\delta g$ are the functional derivatives of the free-energy shift ΔF with respect to G and g, respectively. It is easy to see that the first term on the right-hand side of the above equation is the shift of the conduction-electron spin magnetization ΔM_c and the second term denotes the shift of the impurity spin magnetization ΔM_i. We will later see that the logarithmic singular term in B and T starts to appear in the second-order term of ΔM_i; on the other hand, we have noted that ΔM_c, up to the third order in J, does not contain any logarithmic singular term at all. In our subsequent calculation of ΔM, only the leading logarithmic term in each order of perturbation will be included; the part due to ΔM_c, except the first-order term, will thus be neglected. In Fig. 1, graph (a) is the bare impurity spin magnetization; (b) is the first-order term of ΔM_c. The reason we include it in the calculation is because it is of the same order of magnitude as the first-order term in ΔM_i. Graphs (c) and (d) represent $\Delta M_i=-(\delta\Delta F/\delta g)(\partial g/\partial B)$, where the solid line and the dotted line are, respectively, the conduction propagator and the pseudofermion Green's function. The open square denotes the *s-d* coupling constant $(\vec{\sigma}\cdot\vec{s})J/N$, and the shaded square is the four-point vertex function Γ which represents a summation of parquet graphs to infinite order[7] in the presence of a magnetic field. $\delta\Delta F/\delta g$ is the self-energy of pseudofermion and $-\partial g/\partial B\propto g^2(\omega)$ are the two out-extended pseudofermion lines. At this stage we would like to point out that the graphs in Fig. 1 can be regarded as an exact expression for the impurity spin magnetization within Abrikosov and Suhl's validity range. It is also easy to prove that the logarithmic magnetic-field-dependent terms of Fig. 1(d) come entirely from the $\vec{B}$ dependencies through $g(\omega)$, not through $G(\omega)$. In what follows we neglect the direct effect of B on $G(\omega)$ and take into account the effects of the magnetization of the pseudofermions only.

Figure 1(a) represents the bare magnetization of the localized impurity spin. The evaluation of the

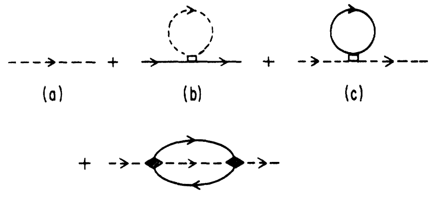

FIG. 1. Diagrams representing the impurity spin magnetization.

diagram is straightforward; it is of the form

$$M_0=\mu_B gSB_s(S\theta/T)=\mu_B g\,\langle S^z\rangle\ , \tag{1}$$

where $\theta=\mu_B gB$, μ_B is the Bohr magneton, and g is the Landé g factor for impurity spin. $B_s S\theta/T$ is the Brillouin function and is defined by

$$B_s(x)=\frac{2S+1}{2S}\coth\frac{(2S+1)x}{2S}-\frac{1}{2S}\coth\frac{x}{2S}\ . \tag{2}$$

Figures 1(b) and 1(c) represent the first-order correction to the bare magnetization. These two diagrams can be written together and yield the contribution to the magnetization, which is

$$M_1=-\frac{\partial}{\partial B}\left[\left(\frac{J}{N}\rho\right)\mu_B gBSB_s\left(\frac{S\theta}{T}\right)\right], \tag{3}$$

where ρ is the density of states at the Fermi surface.

Now we are going to evaluate the graph of Fig. 1(d) where the shaded square is the four-point vertex function Γ which represents a summation of parquet graphs to infinite order[7] in the presence of the magnetic field. The corresponding expression for this can be proved to have the form

$$M_2=\frac{1}{2}\frac{\partial}{\partial B}\left(\frac{1}{Z(\theta)}\iint\frac{d^3p\,d^3q}{(2\pi)^6}\right.$$
$$\times\left.\frac{n(\epsilon_p)n(-\epsilon_q)\,e^{S^z_{\alpha\alpha}\theta/T}-n(-\epsilon_p)n(\epsilon_q)e^{S^z_{\beta\beta}\theta/T}}{\epsilon_p-\epsilon_q+(S^z_{\beta\beta}-S^z_{\alpha\alpha})\theta}\right)$$
$$\times\left|\langle\xi\alpha|\,\Gamma(\epsilon_p;\ \lambda-S^z_{\alpha\alpha}\theta|\,\epsilon_q;\ \epsilon_p-\epsilon_q+\lambda-S^z_{\alpha\alpha}\theta)|\,\eta\beta\rangle\right|^2, \tag{4}$$

where λ is the single-particle energy[7] assigned for the pseudofermion and $S^z_{\beta\beta'}$ are the z-component spin matrices; each index β and β' assumes $2S+1$ values $-S,\,-S+1,\ldots,S$, and $n(\epsilon_p)$ is the Fermi function. $Z(\theta)$ is defined as

$$Z(\theta)=\sum_{M=-S}^{S}e^{\theta M/T}\ .$$

As pointed out by Abrikosov,[7] the vertex function can be approximately decomposed as

$$\langle\xi\alpha|\,\Gamma(\epsilon_p;\ \lambda-S^z_{\alpha\alpha}\theta|\,\epsilon_q;\ \epsilon_p-\epsilon_q+\lambda-S^z_{\alpha\alpha}\theta)|\,\eta\beta\rangle$$
$$=t(\epsilon_p;\ \lambda-\theta|\,\epsilon_q;\ \epsilon_p-\epsilon_q+\lambda-\theta)\delta_{\xi\eta}\delta_{\alpha\beta}$$
$$+\vec{\sigma}_{\xi\eta}\cdot\vec{S}_{\alpha\beta}\,\tau(\epsilon_p;\ \lambda-\theta|\,\epsilon_p;\ \epsilon_p-\epsilon_q+\lambda-\theta)\ . \tag{5}$$

A more rigorous decomposition of Γ is given by More.[8] However, our present approximation assumes that the other scattering amplitudes are small compared to t and τ. Substituting (5) into (4) and after a lengthy manipulation we obtain

$$M=\mu_B g\langle S^z\rangle\left[1-\frac{J}{N}\rho\right.$$
$$\times\left(1+\theta\frac{\partial}{\partial\theta}\ln\langle S^z\rangle\right)-2\left(1+\theta\frac{\partial}{\partial\theta}\ln\langle S^z\rangle\right)\iint\frac{d^3p\,d^3q}{(2\pi)^3}$$
$$\times\left.|\tau(\epsilon_p;\ \lambda-\theta|\,\epsilon_q;\ \epsilon_p-\epsilon_q+\lambda-\theta)|^2\frac{n(\epsilon_p)n(-\epsilon_q)}{(\epsilon_p-\epsilon_q-\theta)^2}\right], \tag{6}$$

where $M=M_0+M_1+M_2$. To obtain (6), we have made the approximation by putting in M_2

$$(\epsilon_p-\epsilon_q+\theta)^{-1}\simeq(\epsilon_p-\epsilon_q-\theta)^{-1}\ .$$

It is very easy to check that this approximation does not destroy the logarithmic behavior of the integrations. In order to analyze M in a nonperturbative manner, we approximate the spin-flip vertex function by Suhl's spin-flip scattering amplitude $\tau(\epsilon_p,\,\theta)$. This approximation seems to be a good one in the calculation of the zero-field susceptibility.[2-4] We assume it should be a valid one even in the presence of a magnetic field. From Ref. 8, $|\tau(\epsilon_p;\ \theta)|^2$ has the form

$$|\tau(\epsilon_p,\,\theta)|^2=|\,F(\epsilon_p,\,\theta)|^2[1+a(\epsilon_p)|\,F(\epsilon_p,\,\theta)|^2]^{-1}\ , \tag{7}$$

where

$$a(\epsilon_p)=4\pi^2S(S+1)\rho^2(\epsilon_p)\ ,$$

$$F(\epsilon_p,\,\theta)=\frac{1}{\rho(\epsilon_p)}\left(\frac{N}{J\rho}-\int_{-1}^{1}\rho(x)\,dx\,\frac{\tanh[(x+\theta)/2T]}{x-\epsilon_p}\right),$$

and $\rho(\epsilon_p)$ is the density of states of conduction electrons given by

$$\rho(\epsilon_p)=\rho(1-\epsilon_p^2)^{1/2}\,,$$

with the Fermi energy $\epsilon_F=1$. Substituting (7) into (6) and carrying out the integrations, we obtain the following expression for M:

$$M=\mu_B g\langle S^z\rangle\left\{1-\frac{J}{N}\rho\left(1+\theta\frac{\partial}{\partial\theta}\ln\langle S^z\rangle\right)\right.$$
$$-\left(1+\theta\frac{\partial}{\partial\theta}\ln\langle S^z\rangle\right)\frac{1}{\pi(2S+1)}$$
$$\times\left.\left[\tan^{-1}\frac{N/J\rho}{\pi(2S+1)}-\tan^{-1}\frac{N/J\rho+2\ln\{\theta,\ T\}}{\pi(2S+1)}\right]\right\}. \tag{8}$$

In the given formula, the symbol $\{\theta,\ T\}$ denotes the largest of the indicated quantities, and $\langle S^z\rangle$ is given by (1) and (2); thus we have

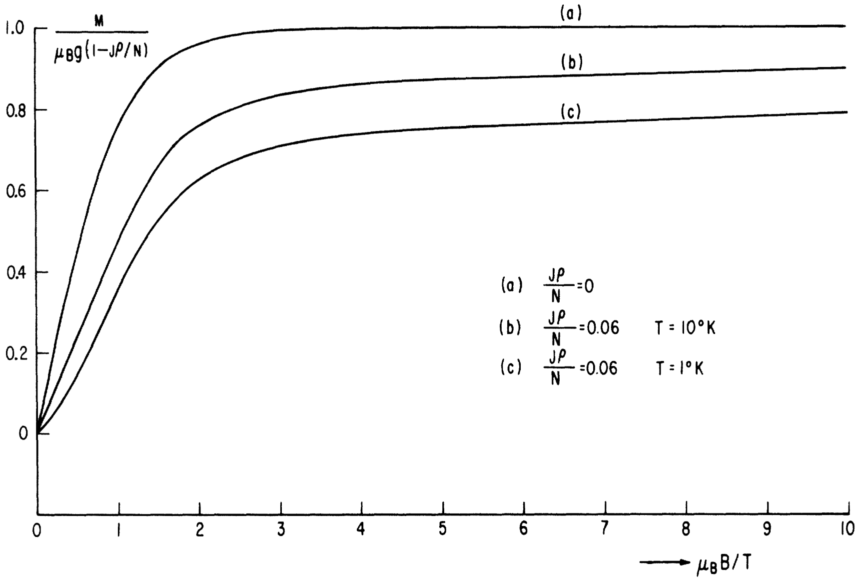

FIG. 2. Variation of the impurity magnetization as function of $\mu_B B/T$.

$$\theta\frac{\partial}{\partial\theta}\ln\langle S^z\rangle = \frac{\theta}{4T\langle S^z\rangle}\times\left[\operatorname{csch}^2\frac{\theta}{2T} - (2S+1)^2\operatorname{csch}^2\frac{(2S+1)\theta}{2T}\right].$$

In the limit $\theta = g\mu_B B \gg T > T_k$, we have

$$M = \mu_B g\langle S^z\rangle\left[1 - \frac{J\rho/N}{1 + (2J\rho/N)\ln(g\mu_B B)}\right]. \tag{9}$$

This is in agreement with the perturbation results of Giovanini *et al.*[1] In the limit $\theta \ll T$, we have

$$M = \mu_B g\langle S^z\rangle\left\{1 - \frac{2}{\pi(2S+1)}\left[\frac{\pi}{2} - \tan^{-1}\frac{N/J\rho + 2\ln T}{\pi(2S+1)}\right]\right\}. \tag{10}$$

This is in agreement with our susceptibility calculation.[3,4] The impurity spin magnetization $M(1 - J\rho/N)^{-1}$, which is normalized at large θ, has been plotted versus $\mu_B B/T$ from 0 to 10 for $S = \frac{1}{2}$ for two different coupling constants as shown in Fig. 2. The essential feature of the curve for $J \neq 0$ is that it does not show any saturated behavior at large $\mu_B B/T$ as is shown in the case for $J = 0$. The calculation agrees qualitatively with the experimental results of Kitchens and Graig[9] on the alloys of paramagnetic metals with Fe as impurity.

Finally we would like to point out that the method we have used is in the limit of the Abrikosov and Suhl approach; only the leading logarithmic term in each order of perturbation theory is included. Therefore our result is not a valid one for $T \ll T_K$ and $B \ll B_C$, where B_C is defined as $\mu_B g B_C = \exp(-N/2J\rho)$.

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