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Static Correlation Function in Dilute Alloys*

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The nonperturbative expression for the static correlation function, $\langle \vec{S}^{\rm el}(r)\cdot\vec{S}^{\rm imp}\rangle$, formulated in an earlier publication, is computed numerically. Our calculation shows that for large distances ($k_F^{-1} < r < D/T_K$) the static correlation function damps down much faster than $1/r^2$. This is in disagreement with the large-distance $-|a|[(\sin k_F r)/k_F r]^2$ behavior predicted by some recent calculations.

I. INTRODUCTION

The static correlation function (henceforth referred to as SCF) in dilute magnetic alloys has been subjected to extensive theoretical investigation in the last few years.[1-6] The SCF is of considerable physical importance, as a spatial average of this function describes the impurity contribution to the magnetic susceptibility in dilute alloys. In a recent publication, Fullenbaum and Falk[3] have examined the SCF on the basis of Nagaoka's theory[7] as well as the singlet-state theories due to Heeger and Jensen[8] and Applebaum and Kondo.[9] They found that for low temperatures the dominant behavior of

the SCF is given by $-|a|\,[(\sin k_F r)/k_F r]^2$ at large distances ($k_F r \gg 1$). Here k_F is the Fermi momentum and a is a constant. On the contrary, by iterating Nagaoka's decoupled Green's function we have found, apart from some oscillatory terms involving Si and Ci functions, a nonoscillatory ($-\text{const}\ J^2/r^3$) term in the second-order expression for the SCF. This nonoscillatory term was shown to be responsible for the well-known Kondo-type $\log(\epsilon_F/T)$ singularity in the susceptibility.[10,11] More recently, Keiter[12] has investigated this correlation function using a graphical perturbation technique. Keiter's leading two terms are in complete agreement with our perturbational calculation. The very-long-range $[(\sin k_F r)/k_F r]^2$ contribution to the SCF was also not found by Keiter.

One of the authors has derived a nonperturbational expression for the SCF based on Nagaoka's theory which is valid at all temperatures.[2] It was also demonstrated that in the high-temperature limit the nonperturbational expression for the SCF reproduces the perturbational results.[1,12] Unfortunately, the nonperturbational expression involves certain integrals containing t matrices which, to the authors' knowledge, are not possible to carry out analytically. The existing controversial theoretical results for the SCF, particularly at large distances, prompted us to carry out a detailed numerical calculation of the spatial behavior of the SCF in the nonperturbative regime ($T < T_K$) and to compare the results with different existing calculations. The paper is organized in the following way: In Sec. II we give a brief derivation of the nonperturbational expression for the SCF based on the Bloomfield-Hamann[13] solution for the Nagaoka equations. In Sec. III we give the results of our numerical analysis of the SCF and compare them with different calculations.

II. NONPERTURBATIONAL FORMALISM OF STATIC CORRELATION

Based on Nagaoka's theory, the SCF $\langle \vec{S}^{el}(r)\cdot\vec{S}^{imp}\rangle$ can be expressed as[7]

$$[\langle \vec{S}^{el}(r)\cdot\vec{S}^{imp}\rangle = \tfrac{2}{3}\sum_{\vec{k}\,\vec{k}'}\int_{-\infty}^{+\infty} d\omega f(\omega)\,[-2\,\mathrm{Im}\Gamma_{\vec{k}\vec{k}'}(\omega)] \times e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}, \tag{1}$$

where

$$\Gamma_{\vec{k}\vec{k}'}(\omega) = \langle C_{k'}, S_z + C_{k'}, S_- | C_k\rangle. \tag{2}$$

Our notation is the same as that of Nagaoka. After performing the ω integration in (1), the SCF can be expressed in terms of two basic functions, $G_A(\omega)$ and $\phi_A^1(\omega)$, as[2]

$$\begin{aligned}\langle \vec{S}^{el}(r)\cdot\vec{S}^{imp}\rangle = -\tfrac{4}{3}\sum_{\vec{k}\,\vec{k}'} e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}[2\pi(\epsilon_k-\epsilon_{k'})]^{-1}\{(1/\pi\rho\gamma)\mathrm{Re}\,[JG_A(\epsilon_k)-\phi_A^1(\epsilon_k)-JG_A(\epsilon_{k'})+\phi_A^1(\epsilon_{k'})]\\ +(J\pi/2N)[m_{\vec{k}'}-S(S+1)]\,[f(\epsilon_{k'})-f(\epsilon_k)]+(J/4N\gamma)[m_{k'}-S(S+1)]\\ \times \mathrm{Im}[JG_A(\epsilon_k)-\phi_A^1(\epsilon_k)-JG_A(\epsilon_{k'})+\phi_A^1(\epsilon_{k'})]\},\end{aligned} \tag{3}$$

where

$$n_k(\omega) = \tfrac{1}{2}[f(\omega)+\tfrac{1}{2}] + (2\pi\gamma)^{-1}\,\mathrm{Im}\,\phi_A^1(\omega), \tag{4}$$

$$m_k(\omega) = (2/\pi^2\gamma^2)\,\mathrm{Re}[JG_A(\omega)-\phi_A^1(\omega)], \tag{5}$$

$$JG_A(\omega) = \gamma\left[\frac{1}{2}\ln\frac{(\omega+D)\,(\omega-D)}{(2\pi i T)^2} - \psi\left(\frac{1}{2}+\frac{\omega}{2\pi i T}\right)\right]^*, \tag{6}$$

$$\phi_A^1(\omega) = -\{1+\delta+\gamma\,[X_R^2(\omega)+S(S+1)\pi^2]^{1/2}\,e^{-i\eta}\}^*. \tag{7}$$

In writing Eqs. (6) and (7) we have made use of the Bloomfield-Hamann solution for the Nagaoka theory. $\psi(\omega)$ is the digamma function and the expressions for $X_R(\omega)$ and $e^{-i\eta}$ can be found in Ref. 13. The nonperturbational expression for the SCF given by Eq. (3) is derived using the singular, nonlinear integral-equation representation of Nagaoka's decoupled Green's-function equations. It is to be noted that the above expression for the SCF does not depend on a specific solution of the integral equation.

III. NUMERICAL RESULTS AND DISCUSSION

We now proceed to compute Eq. (3) using Eqs. (4)–(7). In the calculation of the digamma function we have made use of the asymptotic expression

$$\psi(Z) \sim \ln z - \frac{1}{2Z} - \sum_{n=1}^{\infty}\frac{B_{2n}}{2nZ^{2n}}, \tag{8}$$

where the B_n's are the Bernoulli numbers. In carrying out the $\vec{k}$ summations we have taken a Lorentzian density of states for the conduction band of width $4\times10^4\,^\circ$K; the Kondo temperature $T_K = 18\,^\circ$K; the coupling constant $\gamma = -0.13533$; the magnitude of the impurity spin $S = \frac{1}{2}$; and the Fermi momentum $k_F \simeq 1.57\times10^8$ cm. To ensure the accuracy of our calculation we have divided the $\vec{k}$ summation regions into many parts with appropriate intervals. The calculation of the function $G_A(\omega)$ given by Eq. (6) is straightforward. The calculation of the function $\phi_A^1(\omega)$ is somewhat complicated, as it involves the

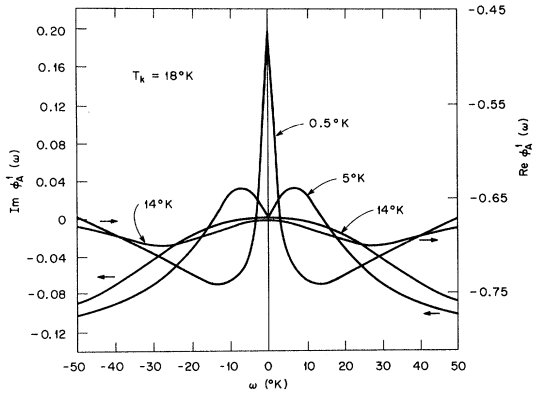

FIG. 1. The ω dependence of $\mathrm{Im}\phi_A^1(\omega)$ and $\mathrm{Re}\phi_A^1(\omega)$.

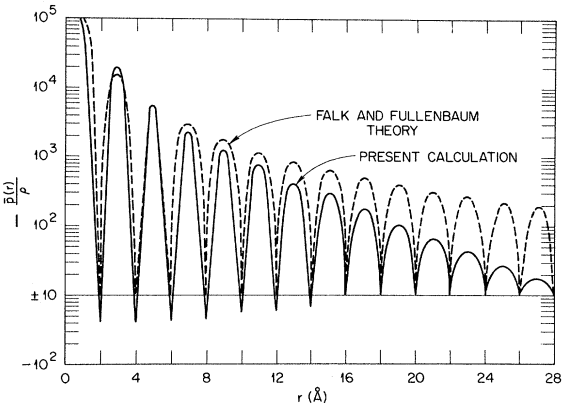

FIG. 2. Spatial dependence of the static correlation function $\bar{p}(r)$ for $T = 5\,^\circ\mathrm{K}$. The solid curve is given by the present calculation and the dotted curve is a $-[(\sin k_F r)/k_F r]^2$ plot normalized to the present value at $k_F r \simeq 8.5$.

phase factor $e^{-i\eta}$. The results of our calculation for $\mathrm{Im}\phi_A^1(\omega)$ and $\mathrm{Re}\phi_A^1(\omega)$ are plotted against ω for $T \gtrless T_K$ in Fig. 1. The double-peaked characteristic of $\mathrm{Im}\phi_A^1(\omega)$ is absent for $T \gtrsim T_K$. For low temperature $\phi_A^1(\omega)$ has a sharp peak near the origin. For $T \gg T_K$, $\phi_A^1(\omega)$ is practically structureless. The structure of $\phi_A^1(\omega)$ is confined within a very narrow energy region ($\sim 200\,^\circ\mathrm{K}$). Once $G_A(\omega)$ and $\phi_A^1(\omega)$ functions are computed, the calculations of $n_k(\omega)$ and $m_k(\omega)$ are trivial. Finally, we calculate the SCF [referred to in the figure as $\bar{p}(r)$] given by Eq. (3) for different distances from the impurity. The spatial dependence of the SCF for temperature $T = 5\,^\circ\mathrm{K}$ is shown in Fig. 2. In order to compare our results with those of Fullenbaum and Falk[3] and others,[4,6] we have plotted the function $-|a|[(\sin k_F r)/k_F r]^2$ normalized to our value at $k_F r \simeq 8.5$. It is evident from our calculation that the static correlation function is an oscillatory function with respect to distance from the impurity, having a very large amplitude in one half-side compared with the other half. However, near the impurity, $\bar{p}(r)$ has a small but finite amplitude on the positive side. Our calculation shows that for large distances, $\bar{p}(r)$ damps down much faster than $1/r^2$. Therefore, we conclude that the *very*-long-range $-[(\sin k_F r)/k_F r]^2$ behavior of the SCF in dilute magnetic alloys for distances $k_F^{-1} < r < D/T_K$ predicted by Fullenbaum and Falk[3] and others[4-6] is in direct disagreement with our numerical calculation for the nonperturbational expression for the SCF as well as with systematic perturbational calculations.[1,2]

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