Temperature-dependent Hartree-Fock theory of the impure spin-$\frac{1}{2}$ Ising-Heisenberg chain

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Hartree-Fock equations for the impure spin-$\frac{1}{2}$ Ising-Heisenberg chain are derived by using the Green-function technique in the pseudofermion representation. The self-consistency equations for the ideal spin-$\frac{1}{2}$ anisotropic Heisenberg antiferromagnet can be recovered as a specific case of the general formalism developed in the present work. In the case of the nonideal XXZ chain, a numerical solution of the self-consistency equations is used to describe the Friedel-type boundary on impurity-induced oscillations of the local magnetization considered previously in the spin-$\frac{1}{2}$ XY model.

I. INTRODUCTION

As a result of the work of Rodriguez[1] and Bulaevskii,[2] the Hartree-Fock approximation (HFA) in the pseudofermion representation has become a widely used tool in the investigation of the ideal spin-$\frac{1}{2}$ antiferromagnetic chains[3–8] described by the Hamiltonian

$$H_0=-J_x\sum_j(S_j^xS_{j+1}^x+S_j^yS_{j+1}^y)-J_z\sum_j S_j^zS_{j+1}^z+h\sum_j S_j^z\,, \tag{1}$$

where J_x and J_z denote the exchange coupling constants and h is the normalized magnetic field.

In particular it was found[8] that the Hartree-Fock calculations of the internal energy U, specific heat C_V, and the low-field longitudinal susceptibility χ_z as functions of the anisotropy parameter $\Delta=J_z/|J_x|$ agree to $O(\Delta)$ with exact results.[9–11] Even for the isotropic Heisenberg antiferromagnet ($\Delta=-1$) Hartree-Fock approximations for U and C_V, as well as for the energy dispersion law of the lowest-lying excitations,[12] introduce only 4–8% error.[2–4,13] The error for χ_z in this case is about 30% at zero temperature but it declines to 11% at temperature $T\sim 0.5|J_x|/k_B$ corresponding to the maximum of the $\chi_z(T)$ curve.[13,14]

In the case of the alternating chains[3,13–20] where exact results are not available at the present time, a similar degree of accuracy of the Hartree-Fock approximation was observed by comparison with the results of the numerical calculations.[14,18–20]

It is then of interest to consider a generalization of that technique in the case of the impure Ising-Heisenberg chain where the analytical results are not available outside the linear spin-wave theory. The latter is known to be an extremely poor approximation for the spin-$\frac{1}{2}$ quasi-one-dimensional magnets.[21,22]

Starting from the analogy between the spin-$\frac{1}{2}$ linear antiferromagnet and the quasi-one-dimensional metal established by the Jordan-Wigner transformation, it has been suggested previously that the presence of the impurity[23] (or boundary[24]) at sufficiently low temperatures, results in the Friedel-type oscillations of the local magnetization.

The exact (zero-temperature) solution of this problem exists only for the spin-$\frac{1}{2}$ XY model of the linear antiferromagnet with the unchanged g factor at the impurity site.[25,26] In the more general case ($\Delta g\neq 0$), it is still possible to obtain the analytical results for the oscillations of the local magnetization at large distances from the impurity.[26] The solution obtained in Refs. 25 and 26 for $J_z=0$ has been used to describe some general features of the oscillations, including the band effects and the disappearance of the perturbation of local magnetization in the absence of the external magnetic field. However, with the notable exception of Cs_2CoCl_4,[27–30] the majority of experimentally available linear antiferromagnets are described by the Ising-Heisenberg rather than by XY model considered in Refs. 24–26.

The inclusion of the Ising term in the model Hamiltonian results in the effective short-range interaction between the pseudofermions and in the different structure of the perturbation potential in the Jordan-Wigner representation. This means that both the shape and amplitude of the boundary or impurity-induced oscillations of the local magnetization are affected by the Ising term, unlike the Friedel oscillations in metal, where, at least in the random-phase approximation, the inclusion of the Coulombic interaction changes the amplitude but not the phase of the oscillations.[31,32]

II. DERIVATION OF THE SELF-CONSISTENCY EQUATIONS FOR THE NONIDEAL CHAIN

Consider the Hamiltonian $H=H_0+V$, where the operator V describes the perturbation of the spin-$\frac{1}{2}$ impurity located at site $j=I$:

$$V=-\Delta J_x\sum_{m=\pm 1}(S_I^xS_{I+m}^x+S_I^yS_{I+m}^y)-\Delta J_z\sum_{m=\pm 1}S_I^zS_{I+m}^z+h(\Delta g/g)S_I^z\,, \tag{2}$$

where ΔJ_x and ΔJ_z describe the change of the coupling constants in the immediate vicinity of the impurity, and $\Delta g/g$ gives the relative change of the spectroscopic splitting factor at the impurity site.

A pseudofermion representation of the Hamiltonian (1) and (2) is

$$H_0=(h+J_z)\sum_{j=1}^{N} n_j-\frac{J_x}{2}\left[\left[C_N^{\dagger}C_1+\sum_{j=1}^{N-1} C_j^{\dagger}C_{j+1}\right]+\text{H.c.}\right]-J_z\left[n_1n_N+\sum_{j=1}^{N-1} n_jn_{j+1}\right]$$
$$+(\gamma/2)[J_x(C_N^{\dagger}C_1+\text{H.c.})+J_z(2n_1n_N-n_N-n_1)]\,, \tag{3a}$$

$$V=-\frac{\Delta J_x}{2}\sum_{m=-1,1}(C_I^{\dagger}C_{I+m}+\text{H.c.})+n_I(\Delta h+\Delta J_z)+\frac{\Delta J_z}{2}(n_{I+1}+n_{I-1})-\Delta J_z n_I(n_{I+1}+n_{I-1})\,, \tag{3b}$$

where N is the number of spins in the chain, $\Delta h=h\,\Delta g/g$, $n_j=C_j^{\dagger}C_j$, and the creation and annihilation operators of the pseudofermions are introduced by the Jordan-Wigner transformation:[1,33]

$$C_j=S_j^{-}\exp\left[-i\pi\sum_{m=1}^{j-1} S_m^{+}S_m^{-}\right], \tag{4a}$$

$$C_j^{\dagger}=S_j^{+}\exp\left[i\pi\sum_{m=1}^{j-1} S_m^{+}S_m^{-}\right], \tag{4b}$$

where $S_j^{\pm}=S_j^x\pm iS_j^y$.

In this work two types of boundary conditions are considered: free-ends chain corresponding to $\gamma=1$ and c-cyclic problem ($C_{N+1}=C_1$),[33] corresponding to $\gamma=0$.

The local magnetization

$$\langle S_j\rangle=\langle n_j\rangle-\tfrac{1}{2} \tag{5}$$

can be expressed through the local density of states $\rho_j(E)$:

$$\langle n_j\rangle=\int_{-\infty}^{\infty}\frac{\rho_j(E)}{1+\exp(\beta E)}dE\,, \tag{6}$$

where

$$\rho_j(E)=-\frac{1}{\pi}\text{Im}G_{jj}(E)\,. \tag{7}$$

and $\beta=1/k_BT$ denotes the inverse temperature in energy units. The Fourier transform of the double-time Green function is defined as $G_{ij}(E)=\langle\langle C_i;C_j^{\dagger}\rangle\rangle_E$, where for arbitrary operators $A(t)$ and $B(t)$ in the Heisenberg representation we define ($\hbar=1$):

$$\langle\langle A;B\rangle\rangle_E=-i\int_{-\infty}^{\infty}\Theta(t)\exp(iEt)\times\langle[A(t),B(0)]_+\rangle dt\,. \tag{8}$$

Considering the equation of motion

$$EG_{ij}(E)=\delta_{ij}-\langle\langle[H,C_i];C_j^{\dagger}\rangle\rangle_E \tag{9}$$

gives

$$EG_{1j}(E)=\delta_{1j}+[h+J_z(1-\gamma/2)]G_{1j}(E)-J_z\langle\langle C_1[n_N(1-\gamma)+n_2];C_j^{\dagger}\rangle\rangle_E$$
$$-\frac{J_x}{2}[(1-\gamma)G_{Nj}(E)+G_{2j}(E)]\,, \tag{10}$$

$$EG_{Nj}(E)=\delta_{Nj}+[h+J_z(1-\gamma/2)]G_{Nj}(E)-J_z\langle\langle C_N[n_1(1-\gamma)+n_{N-1}];C_j^{\dagger}\rangle\rangle_E$$
$$-\frac{J_x}{2}[(1-\gamma)G_{1j}(E)+G_{N-1,j}(E)]\,. \tag{11}$$

For $1<j<N$, but $|j-I|>1$

$$EG_{ij}(E)=\delta_{ij}+(h+J_z)G_{ij}(E)-J_z\langle\langle C_i(n_{i+1}+n_{i-1});C_j^{\dagger}\rangle\rangle_E-\frac{J_x}{2}[G_{i-1,j}(E)+G_{i+1,j}(E)]\,, \tag{12}$$

while

$$EG_{Ij}(E)=\delta_{Ij}+(h+\Delta h+J_z+\Delta J_z)G_{Ij}(E)-(J_z+\Delta J_z)\langle\langle C_I(n_{I+1}+n_{I-1});C_j^{\dagger}\rangle\rangle_E$$
$$-[(J_x+\Delta J_x)/2][G_{I-1,j}(E)+G_{I+1,j}(E)]\,, \tag{13}$$

and for $m=\pm1$

$$EG_{I+m,j}(E)=\delta_{I+m,j}+(h+J_z+\Delta J_z/2)G_{I+m,j}-J_z\langle\langle C_{I+m}(n_{I+m+1}+n_{I+m-1});C_j^{\dagger}\rangle\rangle_E$$
$$-\Delta J_z\langle\langle C_{I+m}n_I;C_j^{\dagger}\rangle\rangle_E-\frac{J_x}{2}[G_{I+m+1,j}(E)+G_{I+m-1,j}(E)]-\frac{\Delta J_x}{2}G_{Ij}(E)\,. \tag{14}$$

Equations (10)—(14) can be decoupled using the Hartree-Fock approximation

$$\langle\langle C_i n_p; C_j^\dagger \rangle\rangle_E \cong \langle n_p \rangle G_{ij}(E) + \langle C_i C_p^\dagger \rangle G_{pj}(E) , \tag{15}$$

which leads to the matrix equation

$$\{\underline{H}^{\mathrm{HF}} - E\underline{\mathbb{1}}\}\underline{G} = \underline{\mathbb{1}} , \tag{16}$$

in which $\underline{\mathbb{1}}$ denotes the $N \times N$ unit matrix, and the temperature-dependent components of the Hamiltonian matrix $\underline{H}^{\mathrm{HF}} = \underline{H}_0^{\mathrm{HF}} + \underline{V}^{\mathrm{HF}}$ are given by the following expressions:

$$(\underline{H}_0^{\mathrm{HF}})_{ik} = [h + J_z(1 - \langle n_{i+1} \rangle - \langle n_{i-1} \rangle]\delta_{ik} - (J_x/2 + J_z\langle C_i C_{i+1}^\dagger \rangle)\delta_{i+1,k} - (J_x/2 + J_z\langle C_i C_{i-1}^\dagger \rangle)\delta_{i-1,k}, \quad 1 < i < N \tag{17}$$

$$(\underline{H}_0^{\mathrm{HF}})_{1k} = [h + J_z(1 - \gamma/2) - J_z(1-\gamma)\langle n_N \rangle - J_z\langle n_2 \rangle]\delta_{1k} - (J_x/2 + J_z\langle C_1 C_2^\dagger \rangle)\delta_{2k} - (1-\gamma)[(J_x/2) + J_z\langle C_1 C_N^\dagger \rangle]\delta_{Nk} , \tag{18}$$

$$(\underline{H}_0^{\mathrm{HF}})_{Nk} = [h + J_z(1 - \gamma/2) - J_z(1-\gamma)\langle n_1 \rangle - J_z\langle n_{N-1} \rangle]\delta_{Nk} - (J_x/2 + J_z\langle C_N C_{N-1}^\dagger \rangle)\delta_{N-1,k} - (1-\gamma)[(J_x/2) + J_z\langle C_N C_1^\dagger \rangle]\delta_{1k} , \tag{19}$$

$$(\underline{V}^{\mathrm{HF}})_{II} = \Delta h + \Delta J_z(1 - \langle n_{I+1} \rangle - \langle n_{I-1} \rangle) , \tag{20}$$

$$(\underline{V}^{\mathrm{HF}})_{I+1,I+1} = \Delta J_z(\tfrac{1}{2} - \langle n_I \rangle) = (\underline{V}^{\mathrm{HF}})_{I-1,I-1} , \tag{21}$$

$$(\underline{V}^{\mathrm{HF}})_{I,I+1} = (\underline{V}^{\mathrm{HF}})^*_{I+1,I} = -(\Delta J_x/2 + \Delta J_z\langle C_I C_{I+1}^\dagger \rangle) , \tag{22}$$

$$(\underline{V}^{\mathrm{HF}})_{I,I-1} = (\underline{V}^{\mathrm{HF}})^*_{I-1,I} = -(\Delta J_x/2 + \Delta J_z\langle C_I C_{I-1}^\dagger \rangle) . \tag{23}$$

All other matrix elements of $\underline{V}^{\mathrm{HF}}$ are equal to zero.

The formal solution of Eq. (16) can be expressed in terms of the eigenvectors $\underline{\phi}^{(m)}$ and eigenvalues E_m of the matrix $\underline{H}^{\mathrm{HF}}$. Assuming that the eigenvectors are orthonormalized

$$G_{jk}(E) = \sum_{m=1}^{N} \frac{\phi_n^{(m)}(\phi_k^{(m)})^*}{E + i0 - E_m} . \tag{24}$$

Equation (24) has the same form as the expression for the time-independent Green function of the one-particle system.[34] This similarity is however somewhat superficial since both $\phi_j^{(m)}$ and E_m depend on the expectations $\langle n_j \rangle$ and $\langle C_j C_{j+1}^\dagger \rangle$, which in turn should be calculated using the Green function $\underline{G}(E)$. In other words Eq. (24) gives yet another form of the HFA equation of motion. It can be brought into the form convenient for the numerical solution by excluding Green function and singular denominators.

Substitution of

$$\mathrm{Im}\, G_{jj}(E) = -i\pi \sum_{m=1}^{N} |\phi_j^{(m)}|^2 \delta(E - E_m) \tag{25}$$

into Eqs. (6) and (7) gives

$$\langle n_j \rangle = \sum_{m=1}^{N} \frac{|\phi_j^{(m)}|^2}{1 + \exp(\beta E_m)} . \tag{26}$$

Similarly

$$\langle C_j C_{j+1}^\dagger \rangle = -\sum_{m=1}^{N} \frac{\phi_j^{(m)}(\phi_{j+1}^{(m)})^*}{1 + \exp(\beta E_m)} . \tag{27}$$

Equations (17)—(23) and (26) and (27) together with

$$\underline{H}^{\mathrm{HF}}\underline{\phi}^{(m)} = E_m \underline{\phi}^{(m)} \tag{28}$$

present the system of self-consistency equations for the nonideal spin-$\frac{1}{2}$ Ising-Heisenberg chain.

For the ideal chain with C-cyclic boundary conditions ($\gamma = 0$) and $\underline{V}^{\mathrm{HF}} = \underline{0}$, one finds

$$(\underline{H}^{\mathrm{HF}})_{ij} = E_0\delta_{ij} + t(\delta_{i,j+1} + \delta_{i,j-1}) , \tag{29}$$

with

$$E_0 = h + J_z(1 - 2\langle n_j \rangle) \tag{30}$$

and

$$t = -J_x/2 - J_z\langle C_{j-1}^\dagger C_j \rangle , \tag{31}$$

where $\langle n_j \rangle$ and $\langle C_{j-1}^\dagger C_j \rangle$ do not depend on the site number j. Then

$$\phi_j^{(k)} = N^{-1/2} e^{ikj}, \quad E_k = E_0 + 2t\cos k \tag{32}$$

so that expressions (26) and (27) give

$$\langle n_j \rangle = N^{-1}\sum_k f_k , \tag{33}$$

$$\langle C_j C_{j+1}^\dagger \rangle = -N^{-1}\sum_k f_k \cos k , \tag{34}$$

where $f_k = [1 + \exp(\beta E_k)]^{-1}$ and $-\pi < k < \pi$ (lattice constant $a = 1$).

After defining the average magnetization per unit site $\langle S^z \rangle = \langle n_j \rangle - \frac{1}{2}$ and the parameter

$$p = 1 - \frac{2J_z}{NJ_x}\sum_k f_k \cos k , \tag{35}$$

the self-consistency equations for the ideal antiferromagnetic chain can be presented in the form introduced by Bulaevskii:[3]

$$\langle S^z\rangle = -\frac{1}{2} + \frac{1}{N}\sum_k \{1+\exp[\beta(h-2J_z\langle S^z\rangle - pJ_x\cos k)]\}^{-1}\,, \tag{36}$$

$$p = 1 - \frac{2J_z}{NJ_x}\sum_k \frac{\cos k}{1+\exp[\beta(h-2J_z\langle S^z\rangle - pJ_x\cos k)]}\,. \tag{37}$$

Derivation of the self-consistency equations for the ideal isotropic chain using the Green-function method was given by Oguchi and Tsuchida.[4] Schneider *et al.*[6] investigated the equations equivalent to (36) and (37) in the anisotropic case.

Thus in the absence of perturbation the method presented here is equivalent to the previous results for the uniform Ising-Heisenberg chain.

III. RESULTS AND DISCUSSION

The self-consistency equations derived above can be solved numerically using the iterative procedure. The results of the numerical solution are shown in Fig. 1 for the isotropic Heisenberg antiferromagnet $J_x=J_z=-J<0$, $\Delta J_x=\Delta J_z=-\Delta J$. As in the case of the XY problem,[23–26] perturbation of local magnetization has an oscillatory spatial dependence with the amplitude decaying with distance from the impurity. Oscillations of local magnetization are accompanied by oscillations of the transition probability amplitude $\langle C_j C_{j+1}^{\dagger}\rangle$ depicted in Fig. 1(b). In addition, in the case of the free-ends boundary conditions ($\gamma=1$), oscillations of the local magnetization and transition amplitude appear near the ends of the chain.

As is illustrated by comparison of Figs. 1(a) and 2, both the shape and amplitude of the oscillations depend on the relative strength of the different components of the perturbation potential, i.e., $h\,\Delta g/g$ and $\Delta J/J$. Oscillations of the local magnetization, as well as Friedel oscillations of the electron density in metals[32] are damped by the temperature increase [compare Figs. 1(a) and 3]. In the high-temperature region the numerical solution of the Hartree-Fock equations follows the Curie-Weiss law

$$\langle S_I^z\rangle \cong -\frac{h(1+\Delta g/g)}{4[T+(J+\Delta J)/2]}\,, \tag{38}$$

$$\langle S_j^z\rangle \cong -\frac{h}{4(T+J/2)}\,, \quad |j-I|\gg 1\,. \tag{39}$$

In the example $\Delta J=J$, $\Delta g=0$, these expressions describe the results of the numerical solution with a precision better than 3% for $T>5J$.

In the opposite case $T\ll J$, if h is also small, an iterative solution of the Hartree-Fock equations for the nonideal antiferromagnetic chain may result in unphysical solutions that correspond to long-range antiferromagnetic ordering at nonzero temperature. This is presumably the consequence of the mean-field nature of the Hartree-Fock approximation (15) used to decouple the equations of motion for the Green functions. Low-temperature parasitic solutions can be easily separated using their dependence on the starting point of the iteration procedure and wrong values of the bulk magnetization and transition amplitude at large distances from the impurity.

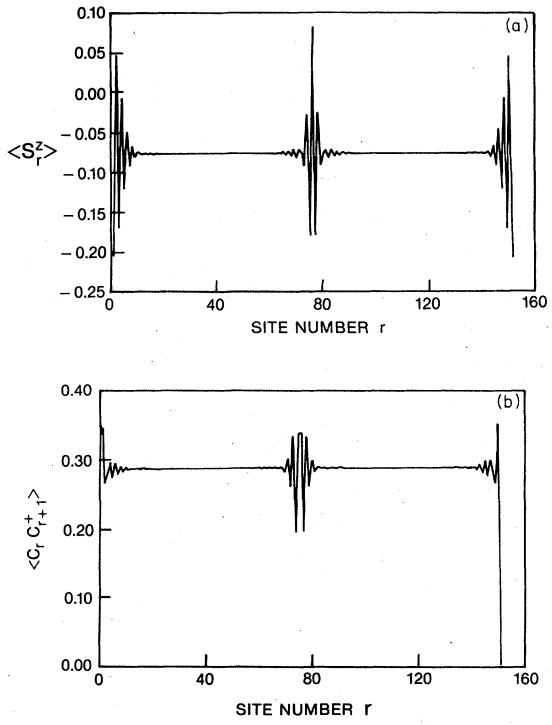

FIG. 1. Boundary and impurity-induced oscillations of (a) the local magnetization and (b) the transition amplitude in the isotropic Hamiltonian antiferromagnet. $N=151$, $I=76$, $J_x=J_z=-J<0$, $T=0.3J/k_B$, $h=0.5J$, $\Delta g=0$, $\Delta J_x=\Delta J_z=-J$, and $\gamma=1$.

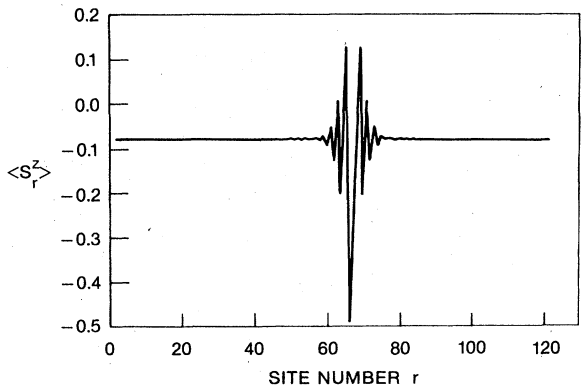

FIG. 2. Impurity-induced oscillations of local magnetization for $N=101$, $I=51$, $J_x=J_z=-J<0$, $T=0.3J/k_B$, $h=0.5J$, $\Delta g/g=2$, $\Delta J_x=\Delta J_z=2J$, and $\gamma=0$.

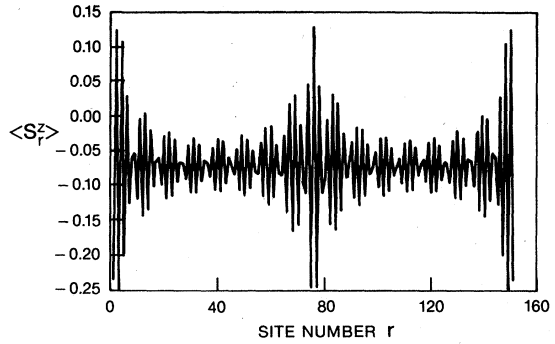

FIG. 3. Interference of the boundary and impurity-induced oscillations in the isotropic Heisenberg antiferromagnet. $T=0.18J/k_B$; other parameters are same as in Fig. 1.

In the above examples $h=0.5J$, $T\geq 0.18J$. In this case the oscillation of $\langle S_j^z\rangle$ can still be considered without too strong temperature damping but the problem of parasitic solutions does not affect the calculations. For the results presented in Figs. 1–3, $\langle S_j^z\rangle \cong \langle S^z\rangle$ and $\langle C_j C_{j+1}^{\dagger}\rangle \cong (p-1)/2$, where $|j-I| \gg 1$ (and also $j\gg 1$, $N-j\gg 1$ if $\gamma=1$), and $\langle S^z\rangle$ and p are determined by the numerical solution of the self-consistency equations (36) and (37) for the ideal chain.

The method described here is not limited to chains with a single impurity. An example of the interference effect on the oscillations of the local magnetization is shown in Fig. 4 for the spin-$\frac{1}{2}$ XY chain. In this case the Hamiltonian matrix does not depend on the state of the system, and for a single defect with $J_z=\Delta J_z=\Delta g=0$, Eqs. (26) and (5) give the same result for the local magnetization as the exact analytical solution.[25] A second impurity is included by the evident modification of the perturbation matrix $\underline{V}^{\mathrm{HF}}$.

When the impurities are brought close to each other [see Fig. 4(b)] the interference effects significantly change the local magnetization of the sites lying to the right side of the first impurity ($I_1=77$). However for $j<I_1$ the local magnetization is not very sensitive to the presence of the second impurity at site $I_2=80$. This is due to the relatively strong change of the single-site energy of site I_1 which effectively separates the chain into two weakly connected parts as discussed elsewhere.[26] This ability of the impurity with a large $h\,\Delta g/g$ to serve as a screen against

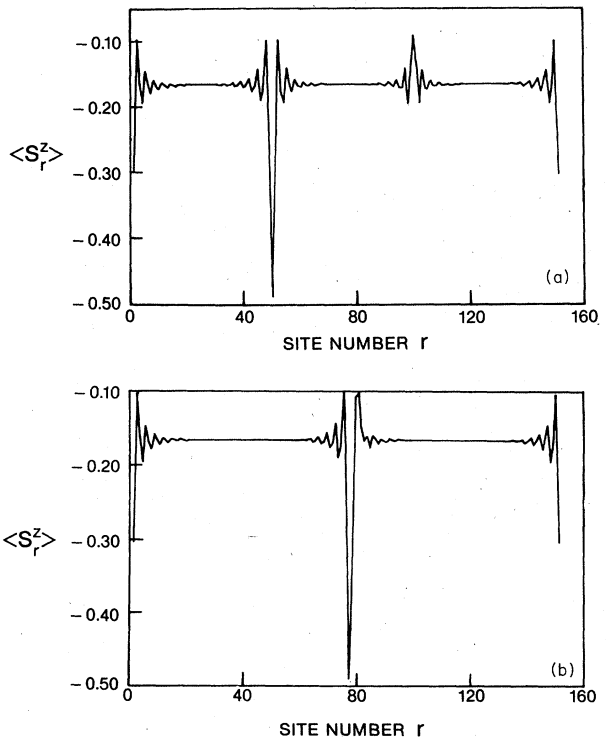

FIG. 4. Local magnetization in the spin-$\frac{1}{2}$ XY chain ($J_z=\Delta J_z=0$) with two impurities located in sites I_1 and I_2. $N=151$, $T=0.025\,|J_x|/k_B$, $h=0.5\,|J_x|$, and $\Delta g/g=2$. (a) $I_1=50$, $I_2=100$; (b) $I_1=77$, $I_2=80$. $(\Delta J_x)_1=-J_x/2$, $(\Delta g/g)_1=2$, $(\Delta J_x)_2=J_x$, and $(\Delta g/g)_2=\frac{1}{2}$.

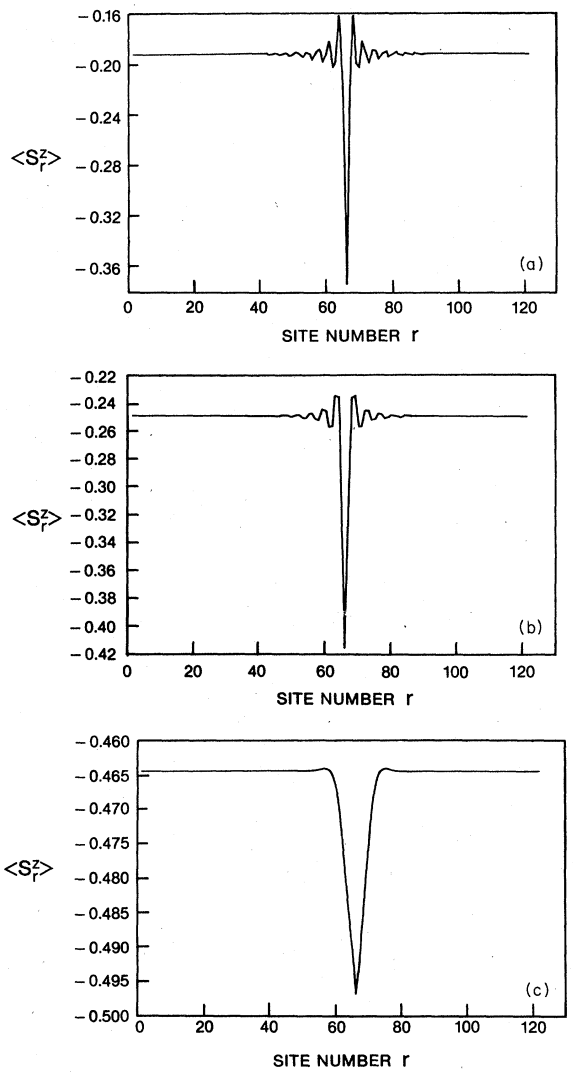

FIG. 5. Friedel-type oscillations of the local magnetization in the anisotropic Heisenberg ferromagnet. $N=121$, $I=66$, $J_x=J>0$, $\Delta J_z=\Delta J_x=0$, $\Delta g/g=1$, $h=0.5J$, and $T=0.02J/k_B$. (a) $J_z=0.1J$; (b) $J_z=0.25J$; (c) $J_z=0.5J$.

the other is a specific feature of the XY chain with the nearest-neighbor interaction and is lost when $J_z \neq 0$.

The effect of the anisotropy of the exchange interaction has been investigated numerically by changing J_z and considering an impurity with $\Delta J_x = \Delta J_z = 0$, $\Delta g \neq 0$ to escape the problem of the simultaneous scaling of ΔJ_x and ΔJ_z. As shown in Fig. 5, the increase of J_z for a given J_x results in additional damping of the oscillations which exist even in the anisotropic ferromagnet if $\Delta < 1$.[35] A similar conclusion is achieved by comparison of the oscillations of the local magnetization in the XY chain and isotropic Heisenberg antiferromagnet.

This result shows the limitation of the analogy between the Friedel oscillations of electron density in metal and the oscillations of the local magnetization in quantum-spin chains. The Ising term in the Hamiltonian (1) results in the repulsive ($J_z < 0$) or attractive ($J_z > 0$) interaction between the quasiparticles given by

$$H_{\text{int}} = -J_z \sum_j n_j n_{j+1} . \tag{40}$$

In the electron gas, Coulombic repulsion of the electrons reduces the amplitude of the Friedel oscillations,[31,32] while the short-range repulsive interaction of the pseudofermions has the opposite effect.

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