Self-consistent spin-wave theory of two-dimensional magnets with impurities

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The self-consistent spin-wave theory is applied to investigate the magnetization distribution around the impurity in isotropic and easy-axis two-dimensional ferro- and antiferromagnets. The temperature dependences of the host magnetization disturbance and impurity magnetization are calculated. The short-range order in the isotropic case is investigated. The importance of dynamical and kinematical interactions of spin waves is demonstrated. [S0163-1829(99)13341-1]

I. INTRODUCTION

In connection with extensive investigations of copper-oxide based superconductors, great attention has been paid to studying magnetism of low-dimensional systems. Of particular interest is the problem of nonmagnetic impurities in magnetic hosts. Numerous experimental results (see, e.g., Refs. 1–3) demonstrate that even small amount of substitution impurities (Zn, Fe, etc.) in CuO_2 planes may influence strongly magnetic properties, e.g., lead to strong suppression of host magnetization. These facts have stimulated a number of theoretical works (see, e.g., Refs. 2–9). In particular, the impurity problem for isotropic two-dimensional (2D) antiferromagnets at $T=0$ was investigated by the standard spin-wave theory.[5] However, detailed consideration of the finite-temperature situation, especially in a wide temperature region, is absent. Moreover, the usual spin-wave theory is here obviously inapplicable, since this does not take into account adequately the short-range magnetic order which is a characteristic feature of low-dimensional magnets.

On the other hand, the impurity problem for three-dimensional (3D) magnets was investigated within the standard spin-wave theory (see, e.g., Ref. 10). It was established that in the case of a weakly coupled magnetic impurity in a ferromagnet the standard spin-wave approximation is insufficient already at $T\sim T_{\rm imp}$ where $T_{\rm imp}\ll T_C$ is the energy of impurity-host coupling. Inclusion of dynamical and kinematic interaction of spin waves within the Tyablikov approximation[10] leads in this case to occurrence of an anomalous temperature dependence of impurity magnetization. Therefore it is interesting to investigate the impurity problem for 2D systems, such as ferro- and antiferromagnets (FM and AFM) with small anisotropy or interlayer coupling (which are required to produce finite values of the magnetic ordering temperature T_M).

In the present paper we consider weakly anisotropic 2D impurity magnetic crystals with the use of the self-consistent spin-wave theory (SSWT). This theory was developed to describe thermodynamics of 2D systems,[11–13] and also successfully applied to quasi-2D (Refs. 14 and 15) and weakly anisotropic 2D magnets.[15] An important advantage of SSWT in comparison with the usual spin-wave theory is that it gives a possibility to describe both ordered and disordered phases and therefore provides a qualitatively correct description of the strong short-range order above T_M. Introducing slave fermions[16] into SSWT allows us to take into account kinematic interactions of spin waves and correctly describe systems at not too low temperatures. In the following sections we calculate the impurity-induced magnetization disturbance for different signs of exchange interactions in the host and between host and impurity.

II. FERROMAGNETIC IMPURITY IN FERROMAGNETIC HOST

The Heisenberg Hamiltonian of a FM crystal with a square lattice, containing a ferromagnetically coupled impurity at the site $i=0$, reads

$$\mathcal{H}=-\frac{1}{2}\sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j+\mathcal{H}_A, \tag{1}$$

where

$$\mathcal{H}_A=-D\sum_i (S_i^z)^2-\frac{1}{2}\sum_{ij} \eta_{ij}S_i^zS_j^z, \tag{2}$$

D and η_{ij} being parameters of single-site and two-site easy-axis anisotropy. In the nearest-neighbor approximation the nonzero exchange integrals are

$$J_{i,i+\delta}=\begin{cases} J', & i=0 \quad \text{or} \quad i+\delta=0 \\ J, & i,i+\delta\neq 0, \end{cases} \tag{3}$$

where δ denotes nearest neighbors, $J>0$, $J'>0$.

Following to Ref. 15 we use in the FM case for $i\neq 0$ the representation[16]

$$S_i^+=\sqrt{2S}a_i, \quad S_i^z=S-a_i^\dagger a_i-(2S+1)c_i^\dagger c_i,$$

$$S_i^-=\sqrt{2S}\left(a_i^\dagger-\frac{1}{2S}a_i^\dagger a_i^\dagger a_i\right)-\frac{2(2S+1)}{\sqrt{2S}}a_i^\dagger c_i^\dagger c_i, \tag{4}$$

where $a_i^\dagger,a_i$ are the Bose ideal magnon operators and $c_i^\dagger,c_i$ are the auxiliary pseudofermion operators at the site i. As discussed in Refs. 16 and 15, the pseudofermion contribution to thermodynamic quantities cancels exactly the contribution of unphysical states with $\langle a_i^\dagger,a_i\rangle>S$. Thus introducing of pseudofermion operators gives a possibility to reduce the problem of accounting for kinematical interaction of spin waves (which arises because of the restricted number of states at each site) to a more simple problem of boson-pseudofermion interaction. Note that due to the imaginary contribution to their chemical potential, $i\pi T$, pseudofermions possess the Bose distribution function rather than the Fermi one, cf. Refs. 16 and 15. For $i=0$ one has to replace in Eq. (4) $S\rightarrow S'$ with S' being the impurity spin.

To satisfy the condition $\overline{S_i}=0$ in the paramagnetic phase we introduce the Lagrange multipliers μ_i at each lattice site, which corresponds to the constraint of the magnon occupation number at $T>T_C$ (see, e.g., formal consideration in Ref. 17 and the discussion in Ref. 15). These multipliers play the role of a local ''chemical potential'' for the boson-pseudofermion systems. Introducing μ_i permits us to correct drawbacks of the standard spin-wave theory which is inapplicable at $T>T_C$ since the magnetization formally becomes negative. At $T<T_C$ we have $\mu_i=0$ and the total magnon occupation number is not conserved.

Further we perform decouplings of the quartic forms which occur after substituting Eq. (4) into Eq. (1). Introducing the averages

$$\xi_{i,i+\delta}=\overline{S_{i+\delta}}+\langle a_i^\dagger a_{i+\delta}\rangle \tag{5}$$

we derive the quadratic Hamiltonian of the mean-field approximation

$$\mathcal{H}=\sum_{i\delta}\ \xi_{i,i+\delta}J_{i,i+\delta}[a_i^\dagger a_i-a_{i+\delta}^\dagger a_i+(2S+1)c_i^\dagger c_i]$$
$$-\sum_i\ \mu_i[a_i^\dagger a_i+(2S+1)c_i^\dagger c_i]+\mathcal{H}_A. \tag{6}$$

As well as in the uniform magnets,[15] the averages $\xi_{i,i+\delta}$ take into account the dynamical interaction of spin waves in the lowest Born approximation. The Fermi operators describe the kinematic interactions of the spin waves.

Following Refs. 18 and 15, we treat the influence of the magnetic anisotropy by neglecting quartic forms in $\mathcal{H}_A$, which yields

$$\mathcal{H}_A=-H_A\sum_i\ S_i^z=-H_A\sum_i\ [S-a_i^\dagger a_i-(2S+1)c_i^\dagger c_i]$$

with the anisotropy field H_A

$$H_A=(2S-1)D+S\sum_\delta\ \eta_{i,i+\delta}. \tag{7}$$

As discussed in Ref. 15, the effect of the anisotropy field H_A differs from that of the true magnetic field since the chemical potentials μ_i are also influenced by H_A. Thus the magnetic phase transition is still present at $H_A>0$, and T_C is shifted to higher values. In the limit $H_A\ll J$ under consideration, effects of single-site and two-site anisotropy are qualitatively the same, although concrete expressions for the field H_A in Eq. (7) are different. In the 2D case H_A is the only factor stabilizing magnetic order ($T_C=0$ at $H_A=0$), but, as already mentioned, SSWT works in the disordered phase also.

For an ideal crystal, $\xi_{i,i+\delta}$ and μ_i do not depend on i and the diagonalization of the Hamiltonian (6) is easily performed.[15] At the same time, for the impurity system this is a complicated task because of the unknown site dependences of $\xi_{i,i+\delta}$ and μ_i which are to be determined self-consistently. However, supposing that except for nearest neighbors of the impurity, $\xi_{i,i+\delta}$ and μ_i practically coincide with the corresponding quantities for the host, ξ_M and μ (this will be confirmed below by our results), we may put in Eq. (6)

$$\xi_{i,i+\delta}=\begin{cases}\xi, & i=0\\ \xi', & i+\delta=0\\ \xi_M, & \text{otherwise}\end{cases},\quad \mu_i-\mu=\begin{cases}\delta\mu_0, & i=0\\ \delta\mu_1, & i+\delta=0\\ 0, & \text{otherwise.}\end{cases} \tag{8}$$

Note that $\xi\neq\xi'$ because of non-Hermiticity of the representation (4). Taking into account Eq. (4) the spin correlation function for impurity spin and its nearest neighbors has the form

$$K\equiv|\langle \mathbf{S}_0\mathbf{S}_\delta\rangle|=\xi\xi'. \tag{9}$$

Under the approximation (8) the Hamiltonian (6) takes the form

$$\mathcal{H}=\mathcal{H}_0+V, \tag{10}$$

where

$$\mathcal{H}_0=J\xi_M\sum_{i\delta}\ [a_i^\dagger a_i-a_{i+\delta}^\dagger a_i+(2S+1)c_i^\dagger c_i]$$
$$+(H_A-\mu)\sum_i\ [a_i^\dagger a_i+(2S+1)c_i^\dagger c_i] \tag{11}$$

is the standard SSWT Hamiltonian without impurities[15] and

$$V=(J'\xi-J\xi_M)\sum_\delta\ [a_0^\dagger a_0-a_\delta^\dagger a_0+(2S'+1)c_0^\dagger c_0]$$
$$+(J'\xi'-J\xi_M)\sum_\delta\ [a_\delta^\dagger a_\delta-a_0^\dagger a_\delta+(2S+1)c_\delta^\dagger c_\delta]$$
$$+\delta\mu_0 b_0^\dagger b_0+\delta\mu_1\sum_\delta\ a_\delta^\dagger a_\delta \tag{12}$$

is the impurity-induced perturbation part. To diagonalize $\mathcal{H}$ we introduce the Green's functions

$$G_{ij}^0(\omega)=\langle\langle a_j|a_i^\dagger\rangle\rangle_\omega^0=\sum_{\mathbf{q}}\ \frac{1}{\omega-E_{\mathbf{q}}}e_i^{i\mathbf{q}(\mathbf{R}_i-\mathbf{R}_j)},$$
$$G_{ij}(\omega)=\langle\langle a_j|a_i^\dagger\rangle\rangle_\omega, \tag{13}$$

where the index 0 means that statistical averages are calculated with $\mathcal{H}_0$,

$$E_{\mathbf{q}}=\xi_M(J_0-J_{\mathbf{q}})+H_A-\mu,\quad J_{\mathbf{q}}=2J(\cos q_x+\cos q_y).$$

In the limit $R\gg1$ we find by using the saddle point approximation (see, e.g., Ref. 10)

$$G_{0R}^0(\omega)\sim\begin{cases}\exp(i\sqrt{\omega/J\xi_M}R)/\omega^{1/4}R^{1/2}, & 1\ll(\omega/J)^{1/2}R,\omega\ll1\\ -\ln(\omega/J) & (\omega/J)^{1/2}R\ll1.\end{cases} \tag{14}$$

The perturbation V can be written in the matrix form

$$V=\sum_{i,,j=0}^{4} V_{ij}a_i^\dagger a_j+\sum_{i=0}^{4} R_i c_i^\dagger c_i, \tag{15}$$

where the indices i,j enumerate the impurity site and its four nearest neighbors. From Eq. (12) we have

$$V=\begin{pmatrix} 4\varepsilon & \gamma & \gamma & \gamma & \gamma \\ \gamma' & \rho & 0 & 0 & 0 \\ \gamma' & 0 & \rho & 0 & 0 \\ \gamma' & 0 & 0 & \rho & 0 \\ \gamma' & 0 & 0 & 0 & \rho \end{pmatrix}, \quad R=(2S+1)\begin{pmatrix} 4\varepsilon \\ \rho \\ \rho \\ \rho \\ \rho \end{pmatrix}, \tag{16}$$

where

$$\gamma'=J'\xi-J\xi_M, \quad \varepsilon=\gamma'+\delta\mu_0/4,$$

$$\gamma=J'\xi'-J\xi_M, \quad \rho=\gamma+\delta\mu_1.$$

Then we have the expression for the perturbed Green's function:[10]

$$\tilde{G}(\omega)=[1-\tilde{G}^0(\omega)V]^{-1}\tilde{G}^0(\omega), \tag{17}$$

where $\tilde{G}(\omega),\tilde{G}^0(\omega)$ are submatrices of matrices $G_{ij}(\omega),G_{ij}^0(\omega)$ with $i,j=0,\ldots,4$. Further we calculate the matrix G from Eq. (17) and the averages $\langle a_i^\dagger a_j\rangle$ from the spectral representation. Then we derive from Eqs. (4) and (8) the system of self-consistency equations

$$\xi=\overline{S_1}-\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}N(\omega)\operatorname{Im}\tilde{G}_{10}^R(\omega),$$

$$\xi'=\overline{S_0}-\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}N(\omega)\operatorname{Im}\tilde{G}_{01}^R(\omega), \tag{18}$$

where $N(\omega)=[\exp(\omega/T)-1]^{-1}$ is the Bose distribution function, $\tilde{G}^R(\omega)=\tilde{G}(\omega+i\delta)$, $\delta\to+0$. The integration region in Eq. (18) is in fact $\alpha\leqslant\omega\leqslant 2\xi_M J_0+\alpha$, $\alpha=H_A-\mu$. The expressions for the site magnetizations take the form

$$\overline{S_0}=S'+\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}N(\omega)\operatorname{Im}\tilde{G}_{00}^R(\omega)+(2S'+1)N(E_0),$$

$$\overline{S_1}=S+\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}N(\omega)\operatorname{Im}\tilde{G}_{11}^R(\omega)+(2S+1)N(E_1), \tag{19}$$

where $E_i=(2S_i+1)J\xi_M+\alpha-\delta\mu_i$ is the pseudofermion energy at the site i ($S_i=S$ for $i\neq 0$ and $S_i=S'$ for $i=0$). In the case of a pure system ($V=0$) we have $\tilde{G}=\tilde{G}^0$ and the values $\overline{S_i},\xi_{i,i+\delta},\mu_i$ are independent of i, so that the system of equations (18), (19) reduces to that of Ref. 15.

In the presence of impurity, the system of equations (18), (19) was solved numerically by the iteration method. First, the site magnetizations were excluded from Eq. (18), and the integrals in the right-hand sides were calculated for the values of short-range order (SRO) parameters corresponding to the pure crystal. Then the equations were iterated until a self-consistent solution was obtained. Finally, the magnetizations of impurity site and its nearest neighbors were calculated by using Eq. (19). The results of numerical calculations of magnetizations $\overline{S_0},\overline{S_1}$ and short-range order parameters ξ,ξ' vs temperature according to Eqs. (18) and (19) for the impurity-host system are presented in Figs. 1 and 2. Figure 1 presents also for comparison the results of the standard spin-wave (SW) theory [which correspond, in our notations, to $\xi_M=\xi=\xi'=S$, pseudofermion occupation numbers $N(E_i)$

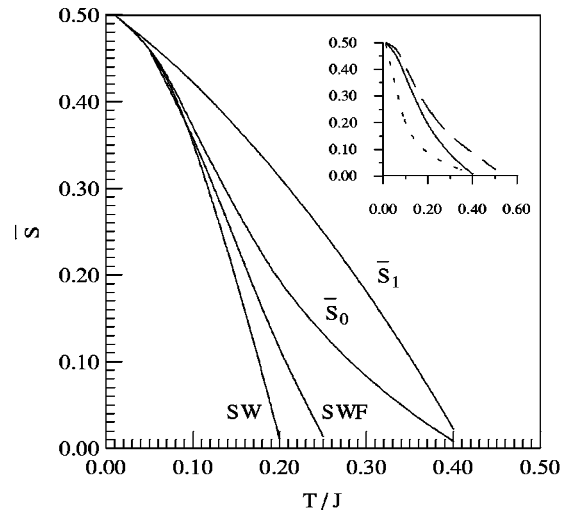

FIG. 1. The temperature dependence of the magnetizations for impurity site $\overline{S_0}$, and for nearest-neighbor sites $\overline{S_1}$ ($S=S'=1/2$, $H_A/J=10^{-3}$, $J'/J=0.15$). The results of the magnetization for the impurity site in the standard (non-self-consistent) spin-wave approach without (SW) and with (SWF) introducing Fermi operators [see Eq. (4)] are presented for comparison. The inset shows the temperature dependence of the impurity site magnetization $\overline{S_0}$ at $H_A/J=10^{-3}$, $J'/J=0.15$ (solid line), $H_A/J=10^{-3}$, $J'/J=0.05$ (short-dashed line), $H_A/J=10^{-2}$, $J'/J=0.15$ (long-dashed line).

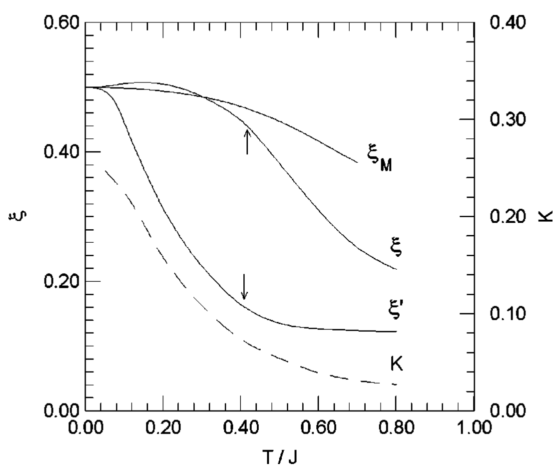

FIG. 2. The temperature dependence of the short-range order parameters ξ,ξ' (solid lines, left scale) and correlation function $K=\langle \mathbf{S}_0\mathbf{S}_\delta\rangle$ (long-dashed line, right scale) for the same parameter values as in Fig. 1. Arrows show the value of the Curie temperature. For comparison, the corresponding short-range order parameter in the ideal crystal, ξ_M, is shown.

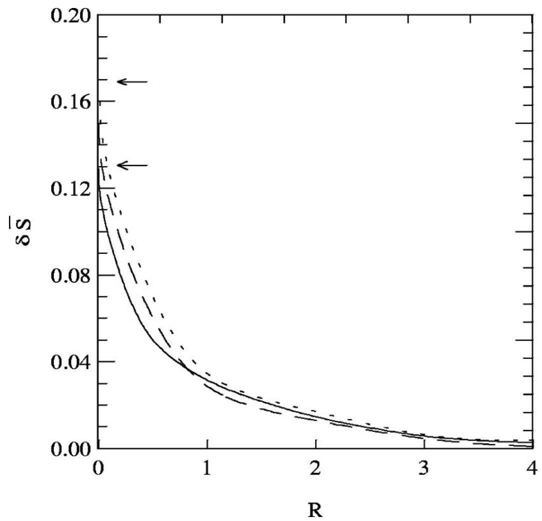

FIG. 3. The distribution of magnetization around the impurity for the same parameter values as in Fig. 1, $T=0.3J$. Arrows show the value of magnetization disturbance at the impurity site ($R=0$).

being replaced by zero] and spin-wave theory with introducing pseudofermions (SWF). We see that the impurity magnetization has an anomalous behavior at temperatures $T \sim J'$. The inset of Fig. 1 shows this dependence at different H_A/J, J'/J. A sharp decrease of impurity-site magnetization at $T\sim J'$ can be easily obtained already in the simple mean-field approximation, but detailed description of this behavior requires more complicated methods. The standard SW, as well as the SWF solutions, does not show this anomaly, so we can conclude that it is caused by both dynamic and kinematic interactions of spin waves. The situation is similar to the 3D case where using the Tyablikov approximation results in a strong modification of the magnetization behavior in this temperature interval.[10] One can see that, owing to a sharp decrease of ξ', the correlations between the impurity site and its nearest neighbors decrease with temperature more rapidly than those in an ideal crystal.

In the ground state the disturbance of magnetization is localized at the impurity site and equals $S'-S$. To calculate the magnetization distribution around the impurity at finite temperatures we need the full matrix G. It may be shown (see, e.g., Ref. 10) that the latter quantity is given by

$$G=G^0+\widetilde{G}^{N0}V\frac{1}{1-\widetilde{G}^0V}\widetilde{G}^{0N}, \tag{20}$$

where $\widetilde{G}^{0N}$ is the submatrix of G^0_{ij} with $i=0,\ldots,4$, $j=0,\ldots,N$, and $\widetilde{G}^{N0}$ is the conjugated matrix. Using Eq. (20) we can find the averages needed. The results of numerical calculation of magnetization disturbance for different values of J'/J, H_A/J are presented in Fig. 3. One can see that at $R>0$ all the results practically coincide; this takes place also in the limiting case where $J'=0$ (or in the case of the vacancy with $S'=0$). One can see that the change of magnetization around the impurity rapidly decreases with increasing distance from the impurity site, so that the magnetization disturbance practically vanishes at the distance of four coordination spheres.

Now we discuss briefly the limit $H_A\to 0$ which corresponds to the 2D isotropic magnets. Although the site magnetizations are changed strongly with changing H_A (the finite-temperature site magnetizations vanish at $H_A\to 0$ and the susceptibility $\chi=\partial\bar{S}/\partial H_A$ is divergent near $T=0$), it may be checked analytically that the derivative $\partial\xi/\partial H_A$ remains finite at $H_A\to 0$. Thus the SRO parameters are smooth functions in the limit $H_A\to 0$ and practically coincide with those calculated above for $H_A=10^{-3}\ J$.

III. ANTIFERROMAGNETIC IMPURITY IN FERROMAGNETIC HOST

Further we consider an AFM impurity in FM host [$J>0$, $J'<0$ in Eq. (3)]. After passing to the local coordinate system at the impurity site, we have to use the representation

$$S_0^+=\sqrt{2S'}b_0^\dagger,\quad S_0^z=-S'+b_0^\dagger b_0+(2S'+1)d_0^\dagger d_0,$$

$$S_0^-=\sqrt{2S'}\left(b_0-\frac{1}{2S'}b_0^\dagger b_0 b_0\right)-2\frac{2S'+1}{2S'}d_0^\dagger d_0 b_0, \tag{21}$$

where $b_0^\dagger,b_0$ are the Bose operators and $d_0^\dagger,d_0$ are the Fermi operators. Then, in the mean-field approximation, the Hamiltonian (1) takes the form

$$\begin{aligned}\mathcal{H}=&\frac{1}{2}J\sum_{i,i+\delta\neq 0}\xi_{i,i+\delta}[a_i^\dagger a_i-a_{i+\delta}^\dagger a_i+(2S+1)b_i^\dagger b_i]\\&+|J'|\sum_\delta\{\xi[a_\delta^\dagger a_\delta-b_0a_\delta+(2S'+1)b_\delta^\dagger b_\delta]\\&+\xi'[b_0^\dagger b_0-b_0^\dagger a_\delta^\dagger+(2S'+1)c_0^\dagger c_0]\}\\&+\sum_{i\neq 0}(H_A-\mu_i)[a_i^\dagger a_i+(2S+1)b_i^\dagger b_i]+(H_A-\mu_0)\\&\times[b_0^\dagger b_0+(2S'+1)c_0^\dagger c_0],\end{aligned} \tag{22}$$

where

$$\xi=\overline{S_0}+\langle d_0^\dagger a_\delta^\dagger\rangle,$$

$$\xi'=\overline{S_1}+\langle a_\delta d_0\rangle.$$

As in ferromagnetic case, we use the approximation $\xi_{i,i+\delta}\simeq\xi_M$ $(i,i+\delta\neq 0)$. To diagonalize Eq. (22) we introduce, following Ref. 10, the ‘‘hole’’ creation and annihilation operators $a_0^\dagger$, a_0 by the canonical transformation

$$a_0=d_0^\dagger,\quad a_0^\dagger=-d_0.$$

As well as in the case of FM impurity, we use the approximation (8). We introduce also the Green's functions (13) and represent the Hamiltonian as Eq. (10) with the parameters of the matrix V, Eq. (16),

$$\gamma'=-J'\xi+J\xi_M,\quad \varepsilon=-J'\xi-J\xi_M+\delta\mu_0/4,$$

$$\gamma=J'\xi'+J\xi_M,\quad \rho=J'\xi-J\xi_M+\delta\mu_1.$$

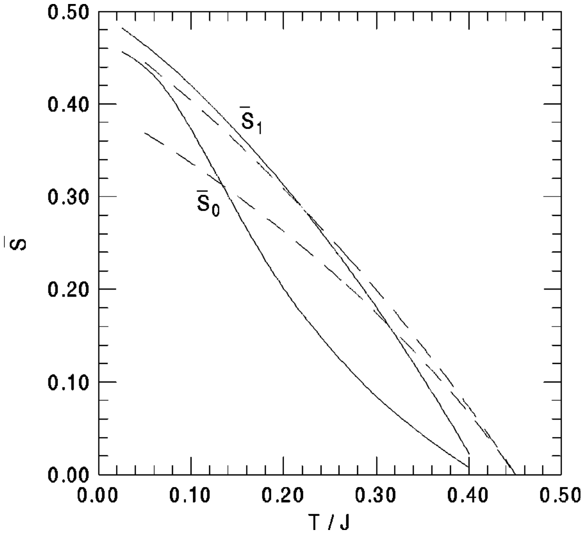

FIG. 4. The temperature dependence of the magnetizations for impurity site $\overline{S_0}$, and for nearest-neighbor sites $\overline{S_1}$ in the case of antiferromagnetic impurity in the ferromagnetic host with $S=S'=1/2$, $H_A/J=10^{-3}$, $J'/J=-0.15$ (solid lines), and $J'/J=-1$ (long-dashed lines).

Then we have the same equation (17) for the full Green's function as in the case of FM impurity; the self-consistency equations also have the same form as Eqs. (18) and (19). Unlike the FM impurity case, the full Green's function has a pole at $\omega=-\omega_0<0$.[10] To take into account the contribution from this pole to the averages needed we deform the integration path in the spectral representation for the Green's function in the complex plane:

$$\langle a_j^\dagger a_i\rangle = -\frac{1}{\pi}\int_{-\infty}^{+\infty} d\omega N(\omega)\,\mathrm{Im}\,G_{ij}^R(\omega)$$

$$= \int_C \frac{d\omega}{2\pi i}N(\omega)G_{ij}(\omega) - TG_{ij}(0). \tag{23}$$

The closed contour C has anticlockwise orientation and is selected in such a way that all the singularities of $G(\omega)$ lie inside C, but all the frequencies $\omega_n = 2\pi nT(n\neq 0)$ lie outside it. The last term in Eq. (23) corresponds to the contribution from $\omega=0$, which is to be subtracted explicitly.

The results of numerical solution of Eqs. (18) and (19) with the use of Eq. (23) for different values of impurity-host coupling are presented in Fig. 4.

The AFM impurity induces the disturbance of host magnetization already at $T=0$. Using the sum rule

$$\pi\sum_i \,\mathrm{Im}[G_{ii}(\omega+i\delta)-G_{ii}^0(\omega+i\delta)] \tag{24}$$

$$=\frac{\partial}{\partial\omega}\mathrm{Im}\ln\det[1-G^0(\omega+i\delta)V] \tag{25}$$

which follows from Eq. (20) and taking into account that $\det[1-G^0(\omega)V]$ has a zero at $\omega=-\omega_0$ we obtain

$$\langle b_0^+ b_0\rangle_{T=0} = \sum_{i>0}\,\langle a_i^+ a_i\rangle_{T=0} \tag{26}$$

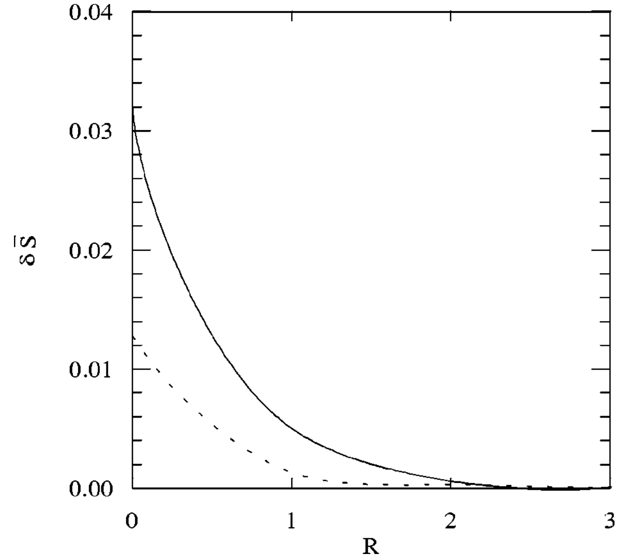

FIG. 5. The distribution of magnetization around the antiferromagnetic impurity in the 2D isotropic ferromagnet at $T=0$, $J'/J=0.15$ (solid line), and $J'/J=0.05$ (dashed line).

so that the total disturbance of magnetization equals $S+S'$.[10] The distribution of magnetization around the impurity site is shown in Fig. 5. At large R the contribution from the pole $\omega=-\omega_0$ gives the main contribution to the magnetization disturbance which is proportional to $\exp(-R\sqrt{\omega_0/J})/R$ and differs from that in the $3D$ case[10] by a preexponential factor only.

IV. THE CASE OF AN ANTIFERROMAGNETIC HOST

Now we consider an antiferromagnet with the Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j + \mathcal{H}_A$$

with $J_{ij}<0,\eta_{ij}<0$. In the case of two sublattices A,B and for the antiferromagnetically coupled impurity spin in the A sublattice we have to use the representation

$$S_i^+ = \sqrt{2S}a_i,\quad S_i^z = S - a_i^\dagger a_i - (2S+1)c_i^\dagger c_i,$$

$$S_i^- = \sqrt{2S}\left(a_i^\dagger - \frac{1}{2S}a_i^\dagger a_i^\dagger a_i\right) - \frac{2(2S+1)}{2S}a_i^\dagger c_i^\dagger c_i \tag{27}$$

for $i\in A$ and

$$S_i^+ = \sqrt{2S}b_i^\dagger,\quad S_i^z = -S + b_i^\dagger b_i + (2S+1)d_i^\dagger d_i,$$

$$S_i^- = \sqrt{2S}\left(b_i - \frac{1}{2S}b_i^\dagger b_i b_i\right) - \frac{2(2S+1)}{2S}d_i^\dagger d_i b_i \tag{28}$$

for $i\in B$ where $a_i^\dagger, a_i$ and $b_i^\dagger, b_i$ are the Bose operators and $c_i^\dagger, c_i$ and $d_i^\dagger, d_i$ are the Fermi operators (for $i=0$ one has again to replace $S\to S'$ in this representation). After standard decouplings the Hamiltonian takes the form

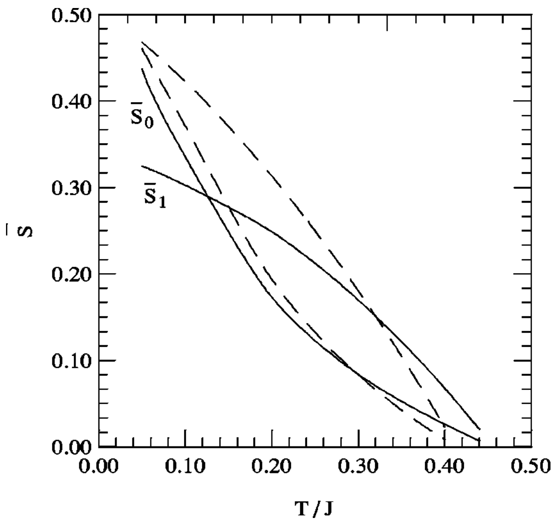

FIG. 6. The temperature dependence of magnetizations for impurity site $\overline{S_0}$ and nearest-neighbor sites $\overline{S_1}$ in an antiferromagnet with $S=S'=1/2$, $H_A/J=10^{-3}$, $J'/J=0.15$. Dashed lines show the corresponding results for a ferromagnet (Fig. 1).

$$\mathcal{H}=\sum_{i\in A,\delta}|J_{i,i+\delta}|\xi_{i,i+\delta}[a_i^\dagger a_i-b_{i+\delta}a_i+(2S_i+1)c_i^\dagger c_i]$$

$$+\sum_{i\in B,\delta}|J_{i,i+\delta}|\tilde{\xi}_{i,i+\delta}[b_{i+\delta}^\dagger b_{i+\delta}-b_{i+\delta}^\dagger a_i^\dagger$$

$$+(2S_i+1)c_i^\dagger c_i]+\sum_{i\in A}(H_A-\mu_i)[a_i^\dagger a_i+(2S_i+1)c_i^\dagger c]$$

$$+\sum_{i\in B}(H_A-\mu_i)[b_i^\dagger b_i+(2S_i+1)d_i^\dagger d_i], \tag{29}$$

where

$$H_A=(2S-1)D+S\sum_i|\eta_{i,i+\delta}| \tag{30}$$

and

$$\xi_{i,i+\delta}=\overline{S_{i+\delta}}+\langle b_{i+\delta}^\dagger a_i^\dagger\rangle,\quad \tilde{\xi}_{i,i+\delta}=\overline{S_i}+\langle a_i b_{i+\delta}\rangle. \tag{31}$$

For the correlation function K we have the same expression (9) as in the FM case with $\xi=\xi_{01},\xi'=\tilde{\xi}_{01}$. To diagonalize Eq. (29) we introduce the operators

$$A_i=\begin{cases}a_i & i\in A\\ b_i^\dagger & i\in B\end{cases}$$

and the Green's functions:

$$\hat{G}_{ij}^0(\omega)=\langle\langle A_i|A_j^\dagger\rangle\rangle_\omega$$

$$=G_{ij}^0(\Omega)\begin{cases}r, & i,j\in A\\ r^{-1}, & i,j\in B\\ 1, & \text{otherwise},\end{cases} \tag{32}$$

where

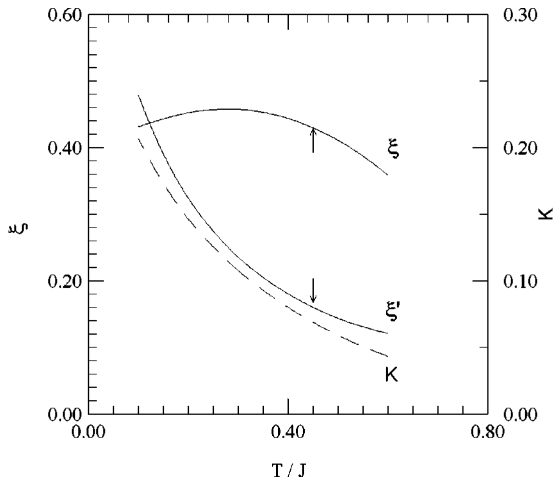

FIG. 7. The temperature dependence of the short-range order parameters ξ,ξ' and correlation function $K=-\langle\mathbf{S}_0\mathbf{S}_\delta\rangle$ for the same parameter values as in Fig. 6. Arrows show the value of the Néel temperature.

$$r=\left(\frac{\lambda+\omega}{\lambda-\omega}\right)^{1/2},\quad \Omega=\lambda-\sqrt{\lambda^2-\omega^2},$$

$$\lambda=|J_0|\xi_M+H_A-\mu.$$

Using the approximation (8) we get the same expression for the Green's function (17) with $\tilde{G}^0(\omega)$ being the 5×5 submatrix of $\hat{G}_{ij}^0(\omega)$, and analogously for $\tilde{G}(\omega)$. In this notation the self-consistent equations for the site magnetizations and short-range order parameters have the same forms as in FM case, see Eqs. (19) and (18). In the case of the pure system we now have $\hat{G}=\hat{G}_0$ and we again reproduce the results of Ref. 15.

The results of numerical calculations for the AFM impurity system case are shown and compared with those for the FM case in Fig. 6. If the impurity spin is weakly coupled to the host, the behavior of magnetization in AFM and FM

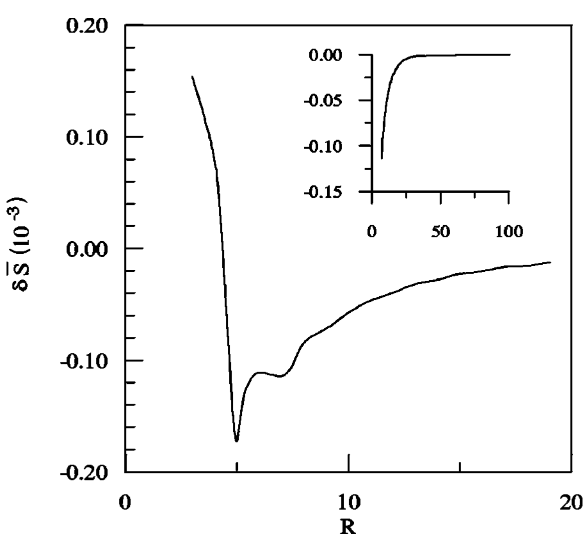

FIG. 8. The distribution of magnetization around impurity in the 2D isotropic antiferromagnet at $T=0$. The inset shows the picture at large R.

situations is very close, except for the region near the magnetic ordering temperature ($T_N > T_C$ because of quantum fluctuations). At the same time, the nearest-neighbor magnetizations are strongly different and demonstrate a behavior that is typical for the corresponding hosts. One can also see that SSWT leads to unambiguous results at low T, where the impurity magnetization turns out to be greater than the host one. The difference between magnetizations of impurity and host increases with decreasing the value of J'/J and decreases with increasing temperature. Thus SSWT predicts strong influence of quantum fluctuations on magnetization in the case of weakly magnetic impurities.

The results of calculating the short-range order parameters ξ, ξ' and the correlation function K are presented in Fig. 7. The parameter ξ has a nonmonotonic temperature dependence. At the same time, the temperature dependence of the correlation function of the impurity spin with its nearest neighbors is monotonic and more rapid than that for correlation functions between spins in the host.

To calculate the total magnetization disturbance we use the sum rule for the Green's functions (32)

$$\pi \sum_i (-1)^i \, \mathrm{Im}[\hat{G}_{ii}(\omega + i\delta) - \hat{G}^0_{ii}(\omega + i\delta)] = \frac{\partial}{\partial \omega} \mathrm{Im} \ln \det[1 - \hat{G}^0(\omega + i\delta) V]. \tag{33}$$

Since $\det(1 - \hat{G}^0 V)$ has no zeros at $\omega < 0$, we obtain at $T = 0$

$$\delta M = S' - S - \frac{1}{\pi} \mathrm{Im} \, \ln \det[1 - \hat{G}^0(\omega + i\delta) V]^0_{-\infty} = S' - S. \tag{34}$$

This result is valid also for a vacancy if we put $S' = 0$. For a ferromagnetically coupled impurity we have to replace in Eq. (34) $S' \to -S'$.

The distribution of magnetization around the impurity in the ground state of a 2D isotropic antiferromagnet is shown in Fig. 8. The magnetization of each sublattice decreases, so that corrections to the host magnetization have alternating signs. The values of sublattice magnetization disturbance are close to those in the spin-wave theory.[5] At large R, the main contribution to the disturbance of sublattice magnetization comes from the frequencies $\omega \ll J$. Expanding Eqs. (20) and (32) up to first order in ω/J, we derive

$$\delta \langle A_0^\dagger A_i \rangle \sim 1/R_i^3. \tag{35}$$

Note that in the 3D case this quantity demonstrates a more rapid decrease $1/R^4$, which may be obtained in the same manner.

V. CONCLUSIONS

To conclude, we have investigated 2D magnets with impurities for different signs of exchange integrals within the framework of self-consistent spin-wave theory.[11,12,15] This theory permits us to calculate both magnetization distribution and the correlation functions (short-range order parameters). For $T = 0$ modifications of the results of the standard spin-wave theory are small. At the same time, for finite temperatures, corrections owing to dynamic and kinematic interactions of spin waves turn out to be important. It should be stressed that despite the absence of long-range order in the isotropic 2D magnets at $T > 0$, the temperature dependence of the impurity-host correlation function K, Eq. (9), is similar to that in the 3D case, although in the latter case the main contribution to K equals $\overline{S_0}\,\overline{S_\delta}$.

The distribution of magnetization in the ground state was investigated in detail. In the nearest-neighbor approximation considered, the host magnetization disturbance decreases rapidly with distance from impurity, and the total change of magnetic moment equals $-S \pm S'$ depending on the sign of J'. More interesting situations occur in the case of the long-range exchange. So, in the case of FM impurity in the FM host with sufficiently strong negative next-nearest impurity-host exchange J'', the total magnetization change equals

$$\delta M = S' - S - 2 z_2 S \tag{36}$$

with z_2 the corresponding coordination number. In the case of FM impurity in the AFM host with large positive J'' we have

$$\delta M = S' - S + 2 z_2 S. \tag{37}$$

It would be of interest also to investigate the problem of a current carrier in the AFM host within a similar approach (e.g., within the t-J model, cf. Ref. 11).

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