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Spin and charge correlations around an Anderson magnetic impurity

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We have studied the correlations between an Anderson magnetic impurity and its surrounding conduction electrons using a Monte Carlo simulation technique. Results for spin and charge correlations for a symmetric Anderson impurity in a free-electron continuum are presented. Our results show the spatial structure of the spin-compensation cloud that forms around the magnetic impurity as the temperature is lowered, and the suppression of the charge-density correlations caused by the Kondo effect.

I. INTRODUCTION

While renormalization-group calculations[1] and Bethe-ansatz solutions[2] have provided detailed information on the thermodynamic properties of magnetic impurities in metals, these methods so far have been unable to provide information about correlation functions involving an impurity and the surrounding conduction electrons. On the other hand, perturbation theory has predicted results for the structure and temperature dependence of the spin-compensation cloud surrounding the impurity that are controversial,[3] so that a nonperturbative approach to compute these quantities is desirable.

In this paper we describe a quantum Monte Carlo procedure for obtaining these correlations. Previous quantum Monte Carlo calculations either were unable to achieve sufficiently low temperatures for interpretive study of the scaling (Kondo) regime,[4] or while achieving low temperatures, focused mainly on the self-correlations of the impurity.[5] Here we point out a procedure, implicit in Ref. 5, that generates a straightforward algorithm for going beyond self-correlations and permits the calculation of the spatial dependence of the correlations between the spin and charge at the impurity with those in conduction states. In Sec. II we present the method, and in Sec. III we present results for the symmetric Anderson model. We conclude in Sec. IV with a short discussion of the significance of these results.

II. FORMULATION

We consider the single-impurity Anderson model:

$$H=\sum_{k,\sigma}\varepsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+\sum_{k,\sigma}V_k(c_{k\sigma}^{\dagger}d_\sigma+\text{H.c.})+\varepsilon_d\sum_{\sigma}n_{d\sigma}+Un_{d\uparrow}n_{d\downarrow}\ . \tag{1}$$

In a path-integral formulation of its thermodynamics,[6] we divide the temperature axis into L slices of size $\Delta\tau=\beta/L$ and eliminate the interaction term in the Hamiltonian by introducing auxiliary Ising variables $\sigma(l)$ (one per time slice).[7] The partition function becomes

$$Z=\mathrm{Tr}_{\{\sigma(l)\}}\exp\left[-\sum_{\mu=\pm1}\mathrm{Tr}\ln g_\mu[\sigma]\right]\ , \tag{2}$$

where g_μ ($\mu=\pm1$ denotes electron spin) is the Green's function. Different Ising configurations give rise to different potentials. The Green's functions for two different configurations are connected by the Dyson equation[5]

$$g'=g+(g-1)(e^{V'-V}-1)g' \tag{3a}$$

and its transpose

$$g'=g+(g'-1)(1-e^{-V'+V})g\ . \tag{3b}$$

The potentials act only on the impurity orbital $|d\rangle$ and are given by

$$V_l^{\mu}=\lambda\mu\sigma(l)\,|\,d\,\rangle\langle\,d\,| \tag{4}$$

with $\cosh(\lambda)=\exp(\Delta\tau U/2)$. Here, l denotes the time-slice index, $1\le l\le L$.

Equations (3) are matrix equations in space and imaginary time. From them we can obtain arbitrary correlation functions in terms of the d-electron Green's function g_{dd} for the fully interacting case and the Green's functions g^0 in the absence of the Coulomb interaction $Un_{d\uparrow}n_{d\downarrow}$. Taking one of the potentials in Eq. (3) as zero and the other due to an actual spin configuration, we have

$$g_{id}=g_{id}^0+g_{id}^0(e^{V}-1)g_{dd}\ , \tag{5a}$$

$$g_{di}=g_{di}^0+(g_{dd}-1)(1-e^{-V})g_{di}^0\ , \tag{5b}$$

$$g_{ij}=g_{ij}^0+g_{id}^0(e^{V}-1)g_{dj}\ , \tag{5c}$$

where i and j refer to positions in space around the impurity. Equations (5) are matrix equations in the time variables ($L \times L$ matrices). From these Green's functions one can obtain all spin and charge correlations. For example, the correlation between the impurity spin and conduction-electron spin at position r_i is given by

$$S(r_i) = \langle\langle \sigma_d^z \sigma^z(r_i) \rangle\rangle = \langle\langle (d_\uparrow^\dagger d_\uparrow - d_\downarrow^\dagger d_\downarrow)(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) \rangle\rangle \ . \tag{6}$$

Here the double angular brackets represent a trace over the fermion variables and an average over σ configurations. Using Wick's theorem to carry out the trace over fermion variables, we obtain

$$S(r_i) = \langle (g_{dd\uparrow} - g_{dd\downarrow})(g_{ii\uparrow} - g_{ii\downarrow}) \rangle - \langle g_{id\uparrow} g_{di\uparrow} + g_{id\downarrow} g_{di\downarrow} \rangle \ , \tag{7}$$

where the single angular bracket denotes an average over the σ configurations. For charge correlations we have

$$C(r_i) = \langle\langle n_d n_c(r_i) \rangle\rangle = \langle (2 - g_{dd\uparrow} - g_{dd\downarrow})(2 - g_{ii\uparrow} - g_{ii\downarrow}) \rangle - \langle g_{id\uparrow} g_{di\uparrow} + g_{id\downarrow} g_{di\downarrow} \rangle \ . \tag{8}$$

As discussed elsewhere,[5,6] the Monte Carlo procedure attempts flips at each time slice l of the σ field and accepts or discards the flip depending on whether the ratio of the determinant $R = R_\uparrow R_\downarrow$ with

$$R_\mu = 1 + [1 - g_{dd}^\mu(l,l)]\{\exp[V_l^\mu(\sigma_{l'}) - V_l^\mu(\sigma_l)] - 1\} \tag{9}$$

is larger or smaller than a random number between 0 and 1. If the move is accepted, all time components of the d Green's function are updated through the relation

$$g'_{dd}(l_1,l_2) = g_{dd}(l_1,l_2) + \frac{[g_{dd}(l_1,l) - \delta(l_1,l)](e^{V_l' - V_l} - 1) g_{dd}(l,l_2)}{1 + [1 - g_{dd}(l,l)][\exp(V_l' - V_l) - 1]} \ . \tag{10}$$

The unperturbed Green's functions are given by

$$g^0(l,l') = T \sum_n e^{-i\omega_n \Delta\tau(l-l')} g^0(i\omega_n) \ , \tag{11}$$

with

$$g_{dd}^0(i\omega_n) = -\frac{1}{i\omega_n - \left[e_d + \frac{U}{2}\right] + \Delta(i\omega_n)} \ , \tag{12a}$$

$$g_{id}^0(i\omega_n) = f_2(r_i, i\omega_n) g_{dd}^0(i\omega_n) = g_{di}^0(i\omega_n) \ , \tag{12b}$$

$$g_{ij}^0(i\omega_n) = -f_1(i\omega_n) + f_2(r_i, i\omega_n) f_2(-r_j, i\omega_n) g_{dd}^0(i\omega_n) \ , \tag{12c}$$

where

$$\Delta(i\omega_n) = \sum_k \frac{|V_k|^2}{i\omega_n - \varepsilon_k} \ , \tag{13a}$$

$$f_1(i\omega_n) = \frac{1}{N} \sum_k \frac{1}{i\omega_n - \varepsilon_k} \ , \tag{13b}$$

$$f_2(r_i, i\omega_n) = \frac{1}{\sqrt{N}} \sum_k \frac{V_k e^{ikr_i}}{i\omega_n - \varepsilon_k} \ . \tag{13c}$$

These functions were evaluated in the following manner. For a wide structureless band with V_k independent of k ($V_k = V/\sqrt{N}$), we have

$$\Delta(i\omega_n) = i\pi V^2 N(0) \mathrm{sgn}(\omega_n) \ , \tag{14a}$$

$$f_1(i\omega_n) = -i\pi N(0) \mathrm{sgn}(\omega_n) \ , \tag{14b}$$

with $N(0)$ the energy density of states per spin at the Fermi energy. For f_2 we need the energy dispersion relation. For an isotropic case with V_k independent[8] of k ($V_k = V/\sqrt{N}$) and for an electron dispersion relation:

$$\varepsilon_k = \frac{k^2}{2m} - \mu \ ,$$

one obtains

$$f_2(r, i\omega_n) = -\frac{V k_F^3}{4\pi (k_F r)\mu} e^{i[1 + (i\omega_n/\mu)] |k_F r|} \ . \tag{15}$$

III. RESULTS

Here we report results for the particle-hole symmetric Anderson model in which $\varepsilon_d = -U/2$. We used units such that the full width of the resonance $2\Delta = 2\pi N(0) |V|^2 = 1$. Simulations for values of $U = 0$, 1, 2, and 4 were done. The corresponding Kondo temperatures for the $U > 0$ cases, obtained from the Bethe ansatz solution,[2] are $T_K = 0.169$, 0.0865, and 0.0216, respectively. A typical Monte Carlo run involved 5000 sweeps through the lattice, and the statistical error for the quantities measured was negligible except where shown. The finite time slice $\Delta\tau$ introduces a systematic error. Simulations with $\Delta\tau = 0.25$ and 0.5 gave results which only differed by a few percent.

As the temperature is lowered, charge fluctuations are suppressed, and the d electrons start to localize and develop a moment. This is shown in Fig. 1(a), where we plot

$$\langle (\sigma_z^d)^2 \rangle = \langle (n_{d\uparrow} - n_{d\downarrow})^2 \rangle \tag{16}$$

versus temperature. The local moment forms at a temperature $T \sim \Delta$ and is stable below that temperature. Its magnitude is a smoothly increasing function of U and tends to unity as $U \rightarrow \infty$ for T small compared with Δ. For $U = 0$, $\langle (\sigma_z^d)^2 \rangle = 0.5$ at all temperatures since we are treating the symmetric case.

For a wide, flat band, where $\sum_k |V_k|^2/(i\omega_n - \varepsilon_k)^2$ is negligible, the total conduction-electron spin polarization in the presence of a small magnetic field H is unaffected by the presence of the impurity and one finds that

$$\frac{\partial}{\partial H}\int \langle n_\uparrow(r)-n_\downarrow(r)\rangle d^3r\Bigg|_{H=0} = \frac{\partial}{\partial H}\int \langle n_\uparrow(r)-n_\downarrow(r)\rangle_0 d^3r\Bigg|_{H=0} . \quad (17)$$

Here $\langle\ \rangle_0$ implies an average for a free-electron system. This is the Clogston-Anderson *compensation theorem.*[9] It implies that the total magnetic susceptibility due the impurity can be written as

$$\chi_d = \int_0^\beta d\tau \langle \sigma_z^d(\tau)\sigma_z^d(0)\rangle , \quad (18)$$

where χ_d is in units of $(g\mu_\beta/2)^2$ and $\sigma_z^d = n_{d\uparrow} - n_{d\downarrow}$.

Figure 1(b) shows $T\chi_d$ versus T. As T decreases below Δ and the moment $\langle(\sigma_z^d)^2\rangle$ forms, the susceptibility due to the impurity initially varies as $\langle(\sigma_z^d)^2/T$. However, as T approaches the Kondo temperature T_K, correlations between the d-electron spin and the conduction-electron spins start to screen the impurity moment and as $T\to 0$ the susceptibility vanishes. It is important to realize that Eqs. (16) and (17) do not imply an absence of correlation between the localized spin and the surrounding conduction-electron spins. On the contrary, it follows directly from them that

$$\chi_d = \frac{1}{T}\left[\langle(\sigma_z^d)^2\rangle + \int \langle \sigma_z^d \sigma_z(r)\rangle d^3r\right] . \quad (19)$$

Thus, an effective moment

$$\mu_{\rm eff}^2(T) = \langle(\sigma_z^d)^2\rangle + \int \langle \sigma_z^d\sigma_z(r)\rangle d^3r \quad (20)$$

is formed from the impurity moment and its spin compensation cloud.

Rewriting Eq. (18) we have for the contribution to this effective moment from the spin compensation cloud

$$S(T) = \int \langle \sigma_z^d \sigma_z(r)\rangle d^3r = T\chi_d - \langle(\sigma_z^d)^2\rangle . \quad (21)$$

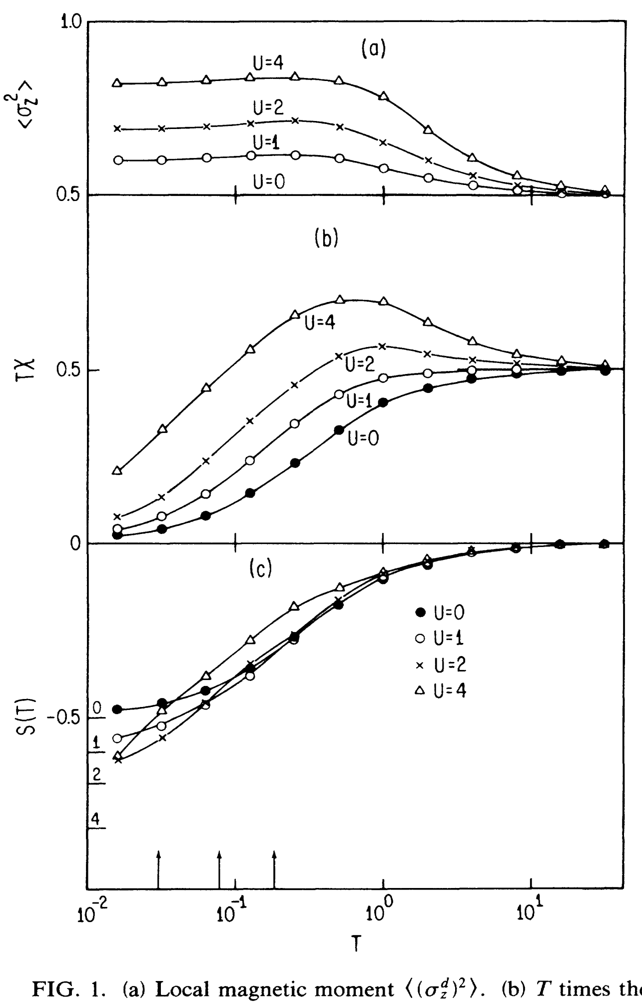

FIG. 1. (a) Local magnetic moment $\langle(\sigma_z^d)^2\rangle$. (b) T times the spin susceptibility and (c) contribution to effective moment from spin compensation cloud [Eq. (21)] for a single symmetric Anderson impurity; $\Delta=0.5$, $U=0$, 1, 2, and 4. The arrows indicate the corresponding Kondo temperatures. The Monte Carlo data are obtained at temperatures $\beta=2^n$, n is an integer.

Figure 1(c) shows $S(T)$ versus T. At temperatures well below T_K, $T\chi_d\to 0$ and $S(T)$ approaches $-\langle(\sigma_d^z)^2\rangle$. In this limit, the spin compensation cloud quenches the local moment leaving a ground-state singlet. For $U=0$, the d-orbital moment $\langle(\sigma_d^z)^2\rangle=0.5$ of the resonance is also quenched as $T\to 0$ by Fermi hole correlations in the surrounding conduction-electron sea. In this case, these correlations vanish on a temperature scale set by the width of the resonance Δ. For $U>0$, there are dynamic correlations as well as Fermi hole correlations which drive S to the significantly more negative $T=0$ value which is needed to quench the d spin. Figure 1(c) shows that the part of the spin compensation cloud produced by dynamic correlations evaporates on a scale set by T_K and, in fact, $S(T)$ is actually reduced from its $U=0$ value at intermediate temperatures. This latter feature reflects the Coulomb modification of the d-electron spectral weight which we will discuss further in our analysis of charge correlations.

In order to examine the spin and charge correlations in more detail, we have numerically calculated $S(r)$ and $C(r)$. Before examining these results for $U\neq 0$, it is useful to consider the $U=0$ case for which

$$C(r) = S(r) + \langle n(r)\rangle \quad (22)$$

and

$$S(r) = -\frac{8\pi\Delta N(0)}{y^2}F^2(y) , \quad (23)$$

with $y=k_F r$ and

$$F(y) = \mathrm{Im}\left[T\sum_{n\,(\geq 0)} \frac{e^{iy[1+(i\omega n/\mu)]}}{\omega_n+\Delta}\right] . \quad (24)$$

Here n_0 is the conduction-electron density $(k_F^3/3\pi^2)$, $\Delta=\pi V^2 N(0)$, and $\mu k_F^2/2m$. When $T\to 0$,

$$F(y) = \mathrm{Im}\int_0^\infty \frac{d\omega}{2\pi}\,\frac{e^{iy[1+(i\omega/\mu)]}}{\omega+\Delta} . \quad (25)$$

Over a wide range of $k_F r$ values, Eq. (25), can be approximated as

$$F(g) \simeq \sin y \int_0^\infty \frac{d\omega}{2\pi} \frac{e^{-y\omega/2\mu}}{\omega+\Delta}$$
$$= \frac{\sin y}{2\pi} e^{(\Delta/2\mu)y} E_1(\Delta y/2\mu) \ . \tag{26}$$

Here $E_1(x)$ is the exponential integral which has the limiting forms

$$E_1(x) \cong \gamma + \ln(x) \ , \quad x \ll 1 \tag{27a}$$

$$E_1(x) \cong \frac{e^{-x}}{x} \left[1 - \frac{1}{x} + \frac{2!}{x^2} - \frac{3!}{x^3} + \cdots \right] , \quad x \gg 1 \tag{27b}$$

with $\gamma = 0.577$, Euler's constant. Equation (27b) leads to the asymptotic result[10]

$$S(r) \cong -\frac{2}{\pi^3} \frac{\mu}{\Delta k_F} \frac{\sin^2(k_F r)}{r^4} \ , \tag{28}$$

which is valid when $k_F r$ is large compared to $2\mu/\Delta$.

In Fig. 2(a) we have plotted $4\pi(k_F r)^2 S(r)/n_0$ versus $k_F r$ for $\mu = 1$, $\Delta = 0.5$, and $T = 0$. Here the spin density has been normalized with respect to the electron density $n_0 = k_F^3/3\pi^2$. The dot-dashed curve is the envelope of the approximate result obtained from Eq. (26). The short-dashed curve and the long-dashed curve correspond to the limiting forms Eq. (27a) and Eq. (27b), respectively. We see that the bulk of the correlations lay inside the region where the asymptotic form, Eq. (28), is applicable. We have also calculated $S(r)$ at finite temperature using Eq. (24) and find that the correlations are exponentially damped on a length scale set by the thermal length v_F/T. Figure 2(b) shows similar results for $\mu = 6$, $\Delta = 0.5$, and $T = 0$. In this case, $2\mu/\Delta = 24$ and the region shown is well inside the asymptotic region appropriate to Eq. (29).

Integrating $S(r)$ we have

$$I(y) = \int_{k_F r \le y} d^3 r S(r) \tag{29}$$

for the spin compensation contained inside of a radius $k_F r = y$. For $U = 0$ at $T = 0$, we have from the sum rule, Eq. (21), $I(\infty) = S(0) = -0.5$. The function $I(y)$ versus y is plotted in Figs. 3(a) and 3(b) for $\mu = 1$ and 6, respectively. From these curves we find that of order 70% of the spin compensation is contained inside the region $k_F r = 2\mu/\Delta$. When $U \neq 0$, we use the same 70% criterion to characterize the size of the spin compensation cloud.

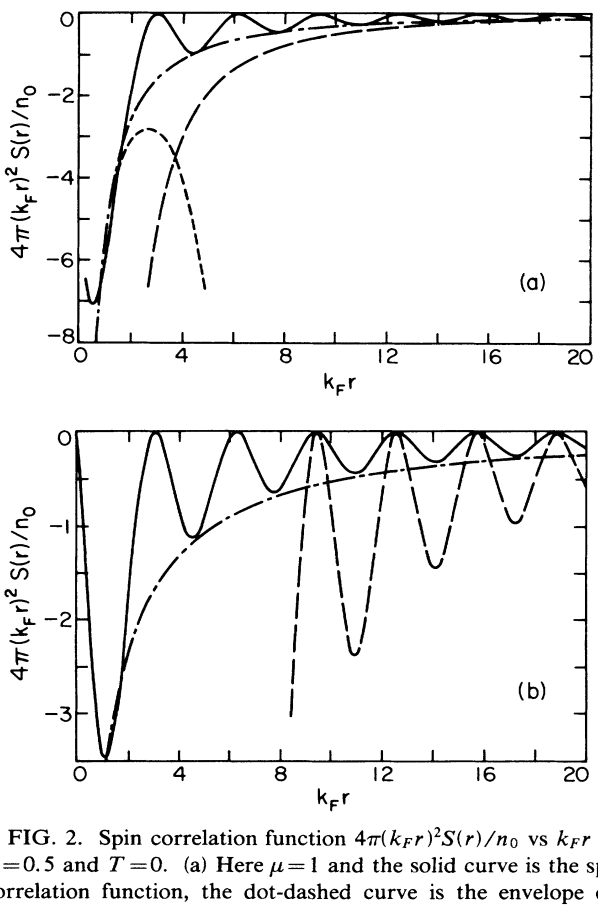

FIG. 2. Spin correlation function $4\pi(k_F r)^2 S(r)/n_0$ vs $k_F r$ for $\Delta = 0.5$ and $T = 0$. (a) Here $\mu = 1$ and the solid curve is the spin correlation function, the dot-dashed curve is the envelope obtained from Eq. (26), and the short dashed curve and the dashed curve correspond to the short and long distance approximate forms, Eqs. (27a) and (27b), respectively. (b) Here $\mu = 6$ corresponding to a bandwidth large compared to Δ.

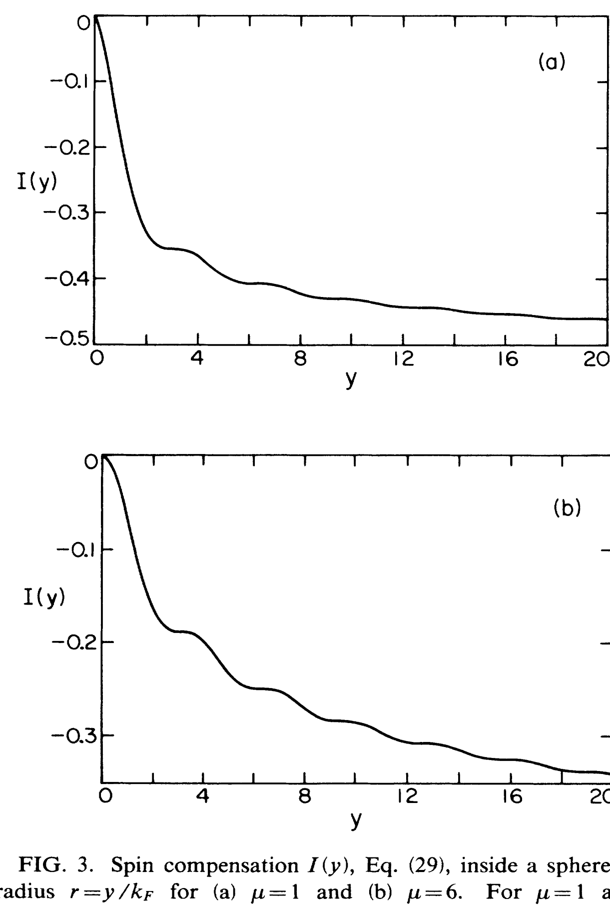

FIG. 3. Spin compensation $I(y)$, Eq. (29), inside a sphere of radius $r = y/k_F$ for (a) $\mu = 1$ and (b) $\mu = 6$. For $\mu = 1$ and $\Delta = 0.5$, $2\mu/\Delta = 4$, while for $\mu = 6$, $2\mu/\Delta = 24$.

We find, as originally discussed by Mezei and Grüner[11] for the charge correlations and Ishii[10] for the spin correlations, that the Kondo resonance which arises for $U \neq 0$ leads to an extension of these correlations to a region set by $2\mu/T_K$ when $T < T_K$.

Using the approach discussed in Sec. II, we have calculated $S(r)$ for various values of the Coulomb interaction U and the temperature T. Figure 4 shows the spatial dependence of the spin correlations $4\pi(k_F r)^2 S(r)/n_0$ for $\mu=6$ and $U=0$, 1, 2, and 4 at temperatures $\beta=8$, 16, and 32. Qualitatively, the spin correlations are not dramatically changed by the presence of U; in particular, the phase and period of the oscillations remain the same. For $U=0$, the correlations are always negative, while for a finite U, ferromagnetic correlations are induced in some regions. At short distances a small U enhances negative spin correlations, but a larger U actually makes them smaller. For $U=4$ and $\beta=8$, the spin correlations at short distances are smaller than for $U=0$, and they become larger as β increases. Only for large distances at the lowest temperature ($\beta=32$) are the antiferromagnetic correlations monotonically increasing with U. In contrast, the ferromagnetic correlations are always monotonically increasing with U. For $\mu=6$, the range of $k_F r$ values shown lay well inside the thermal decay length μ/T.

In Fig. 5 we plot the same data as in Fig. 4 in a way that displays more clearly the temperature dependence. As U increases the temperature dependence becomes stronger, as one would expect: for $U=0$ the relevant temperature scale is Δ, while for $U \neq 0$ it is T_K. However, the ferromagnetic spin correlations are essentially temperature independent. A direct spatial integration of $\langle \sigma_z^d \sigma_z(r) \rangle$ gives results for $S(T)$, Eq. (21), which agree with the sum rule $T\chi_d - \langle (\sigma_z^d)^2 \rangle$, numerically confirming the compensation theorem. The scale over which 70% compensation is obtained is set by $2\mu/T_K$ in agreement with Ishii's result.[10]

We have also studied the effect of the Fermi energy (bandwidth) on the spin correlations. Figure 6 shows results for $\mu=1$. For this value of μ, the thermal decay length is set by β, and we see that the long-distance correlations are washed out as β decreases from 32 to 8. We also see that for $\mu=1$, the region in which the antiferromagnetic correlations monotonically increasing with U occurs at shorter distances than in the previous case. We find that 70% spin compensation, Eq. (29), occurs over a range set by $2\mu/T_K$ which is approximately 12, 23, and 92 for $U=1$, 2, and 4, respectively.

These results for $S(r)$ show that the d-site Coulomb interaction U produces ferromagnetic correlations which are independent of temperature for $T < \Delta$ and antiferromagnetic correlations which are fully established only for $T < T_K$ where they lead to the spin compensation shown in Fig. 1(c). These latter correlations are associated with the development of the spin-compensation cloud and eventually the formation of a ground-state singlet. In order to obtain more insight into the ferromagnetic correlations which arise when $U \neq 0$, it is useful to write the spin correlation function in terms of the spin-up and spin-down charge-density operators:

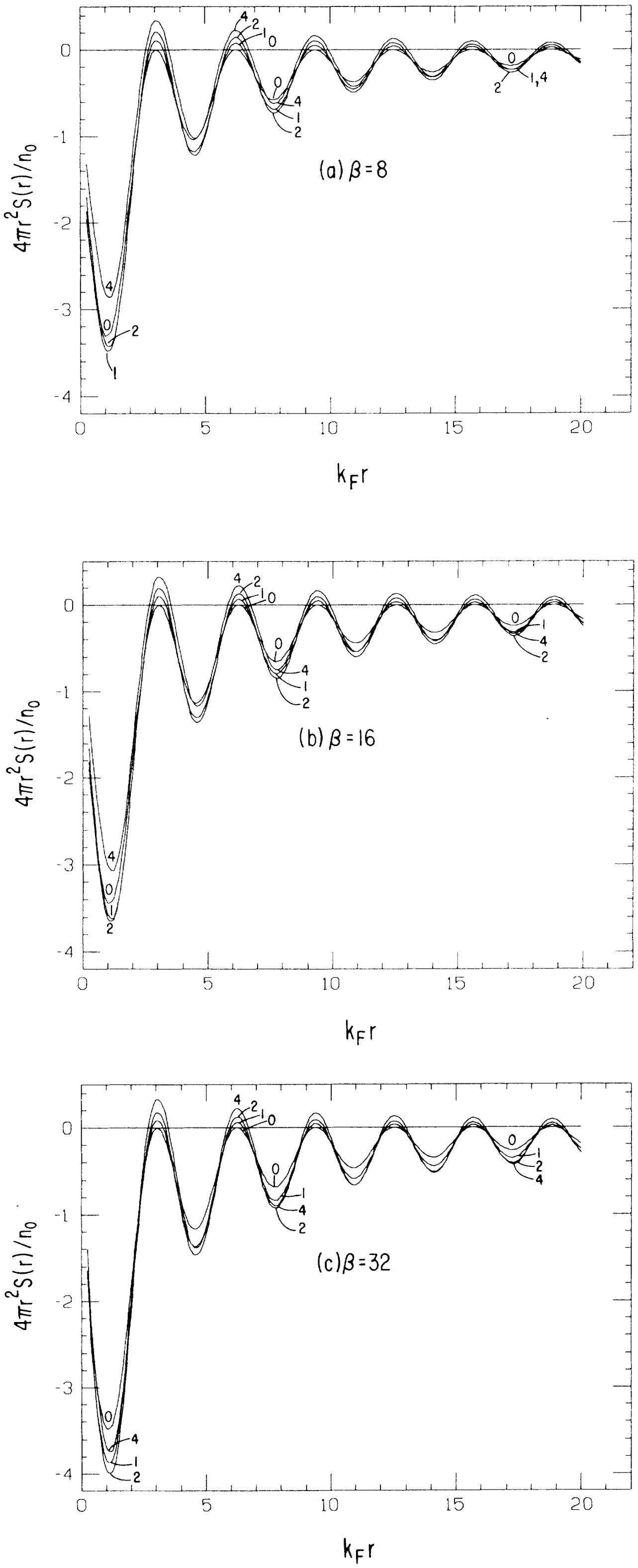

FIG. 4. Spatial dependence of impurity-spin–conduction-electron-spin correlations $S(r)$, Eq. (6), multiplied by $4\pi k_F^2 r^2/n_0$ for $\mu=6$, $U=0$, 1, 2, and 4 and (a) $\beta=8$, (b) $\beta=16$, and (c) $\beta=32$. The inverse Kondo temperatures $1/T_K$ are $\beta_K=5.9$, 11.6, and 46.3 for $U=1$, 2, and 4, respectively.

$$S(r)=2[\langle n_{d\uparrow}n_{\uparrow}(r)\rangle-\langle n_{d\downarrow}n_{\uparrow}(r)\rangle]\ . \tag{30}$$

For $U=0$,

$$\langle n_{d\uparrow}\rangle\langle n_{\uparrow}(r)\rangle-\langle n_{d\downarrow}\rangle\langle n_{\uparrow}(r)\rangle=0 \tag{31}$$

and $S(r)$ is determined entirely by the exchange contribution arising from the Pauli principle, Eq. (23). Thus the structure of $S(r)$ in Fig. 5(a) simply reflects the Fermi hole in $n_{\uparrow}(r)$ created around the impurity when $n_{d\uparrow}$ is occupied. In the presence of U, both terms in Eq. (30) are modified. In lowest order the correction to $S(r)$ arises from the second term

$$\langle n_{d\downarrow}n_{\uparrow}(r)\rangle=\langle n_{d\downarrow}\rangle\langle n_{\uparrow}(r)\rangle -U\int_0^{\beta}d\tau\langle n_{d\uparrow}(\tau)n_{\uparrow}(r)\rangle\langle n_{d\downarrow}(\tau)n_{d\downarrow}\rangle\ . \tag{32}$$

Physically, in the presence of U, the occupation of the d site by a down spin repels d spin-up electron density, giving rise to the ferromagnetic correlations shown in Figs. 5(b) and 5(c). This part of the response is set by the polarization which, as shown in Ref. 5, reaches its low temperature value when β is large compared with Δ^{-1}.

We now discuss the spatial dependence of the charge correlations described by $C(r)$, Eq. (8). As for the spin operators, we normalized the charge operators by n_0 and for convenience subtracted from C its asymptotic limit $\langle n(\infty)\rangle=n_0$ so the resulting correlation function decays to zero. Figure 7 shows that there is a large suppression of the Friedel-like oscillations as U increases. This effect was originally discussed by Mezei and Grüner.[11] They argued that the conduction-electron charge-density oscillations are reduced due to the change in the d-electron spectral weight in the Kondo regime. At low temperatures, the d-electron spectra weight develops a narrow resonance having a width of order T_K at the Fermi energy. For distances less than v_F/T_K, the charge density oscillations are suppressed. They recover gradually to the full Freidel value at large distances at zero temperature. At

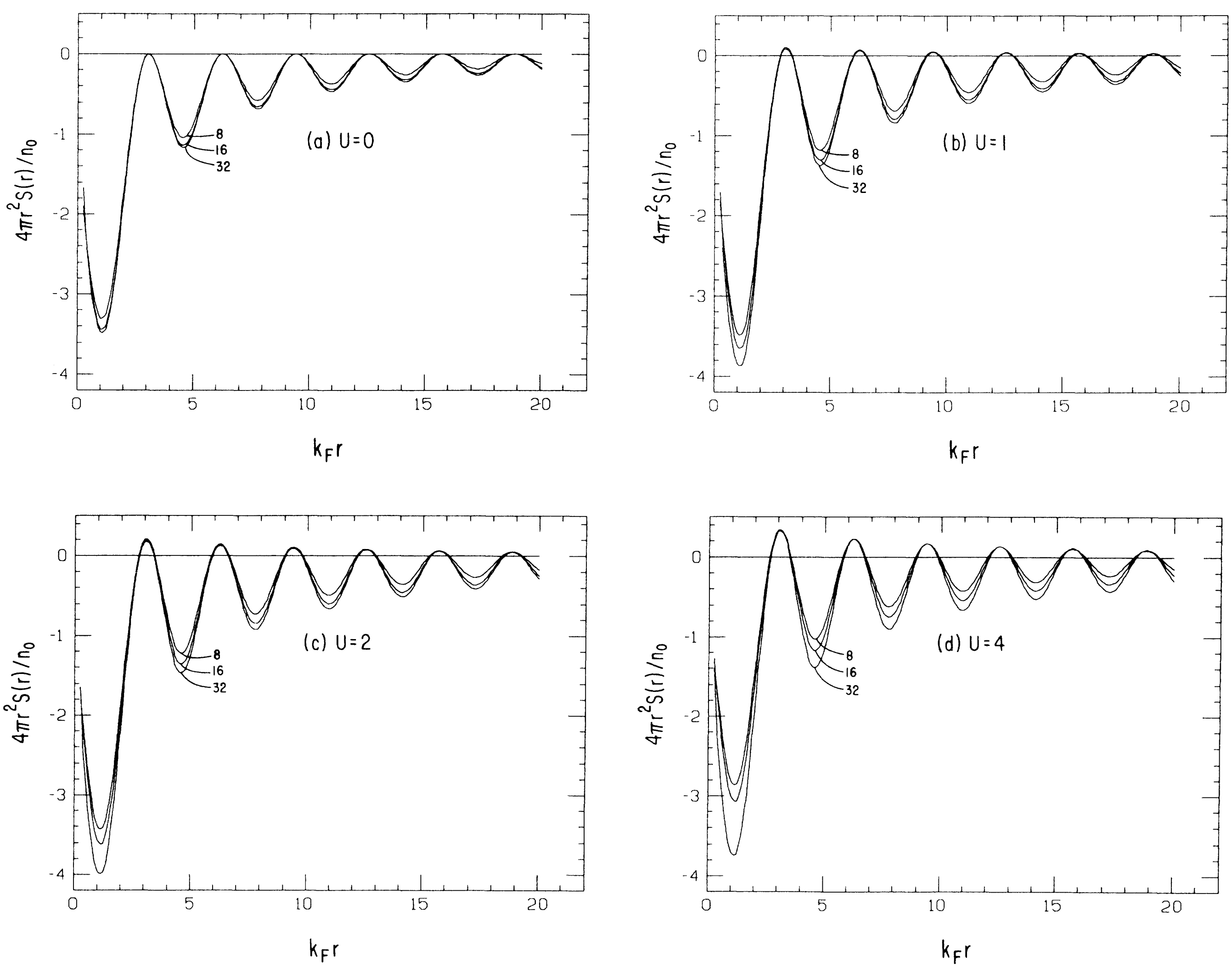

FIG. 5. Spin-spin correlations $4\pi k_F^2 r^2 S(r)/n_0$ for $\mu=6$, $\beta=8$, 16, and 32 and (a) $U=0$, (b) $U=1$, (c) $U=2$, and (d) $U=4$.

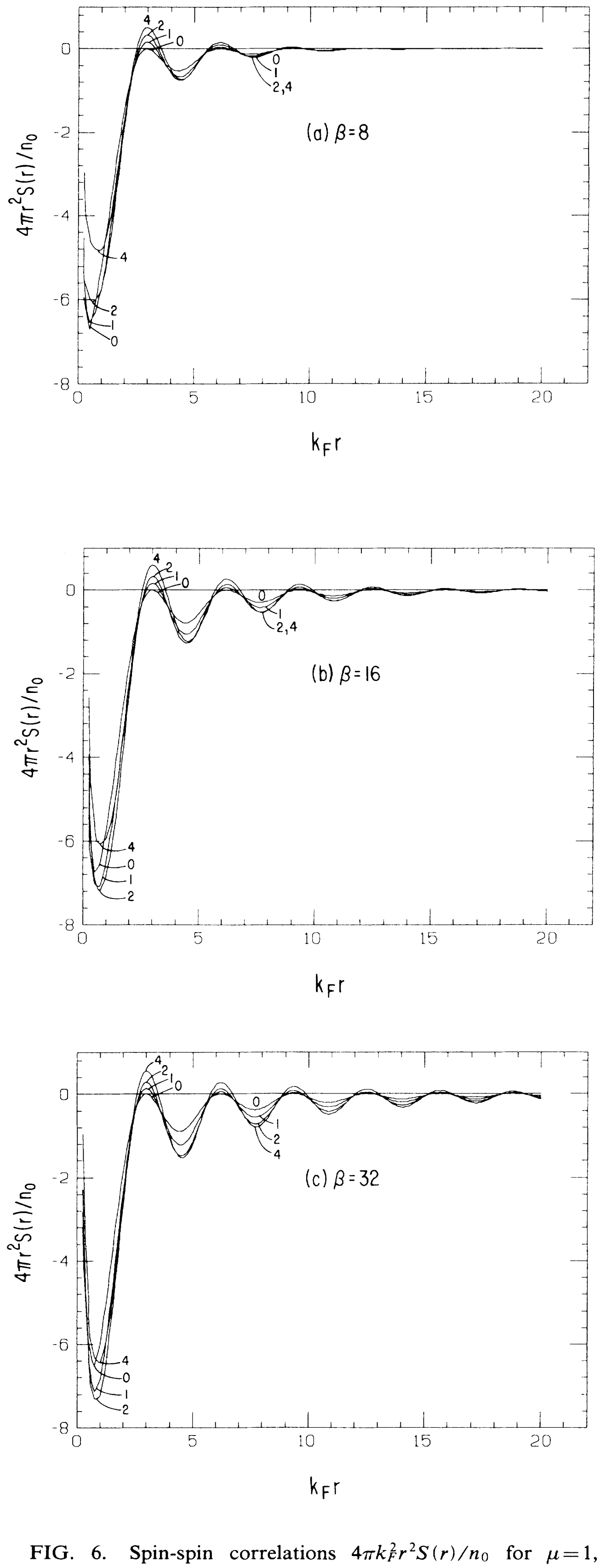

FIG. 6. Spin-spin correlations $4\pi k_F^2 r^2 S(r)/n_0$ for $\mu=1$, $U=0$, 1, 2, and 4 and (a) $\beta=8$, (b) $\beta=16$, and (c) $\beta=32$.

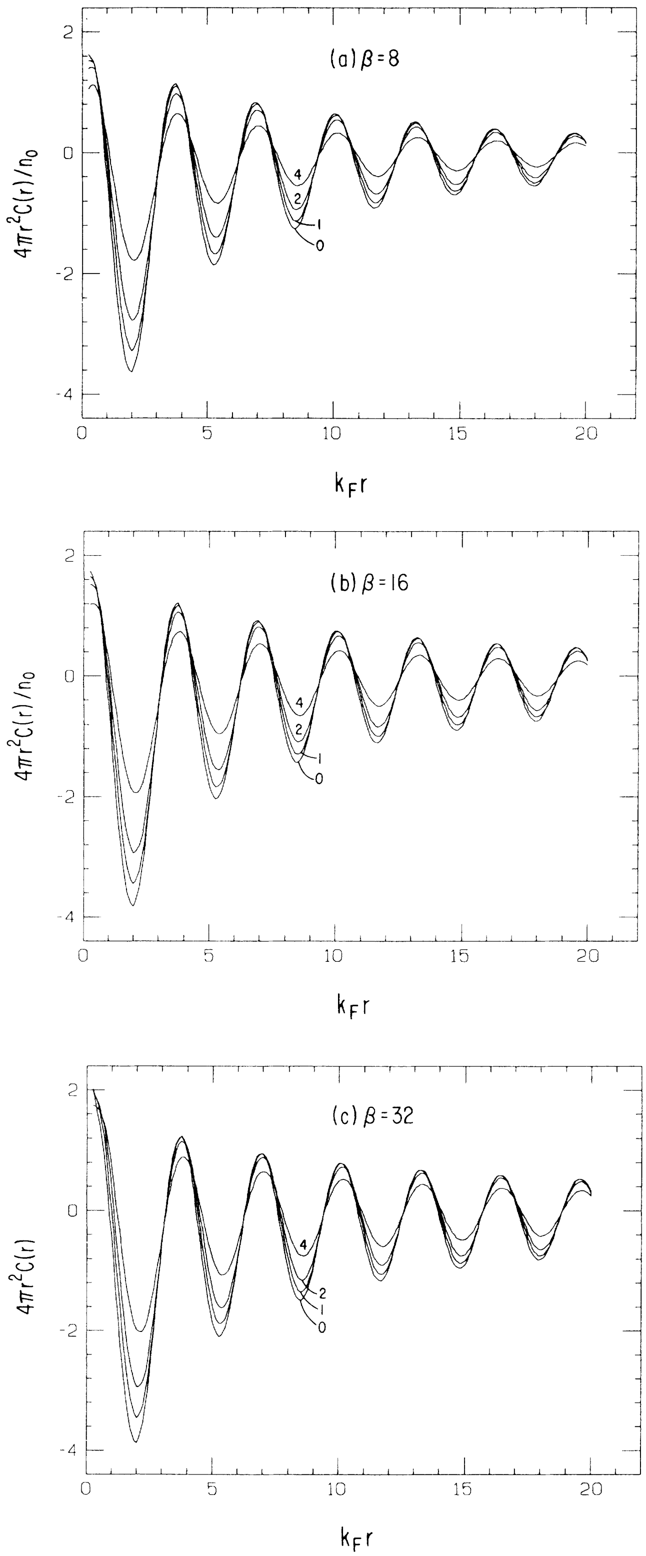

FIG. 7. Impurity-charge–conduction-electron-charge correlations $C(r)$, Eq. (8), multiplied by $4\pi k_F^2 r^2/n_0$ vs $k_F r$ for $\mu=6$, $U=0$, 1, 2, and 4 and (a) $\beta=8$, (b) $\beta=16$, and (c) $\beta=32$. Here we have subtracted off the asymptotic value so the function goes to zero at large distances. One sees that the charge correlations are monotonically suppressed as U is increased at all distances.

finite temperature, however, charge oscillations are suppressed also at large distances due to the temperature dependence of the d-electron spectral weight.[12]

IV. CONCLUSIONS

We have studied the behavior of spin and charge correlations in the compensation cloud around an Anderson impurity. The results for the spin correlations showed the following features. (a) The phase and period of the oscillations in the spin correlations are not changed by the Coulomb interaction. (b) The Coulomb interaction induces ferromagnetic spin correlations in some regions, which are monotonically increasing with U. (c) The antiferromagnetic spin correlations can be *suppressed* by the interaction at short distances at intermediate temperatures. (d) The ferromagnetic spin correlations are nearly temperature independent, while the antiferromagnetic ones show increasing temperature dependence as U increases. (e) As the bandwidth is decreased, the region of space where the anomalous behavior of the antiferromagnetic correlations (decreasing with increasing U) is observed is reduced. (f) As discussed by Ishii,[10] the spin-compensation cloud extends over a wide region around the impurity, set by the Kondo length μ/T_K. One might hope that neutron scattering experiments would be able to measure the spin correlations directly and provide confirmation of our observations. For the charge correlations, we obtained a monotonic suppression with the interaction which is in qualitative agreement with experimental observations[12] as well as phenomenological calculations.[11]

In summary, we have shown that Monte Carlo simulations can provide detailed information about spin and charge correlations for systems of magnetic impurities. Application of this technique to realistic band structures is straightforward since all that changes are the quantities f_1 and f_2 [Eqs. (13)] that enter into the unperturbed Green's function. Thus, this procedure can provide quantitative information on correlations in specific dilute magnetic alloys.

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$$x=k_F r(1+\omega_n/\mu)^{1/2}\,.$$

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