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Temperature Dependence of Magnetic Susceptibility in Dilute Magnetic Alloys

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For a system consisting of the conduction electrons and a localized spin which are coupled by the antiferromagnetic exchange interaction, $J<0$, magnetic susceptibility due to the spin has been considered by several authors.[1),2)] The closed form solution of Suhl's equation (or Nagaoka's equation) for the scattering t matrix was found.[3),4)] In this note, it will be shown that the magnetic susceptibility can be expressed, in terms of the scattering matrix, in an analytic form and the obtained result agrees with the Hamann's result at zero temperature for spin 1/2 impurities.

The Hamiltonian of the system is given by

$$H=\sum_{k,\mu}\xi_K C^*_{k\mu}C_{k\mu} + \frac{|J|}{2N}\sum_{\substack{KK'\\ \mu\mu'}}(\mu|\boldsymbol{\sigma}\cdot\boldsymbol{S}|\mu')C^*_{K\mu}C_{K'\mu'}\equiv H_0+H',$$

where $\boldsymbol{\sigma}$ is the Pauli matrix and ξ_K is the one-electron energy measured from the chemical potential. In what follows, the degenerate ground state of H and the unperturbed degenerate ground state of H_0 are denoted by $|\lambda\rangle$ and $|\lambda 0\rangle$, respectively. Simple calculations show that the double time Green's function, which is defined by

$$G_{k\mu\lambda,k\mu'\lambda'}(\omega)\equiv\frac{(-i)}{(2\pi)}\int_0^\infty e^{i\omega t}dt \times\langle\lambda'|[C_{k\mu'}(t),C^*_{k\mu}(0)]_+|\lambda\rangle$$
$$=\frac{\delta_{\mu\mu'}\delta_{\lambda,\lambda'}}{2\pi(\omega-\xi_K)}+\frac{1}{2\pi(\omega-\xi_K)^2}\times T^A_{k\mu'\lambda',k\mu\lambda}(\omega)\quad\text{for } k>k_F$$

(k_F is the Fermi wave number) and

$$\bar{G}_{k\mu\lambda,k\mu'\lambda'}(\omega)\equiv\frac{(-i)}{(2\pi)}\int_0^\infty e^{i\omega t}dt \times\langle\lambda'|[C^*_{k\mu'}(t),C_{k\mu}(0)]_+|\lambda\rangle$$
$$=\frac{\delta_{\mu\mu'}\delta_{\lambda,\lambda'}}{2\pi(\omega-|\xi_K|)}+\frac{1}{2\pi(\omega-|\xi_K|)^2}\times T^B_{k\mu'\lambda',k\mu\lambda}(\omega)\quad\text{for } k<k_F,$$

are related at zero temperature to the T matrix of the one-particle (or one-hole) scattering state as follows,*)

$$T^{A}_{k\mu'\lambda',k\mu\lambda}(\omega)=T^{S}_{k\mu'\lambda',k\mu\lambda}(\omega)$$
$$\equiv\langle\phi_{k\mu'\lambda'}|\frac{1}{\omega-H}-\frac{1}{\omega-H_0}|\phi_{k\mu\lambda}\rangle$$

and

$$T^{B}_{k\mu'\lambda',k\mu\lambda}(\omega)=-T^{S}_{k\mu'\lambda',k\mu\lambda}(\omega)$$
$$\equiv-\langle\phi_{k\mu'\lambda'}|\frac{1}{\omega-H}-\frac{1}{\omega-H_0}|\phi_{k\mu\lambda}\rangle, \tag{1}$$

where

$$|\phi_{k\mu\lambda}\rangle=\begin{cases}C^*_{k\mu}|\lambda\rangle & (k>k_F)\\ C_{k\mu}|\lambda\rangle & (k<k_F)\end{cases}$$

is the incident state of one-particle (or one-hole) state. Here we took the origin of the energy as $H|\lambda\rangle=0$ and $H_0|\phi_{k\mu\lambda}\rangle=|\xi_K||\phi_{k\mu\lambda}\rangle$. Let us assume that Eq. (1) essentially holds at finite temperature.**) Then, we obtain

$$\langle\lambda'|\sum_k C^*_{k\mu}C_{k\mu}|\lambda\rangle-\langle\lambda'0|\sum_k C^*_{k\mu}C_{k\mu}|\lambda0\rangle$$
$$=-\frac{1}{\pi}\int_{-\infty}^{\infty}\left(f(\omega)-\frac{1}{2}\right)d\omega$$
$$\times\mathrm{Im}\sum_k\frac{1}{(\omega-\xi_K)^2}T^{A}_{k\mu\lambda,k\mu\lambda'}(\omega)$$
$$=-\frac{1}{\pi}\int_{-\infty}^{\infty}\left(f(\omega)-\frac{1}{2}\right)d\omega$$
$$\times\mathrm{Im}\sum_k\langle\phi_{k\mu\lambda'}|\frac{1}{\omega-H}-\frac{1}{\omega-H_0}|\phi_{k\mu\lambda}\rangle, \tag{2}$$

where $f(\omega)$ is the Fermi function. Equation (2) reduces to

$$\langle\lambda'|\sum_k C^*_{k\mu}C_{k\mu}|\lambda\rangle-\langle\lambda'0|\sum_k C^*_{k\mu}C_{k\mu}|\lambda0\rangle$$
$$=\frac{1}{\pi}\int\left(\frac{\partial f(\omega)}{\partial\omega}\right)d\omega$$
$$\times\mathrm{Im}\{\sum_k\langle k|\ln\mathfrak{G}^S\mathfrak{G}_0^{-1}|k\rangle(P_0)_{\mu\lambda',\mu\lambda}$$
$$+\sum_k\langle k|\ln\mathfrak{G}^t\mathfrak{G}_0^{-1}|k\rangle(P_1)_{\mu\lambda',\mu\lambda}. \tag{3}$$

Here we used the notations

$$\langle\phi_{k\mu\lambda}|(\omega-H)^{-1}|\phi_{k\mu\lambda}\rangle$$
$$=\langle k|\mathfrak{G}^S|k\rangle(P_0)_{\mu\lambda',\mu\lambda}+\langle k|\mathfrak{G}^t|k\rangle(P_1)_{\mu\lambda',\mu\lambda}$$

and

$$\langle\phi^0_{k\mu\lambda}|(\omega-H_0)^{-1}|\phi^0_{k\mu\lambda}\rangle=\langle k|\mathfrak{G}^0|k'\rangle,$$

where P_1 and P_0 are the triplet and singlet projection operators

$$(P_1=(2S+1)^{-1}[S+1+(\boldsymbol{S}\cdot\boldsymbol{\sigma})],$$
$$P_0=(2S+1)^{-1}[S-(\boldsymbol{S}\cdot\boldsymbol{\sigma})])$$

and $|\phi^0_{k\mu\lambda}\rangle$ denotes the unperturbed one-particle (or one-hole) state. Equation (3) comes from the following operator equations:

$$(\omega-H)^{-1}=\frac{\partial}{\partial\omega}\log(\omega-H),$$
$$\log A=-\log(1/A),$$
$$\log(AP_0+BP_1)=(\log A)P_0+(\log B)P_1$$

and

$$\mathrm{Tr}\log AB=\mathrm{Tr}\log A+\mathrm{Tr}\log B.$$

Making the S-wave approximation

$$T^{A}_{k\mu\lambda,k'\mu'\lambda'}(\omega)$$
$$\equiv t^S(\omega)(P_0)_{\mu'\lambda',\mu\lambda}+t^t(\omega)(P_1)_{\mu'\lambda',\mu\lambda},$$

we have

$$\tfrac{1}{2}\langle\lambda'|\sum_k(C^*_{k\uparrow}C_{k\uparrow}-C^*_{k\downarrow}C_{k\downarrow})|\lambda\rangle$$
$$-\tfrac{1}{2}\langle\lambda'0|\sum_k(C^*_{k\uparrow}C_{k\uparrow}-C^*_{k\downarrow}C_{k\downarrow})|\lambda0\rangle$$
$$=(S_z)_{\lambda',\lambda}A, \tag{4a}$$

where

$$A=\frac{1}{\pi(2S+1)}\int\left(\frac{\partial f(\omega)}{\partial\omega}\right)d\omega\times$$

*) K. Kawamura already established this result at the meeting of physical society of Japan held in Hiroshima (1967).

) H. Suhl showed that this is correct by taking S-wave approximation [Physics **2 (1965), 39].

$$\times \mathrm{Im}\ \ln\left(\frac{1+F(\omega)t^S(\omega)}{1+F(\omega)t^t(\omega)}\right) \qquad (4b)$$

and

$$F(\omega)\equiv\sum_k(\omega-\xi_k)^{-1}.$$

According to Suhl's work,[5] the magnetic susceptibility χ due to a localized spin is expressed by*)

$$\chi/\chi_0=1+2A\,, \qquad (5)$$

where χ_0 is the free spin value. With the aid of the solution of Suhl's equation (or Nagaoka's equation), we have

$$\chi/\chi_0=1-\frac{2}{\pi(2S+1)}$$
$$\times \mathrm{Tan}^{-1}\frac{(2S+1)(\pi G(T))}{1-S(S+1)(\pi G(T))^2}, \qquad (6)$$

where

$$G(T)=\left(\log\frac{T}{T_K}\right.$$
$$\left.+\sqrt{\left(\log\frac{T}{T_K}\right)^2+S(S+1)\pi^2}\right)^{-1}$$

and

$$T_K=1.14D\exp\left(-\frac{1}{\rho|J|}\right),$$

D and ρ denoting the band width and the state density of conduction electrons, respectively. Equation (6) includes the following results:

$$\chi/\chi_0=1-\left(\log\frac{T}{T_K}\right)^{-1} \quad \text{for } T\gg T_K\,,$$

$$\chi/\chi_0=1-\frac{2}{(2S+1)}\left(1-\frac{(2S+1)}{2|\log(T/T_K)|}\right)$$
$$\text{for } T\ll T_K\,,$$

$$\chi(T_K)/\chi_0=1-\frac{1}{(2S+1)}$$

and

$$[\chi(T=\infty)-\chi(T_K)]$$
$$\div[\chi(T_K)-\chi(T=0)]=1\,.$$

1) D. J. Scalapino, Phys. Rev. Letters **16** (1966), 937.
2) D. R. Hamann, Phys. Rev. **158** (1967), 570.
3) J. Kondo, Prog. Theor. Phys. **40** (1968), 695.
4) P. E. Bloomfield and D. R. Hamann, **164** (1967), 856.
J. Zittarz and E. Müller-Hartmann, Z. Phys. **212** (1968), 380.
5) H. Suhl, *Rendiconti della Scuola Internazionale di Fisica Enrico Fermi XXXVII Corso* (Academic Press, Inc., New York, 1967).

*) H. Suhl took the approximation that the "renomalized" coupling constant f_r defined by $\langle\lambda|Sz|\lambda'\rangle=f_r(Sz)\lambda\lambda'$ is equal to 1. In this approximation, Eq. (5) is correct.