PHYSICAL REVIEW B, VOLUME 63, 134408

Green's function theory of the spin-1 low-dimensional quantum *XY* ferromagnet

M. E. Gouvêa and A. S. T. Pires
Departamento de Física, ICEx, Universidade Federal de Minas Gerais, Belo Horizonte, CP 702, CEP 30123-970, MG, Brazil
(Received 12 September 2000; published 5 March 2001)

We calculate the spin-spin correlations and the magnetic susceptibility of the quantum one- and two-dimensional XY models with $S=1$, using the two-time Green's function method and performing a decoupling proposed by Kondo and Yamaji for cases with no long-range order. A set of self-consistent equations of the correlation functions are derived and solved numerically. We present results for the correlation functions, susceptibilities, and specific heat for the whole range of temperature.

DOI: 10.1103/PhysRevB.63.134408 PACS number(s): 75.10.Hk, 75.40.Cx

I. INTRODUCTION

Several techniques have been proposed to study magnetic models. However, some of these theories work well only into a specific and limited range of low or high temperatures. On the other hand, the two-time Green's function method[1] is known as the standard method which gives reasonable results for the thermodynamic properties over the whole temperature range. In the application of this method, the Tyablikov decoupling approximation[2] is usually used to obtain the approximate solution from an infinite set of coupled Green's functions. This method invokes the existence of long-range order. The decoupling procedure gives a spin-wave spectrum which depends on $\langle S^z \rangle$. This method has been recently used by Siurakshina *et al.*[3] to study the three-dimensional (3D) $S=1/2$ Heisenberg model with spatially anisotropic coupling on a simple cubic lattice

However, $\langle S^z \rangle$ vanishes in one and two dimensions (except for Ising-like anisotropies in 2D and some long-range-order interactions). In order to apply the two-time Green's function method to cases without long-range order, Kondo and Yamaji[4] and Knapp and ter Haar[5] proposed a decoupling at a stage one step further than Tyablikov. The decoupled Green's functions depend on averages such as $\langle S_0^z S_1^z \rangle$ and $\langle S_0^z S_2^z \rangle$ which are determined by self-consistency requirements. Then, the thermodynamic quantities can be calculated from the knowledge of these solutions.

As pointed out by Shimahara and Takada,[6] the advantages of the Kondo-Yamaji theory (KY) lie in the following points: (i) the KY theory is based on a clear physical picture; (ii) the KY theory interpolates between the high- and low-temperature limits with a unified picture over the whole temperature region; (iii) the KY theory does not violate the sum rule and the rotational symmetry.

Knapp and ter Haar[5] applied this higher order decoupling in a treatment of the 3D Heisenberg model paramagnetic phase. Later, Scales and Gersch[7] applied the procedure to study the 1D, 2D, and 3D antiferromagnetic Heisenberg models. Kondo and Yamaji[4] studied the one-dimensional $S=1/2$ isotropic ferro- and antiferromagnetic Heisenberg models. Their treatment gives reasonable features for the thermodynamic properties at all temperatures for both signs of the exchange. At high temperatures, they reproduced the correct results obtained by the high-temperature expansion method. On the other hand, the results at low temperature are similar to those of the modified spin-wave theory[8] and agree quite well to other results obtained by different techniques such as a numerical calculation for a finite chain.[9]

Later, Yamaji and Kondo[10] applied the technique to study the 2D ferromagnetic Heisenberg model. Uchinami *et al.*[11] studied the $S=1/2$ XY model by using the same method. The value of the nearest-neighbor correlation functions in 1D calculated by Uchinami *et al.* is in good agreement with the exact values calculated by Katsura *et al.*[12] Shimahara and Takada[6] applied the KY method with a semiphenomenological improvement to the 2D ferro- and antiferromagnetic Heisenberg models. Winterfeld and Ihle[13] extended Shimahara and Takada's procedure for the $S=1/2$ 2D antiferromagnetic model in order to obtain the dynamical spin-correlation function of this model. Bao *et al.*[14] generalized the KY technique to the 1D antiferromagnetic Heisenberg chain. The gap (predicted by Haldane) at null wave vector in the excitation spectrum appeared naturally in the analytical result. Kawabe[15] and later Fukumoto and Oguchi[16] studied the spin-1/2 antiferromagnetic XXZ model on a square lattice. Dong and Feng[17] studied the spin liquid state of the 2D Heisenberg antiferromagnet on a triangular lattice. The ground-state energy was found to be in very good agreement with the results obtained within the variational Monte Carlo method based on the resonating-valence-bond state. Song *et al.*[18] improved the decoupling approximation of the KY theory and applied it to study the spin-1/2 2D antiferromagnetic Heisenberg model with broken bonds at finite temperature. Ihle *et al.*[19] combined the spin-rotation invariant Green's function approach (using the same KY decoupling) to Lanczos diagonalization to study the order-disorder transition in the $S=1/2$ antiferromagnetic Heisenberg model with spatial anisotropy.

In this paper, we apply the KY procedure to the $S=1$ XY model described by the Hamiltonian

$$H=-2J\sum_{\langle ij\rangle}(S_i^x S_j^x + S_i^y S_j^y), \tag{1}$$

where the summation is taken over all nearest-neighbor pairs. We will discuss the one- and two-dimensional cases. The $S=1/2$ case has been rigorously solved for a linear chain[20] and treated in the framework of the KY theory by Uchinami *et al.*[11]

However, as pointed out by Bao *et al.*,[14] the KY decoupling procedure gives different results for integer and half-odd integer spins due to the distinct relations holding for the spin components S_i^α in each case: this difference justifies a study of the $S=1$ case. The 1D XY model is very interesting. In contrast to the Heisenberg isotropic ferromagnet model, the ground state here is no longer trivial. In fact, because $\langle N^{-1}\Sigma_n S_n^z\rangle=\langle S_T^z\rangle=0$, the ground state corresponds in the Bethe-ansatz picture to the lowest eigenvalue of the block of order

$$\binom{N}{N/2}.$$

In the $S=1/2$ case, the model can be transformed to noninteracting spinless fermions and solved exactly. For large values of spin S, Villain[21] has introduced a transformation leading to a semiclassical spin-waves theory which was used to study the 1D and 2D XY models. However, his procedure does not give the correct predicition for $S=1/2$. This failure in Villain's theory could be expected because the elementary excitations of his theory are magnons, whereas in the $S=1/2$ case the excitations are particle-hole pairs. Besides, Villain's treatment applies only to the low-temperature regime and the procedure we are going to use in this work, the Green's function technique, can be used for the whole temperature range. The 2D classical XY model has been studied intensively due the existence of the Kosterlitz-Thouless topological phase transition[22,23] in these models: the power-law behavior of the spin-correlation function has been obtained by several approaches but the quantum case can have different properties[24] and still deserves more attention.

In Sec. II, we outline the method and present the basic self-consistent equations for the spin-pair correlations and decoupling parameters as a function of the temperature. The self-consistent equations are solved analytically in the high-temperature limit in Sec. III. In Sec. IV the self-consistent equations are solved numerically in a wide temperature region using as starting point the high-temperature solutions obtained in the previous section.

II. GREEN'S FUNCTION FORMALISM

The two-time Green's function is defined as

$$\begin{aligned} G(i-j,t-t') &= -\imath\theta(t-t')\langle[A_i(t),B_j(t')]\rangle \\ &= \langle\langle A_i(t);B_j(t')\rangle\rangle, \end{aligned} \tag{2}$$

where $\theta(t)$ is the step function and $\langle\cdots\rangle$ denotes a thermal average. The time-Fourier transform of Eq. (2) satisfies the equation

$$\omega\langle\langle A;B\rangle\rangle=\frac{1}{2\pi}\langle[A,B]\rangle+\langle\langle[A,H];B\rangle\rangle \tag{3}$$

and the correlation function can be obtained by the spectral representation as

$$\langle AB\rangle=\imath\int_{\infty}^{\infty}d\omega[\langle\langle A;B\rangle\rangle_{\omega+\imath\varepsilon}-\langle\langle A;B\rangle\rangle_{\omega-\imath\varepsilon}]\frac{1}{e^{\beta\omega}-1}. \tag{4}$$

The equations of motion of the Green's function for our model are

$$\omega\langle\langle S_0^x;S_n^x\rangle\rangle=-\imath 2J\sum_\delta \langle\langle S_0^zS_\delta^y;S_n^x\rangle\rangle \tag{5}$$

and

$$\omega\langle\langle S_0^z;S_n^z\rangle\rangle=-\imath 2J\sum_\delta \{\langle\langle S_\delta^xS_0^y-S_\delta^yS_0^x;S_n^z\rangle\rangle\} \tag{6}$$

where δ denotes the vector to the nearest-neighbor site. The higher-order Green's function on the right-hand side of Eq. (5) satisfies the equation

$$\begin{aligned} \omega\langle\langle S_0^zS_\delta^y;S_n^x\rangle\rangle=&\frac{\imath}{2\pi}(-\langle S_0^zS_\delta^z\rangle\delta_{n,\delta}+\langle S_0^yS_\delta^y\rangle\delta_{n,0}) \\ &+\imath 2J\sum_{\delta'}\{\langle\langle S_{\delta'}^yS_\delta^yS_0^x-S_0^yS_\delta^yS_{\delta'}^x \\ &+S_0^zS_\delta^zS_{\delta+\delta'}^x;S_n^x\rangle\rangle\}. \end{aligned} \tag{7}$$

We remark that, for $S=1/2$, some terms cancel each other in Eq. (7). According to the KY method, we decouple the higher-order Green's functions on the right-hand side of Eq. (7) as

$$\begin{aligned} \langle\langle S_i^yS_j^yS_k^x;S_n^x\rangle\rangle&=\alpha^x\langle S_i^yS_j^y\rangle\langle\langle S_k^x;S_n^x\rangle\rangle, \\ \langle\langle S_i^zS_j^zS_k^x;S_n^x\rangle\rangle&=\alpha^x\langle S_i^zS_j^z\rangle\langle\langle S_k^x;S_n^x\rangle\rangle. \end{aligned} \tag{8}$$

The decoupling parameter α^x has been introduced in order to not violate the sum rule of the correlation function and is determined so as to satisfy $C_0^x\equiv\langle(S_i^x)^2\rangle=\langle(S_i^y)^2\rangle=1-\langle(S_i^z)^2\rangle/2$. From Eqs. (5), (7), and (8) and taking the Fourier transform with respect to the lattice points, we find

$$G_q^x(\omega)=\frac{A_q^x}{\omega^2-(\omega_q^x)^2}, \tag{9}$$

where

$$A_q^x=2zJ(C_1^x-\gamma_qC_1^z), \tag{10}$$

$$(\omega_q^x)^2=(2J)^2\alpha^xz[\varepsilon_q(1-\gamma_q)+\Delta], \tag{11}$$

where z is the coordination number, $\gamma_q=(1/z)\Sigma_\delta e^{\imath\vec{k}\cdot\vec{\delta}}$, and the parameters ε_q, Δ_q, and the correlations C_n^σ ($\sigma=x,z$, $n=0,1,2$) are defined by

$$\varepsilon_q=z[C_1^x-(1+\gamma_q)C_1^z], \tag{12}$$

$$\Delta=z(C_1^z-C_1^x)+C_0^x+C_2^x, \tag{13}$$

$$C_1^\sigma = \frac{1}{z}\sum_\delta \langle S_0^\sigma S_\delta^\sigma \rangle, \tag{14}$$

$$C_2^x = \frac{1}{z(z-1)}\sum_{\delta,\delta'} \langle S_0^x S_{\delta+\delta'}^x \rangle. \tag{15}$$

From Eq. (6), we obtain

$$\omega\langle\langle S_0^x S_\delta^y ; S_n^z\rangle\rangle = -\frac{\imath}{2\pi}[\langle S_0^x S_\delta^x\rangle(\delta_{n,0}-\delta_{n,\delta})] + \imath 2J\sum_{\delta'} \times\{-\langle\langle S_0^x S_\delta^z S_{\delta+\delta'}^x ; S_n^z\rangle\rangle + \langle\langle S_0^z S_\delta^y S_{\delta'}^y ; S_n^z\rangle\rangle\} \tag{16}$$

and a similar expression for the other Green's function. The decoupling is now written as

$$\langle\langle S_i^x S_j^z S_k^x ; S_n^z\rangle\rangle = \alpha^z \langle S_i^x S_k^x\rangle\langle\langle S_j^z ; S_n^z\rangle\rangle,$$

$$\langle\langle S_i^z S_j^z S_k^x ; S_n^x\rangle\rangle = \alpha^x \langle S_i^z S_k^z\rangle\langle\langle S_j^x ; S_n^x\rangle\rangle, \tag{17}$$

where the determination of the α^z is discussed in Sec. IV From Eqs. (6), (16), and (17) and using the following relation for $S=1$:

$$S_n^x S_n^x + S_n^y S_n^y = 2 - S_n^z S_n^z, \tag{18}$$

we obtain

$$G_q^z(\omega) = \frac{A_q^z}{\omega^2 - (\omega_q^z)^2}, \tag{19}$$

where

$$A_q^z = 4zJC_1^x(1-\gamma_q), \tag{20}$$

$$(\omega_q^z)^2 = (2J)^2 2zB(1-\gamma_q), \tag{21}$$

with $B = 1+\alpha^z(C_2^x - C_0^z/z + C_1^z)$.

The relations (14) and (15) lead to the five self-consistent equations

$$C_0^\sigma = \frac{1}{N}\sum_q \frac{A_q^\sigma}{2\omega_q^\sigma}\coth\left(\frac{\beta\omega_q^\sigma}{2}\right), \tag{22}$$

$$C_1^\sigma = \frac{1}{N}\sum_q \frac{\gamma_q A_q^\sigma}{2\omega_q^\sigma}\coth\left(\frac{\beta\omega_q^\sigma}{2}\right), \tag{23}$$

$$C_2^x = \frac{1}{N}\sum_q \frac{z\gamma_q^2-1}{z-1}\,\frac{A_q^\sigma}{2\omega_q^\sigma}\coth\left(\frac{\beta\omega_q^\sigma}{2}\right). \tag{24}$$

The static susceptibilities can be evaluated by the expression

$$\frac{\chi^\sigma}{N} = -\lim_{q\to 0} G_q^\sigma(\omega=0) = \frac{A_{q=0}^\sigma}{(\omega_{q=0}^\sigma)^2} \tag{25}$$

or, explicitly,

$$\frac{\chi^x}{N} = \frac{(C_1^x - C_1^z)}{2J\alpha^x\Delta}, \tag{26}$$

$$\frac{\chi^z}{N} = \frac{C_1^x}{2J\left[1+\alpha^z\left(C_2^x - \frac{C_z^0}{z} + C_1^z\right)\right]}. \tag{27}$$

III. ANALYTIC RESULTS IN THE HIGH-TEMPERATURE LIMIT

In this limit, we can develop $\coth(\beta\omega_q^\alpha/2)$ in Eqs. (22)–(24) as a Taylor expansion in powers of β obtaining

$$\frac{2}{T} \approx \sum_q A_q^\alpha\left(\frac{T}{(\omega_q^\alpha)^2} + \frac{1}{12T}\right); \tag{28}$$

$$C_1^z \approx -\frac{zC_1^x}{3\Theta}\sum_q \gamma_q^2; \tag{29}$$

$$C_1^x \approx \frac{\Theta}{2\alpha^x}\sum_q \frac{\gamma_q(C_1^x - \gamma_q C_1^z)}{2/3 - z\gamma_q C_1^x}; \tag{30}$$

$$C_2^x \approx \frac{\Theta C_1^x}{2\alpha^x C_0^x}\sum_q \frac{z\gamma_q^2 - 1}{1 - \frac{2C_1^x\gamma_q}{C_0^x}}, \tag{31}$$

where $\Theta = T/J$ is the reduced temperature, and we have used $C_0^x = C_0^z = 2/3$ in the high-temperature limit. In 1D, the above expressions lead to

$$\alpha^z = \alpha^x = 1, \tag{32}$$

$$C_1^x \approx \frac{8}{9\Theta}; \quad C_1^z \approx -\frac{C_1^x}{3\Theta}; \quad C_2^x \approx \frac{32}{27\Theta^2}. \tag{33}$$

Inserting these asymptotic solutions in Eqs. (26) and (27), we obtain, in the high-temperature limit, $\chi_x \sim \chi_z \sim 2/(3T)$, in accordance to the Curie-Weiss law.

IV. NUMERICAL RESULTS

The basic Eqs. (22)–(24) of the present theory are quite complicated and therefore we were able to obtain analytical evaluations of the spin-pair correlations C_0^x, C_0^z, C_1^x, C_1^z, C_2^x, and the decoupling parameters α^x and α^z only in the high-temperature region. For lower temperatures, we had to use numerical methods to solve those transcendental equations for the 1D and 2D cases, as discussed in the following two subsections.

A. Linear *XY* chain

In order to solve the set of five self-consistent equations given by Eqs. (22)–(24) in 1D, we use $z=2$ and $\gamma_q = \cos q$. However, we have seven parameters (five spin correlations and two decoupling parameters) to determine and only five

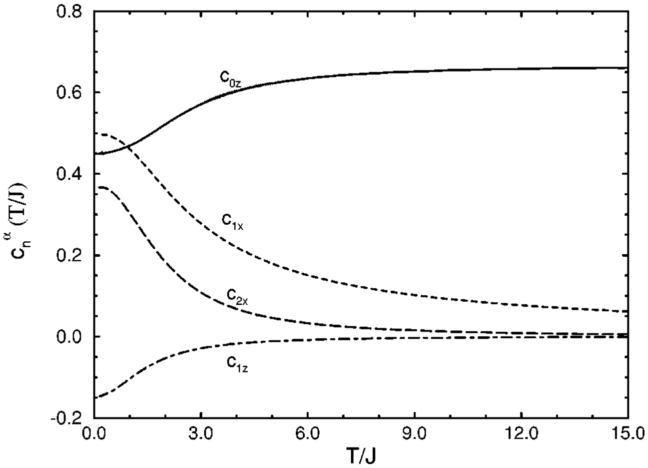

FIG. 1. Temperature dependence of the correlation functions for the 1D XY model with $S=1$, as explained in the text.

equations to use. One additional equation is provided by the sum rule $C_0^x=1-C_0^z/2$, but another equation is still required in order to determine all parameters.

We note that decoupling approximations like we have used here, are proposed for convenience and there is no standard approach to determine, *a priori*, which values the parameters α^x and α^z should assume. This issue was discussed by Kawabe[15] in his analysis of the $S=1/2$ 2D ferromagnetic XY model. The XXZ antiferromagnetic 2D model (spin 1/2) was studied by Fukumoto and Oguchi[16] who, in fact, introduced two decoupling parameters in the way described here. However, those authors restricted their study to the neighborhood of the isotropic Heisenberg point-avoiding the XY regime—and setting $C_0^x=C_0^z=S(S+1)/3$ in the whole temperature range using these conditions to determine the two decoupling parameters. In our XY case, due to the easy-plane anisotropy, it does not seem a ''natural'' choice to require that, for all temperatures, the spin correlation C_0^x has the same value as the C_0^z correlation: it is more reasonable to expect that, as the temperature decreases, the in-plane C_0^x correlation becomes greater than the out-of-plane correlation. In fact, we tried to solve our five self-consistent equations imposing $C_0^x=2/3$ and $C_0^z=2/3$ as conditions to determine α^x and α^z and obtained an unphysical result since all the spin-pair correlations were decreasing with decreasing temperature. We then adopted two slightly different arbitrary ways to determine the decoupling parameters and solve our problem: (i) we chose to use $\alpha^x=\alpha^z$, and, (ii) to fix one of the parameters, α^z, at its high-temperature value ($\alpha^z=1$), and determine the other one by imposing the sum rule, $C_0^x=1-C_0^z/2$, as discussed in Sec. (II).

For each choice, we can then solve the five self-consistent equations numerically with the iteration technique using Eqs. (32) as the initial conditions. The correlations obtained with the two ways of determining the decoupling parameters do not differ appreciably in the whole temperature range. Figure 1 shows the C_0^z, C_1^x, C_1^z, and C_2^x spin correlations as obtained numerically: notice that, as expected, the $C_0^z=\langle S_n^z S_n^z\rangle$ decreases with decreasing temperature. In order to

TABLE I. Values for the C_0^x, C_0^z, C_1^x, C_1^z, and C_2^x correlations at $T=0$ extracted from Villain's (Ref. 21) spin-wave theory (SW) and self-consistent harmonic approximation (SCHA) compared to the results obtained in the present work.

	C_0^x	C_0^z	C_1^x	C_1^z	C_2^x
SW theory	0.6817	0.6366	0.4958	−0.2122	0.446
SCHA	0.7765	0.4470	0.4935	−0.1491	
Present	0.7752	0.4496	0.4974	−0.1497	0.3657

ascertain some accuracy to the approximations done in this work, let us compare the results obtained by us for $T\to 0$ to the ones obtained by Villain[21] at $T=0$. Table I shows the results of the present work and those obtained by Villain by using a spin-wave (SW) theory and, also, by a self-consistent harmonic approximation (SCHA). Up to our knowledge, exact results or Monte Carlo simulations for the quantum $S=1$ XY model, in 1D or 2D, are not available in the literature and thus we cannot make a more precise checking of our methodology. Recently, Schulz[25] studied the XY model for $S=1$ at $T=0$ using a continuum representation, but he derived only the asymptotic behavior for the correlation functions. The expressions obtained by Villain, from SW and SCHA techniques, do also include approximations and are quite complicated (this being the reason by which we did not try to plot his predictions for $T>0$ together with our results in Fig. 1) but the agreement between his results and ours is very good—mainly for the comparison using the SCHA values. The calculation of C_2^x using Villain's SCHA result is cumbersome even at $T=0$ and, then, this value is not specified in Table I.

The internal energy of the XY model is proportional to the spin-pair correlation C_1^x and the specific heat c_v can be easily obtained from

$$\frac{c_v}{JN}=-z\frac{dC_1^x}{dT}. \tag{34}$$

Figure 2 shows $c_v\times T/J$ and we can observe a broad maxi-

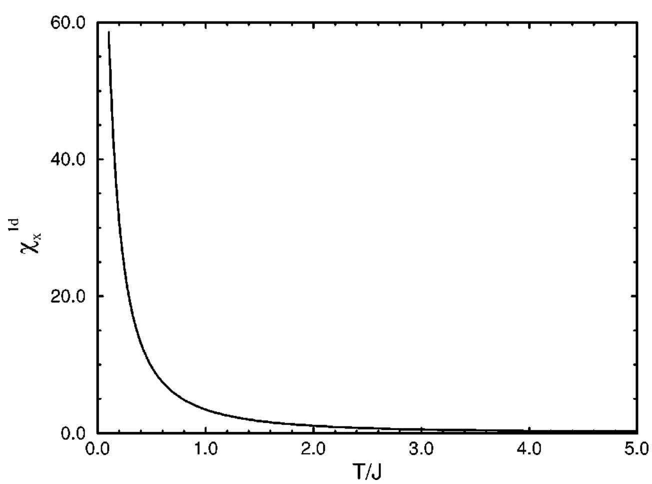

FIG. 2. Temperature dependence of the internal energy U and of the specific heat c_v for the 1D XY model with $S=1$.

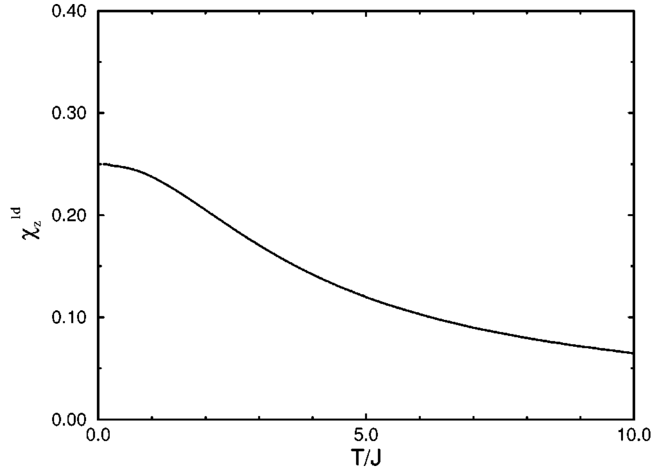

FIG. 3. Temperature dependence of the transverse uniform susceptibility χ^x for the 1D XY model with $S=1$.

mum around $T/J \sim 1.4$.

The static susceptibilities can be calculated from Eqs. (26) and (27) and are shown in Figs. 3 and 4. The longitudinal susceptibility, χ_z is well behaved for all T/J values shown. For low temperatures, χ_z is much smaller than χ_x which seems to diverge as $T\to 0$. Such a divergence would be a sign for a phase transition and deserves to be studied in more detail. Then, let us analyze the behavior of the function Δ appearing in the denominator of χ_x. We then use Eq. (13) to write

$$\Delta = \frac{z}{N}\sum_{\vec{q}} \frac{\gamma_{\vec{q}} A^z_{\vec{q}}}{2\omega^z_{\vec{q}}}\coth\left(\frac{\beta\omega^z_{\vec{q}}}{2}\right) - \frac{1}{N}\sum_{\vec{q}} \frac{A^x_{\vec{q}}}{2\omega^x_{\vec{q}}}\coth\left(\frac{\beta\omega^x_{\vec{q}}}{2}\right) \times\left[z\gamma_{\vec{q}} - 1 - \frac{z\gamma^2_{\vec{q}}-1}{z-1}\right]. \tag{35}$$

The first term on the right-hand side of Eq. (35) corresponds to zC^z_1 and is negative for all T (see Fig. 1): from the definitions of each function used to build this term, we can conclude that it is well behaved in all q region and that its negative value comes from the contribution at large q wave vectors. The last term in Eq. (35) depends on $\omega^x_{\vec{q}}$, given by Eq. (11), and can have singularities for $q\to 0$ if Δ becomes null or negative: an analysis of Fig. 1 leads to the conclusion that Δ decreases as T decreases. Considering this, it is convenient to write separately the small q contributions to the last term of Eq. (35):

$$\Delta = zC^z_1 - \frac{T}{4JN\alpha^x z}\sum_{small\, q}\frac{2J(C^x_0+C^x_2-\Delta)+zJC^z_1 q^2}{\Delta+\dfrac{\varepsilon_q q^2}{2}} \times\left[(z-2)-\frac{z(z-3)q^2}{2(z-1)}\right] - \frac{1}{N}\sum_{large\, q}\frac{A^x_{\vec{q}}}{2\omega^x_{\vec{q}}}\coth\left(\frac{\beta\omega^x_{\vec{q}}}{2}\right) \times\left[z\gamma_{\vec{q}}-1-\frac{z\gamma^2_{\vec{q}}-1}{z-1}\right]. \tag{36}$$

We conclude that the third term on the right-hand side of Eq. (36) is positive (including the sign multiplying it) and this term must be the main one in determining the $\Delta>0$ character for large T. The contribution that could cause problems to the evaluation of Δ and χ_x is the one including the small q contribution at low temperatures (when Δ becomes small). However, we have $z=2$ in 1D and the $\Delta\to 0$ limit of the second term in Eq. (36) is given by

$$-\frac{T}{2J\alpha N}\sum_{small\, q}\frac{(C^x_0+C^x_2)q^2}{\varepsilon_q q^2} \tag{37}$$

which is finite and small. This analysis shows that for $z=2$ there are no singularities in the calculation of Δ and that it possibly only vanishes at $T=0$. We then conclude that, in one dimension, χ_x is finite for finite T and, as it should be, there is no phase transition.

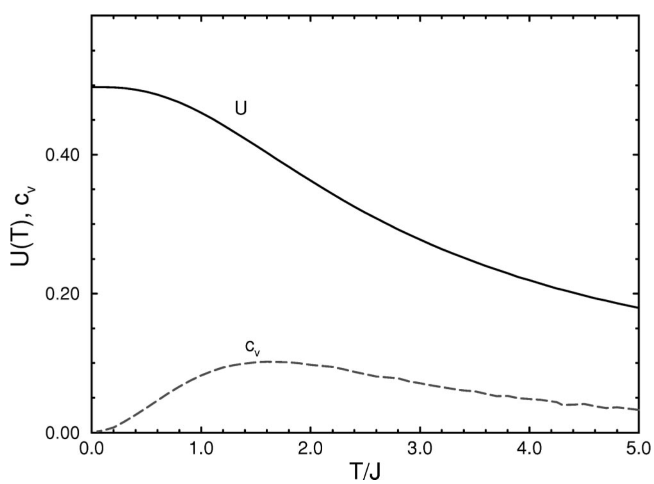

FIG. 4. Temperature dependence of the longitudinal uniform susceptibility χ^z for the 1D XY model with $S=1$.

B. *XY* square lattice

We start our discussion of the 2D results by analyzing the behavior of Δ as the temperature decreases. As discussed in the last subsection, the relevant term to the analysis of any anomaly in Δ is the second one on the right-hand side of (36). For $z=4$, the $\Delta\to 0$ and $q\to 0$ limit of this term,

$$-\frac{T}{4J\alpha}\sum_{small\, q}\frac{1}{\Delta+\varepsilon_q\dfrac{q^2}{2}}\left[(C^x_0+C^x_2-\Delta) - \frac{(C^x_0+C^x_2-\Delta)+6C^z_1}{3}q^2\right], \tag{38}$$

diverges meaning that Δ vanishes at a finite temperature. Our numerical solution of the self-consistent Eqs. (22)–(24): for 2D agrees with this conclusion because we obtain $\Delta=0$ in the neighborhood of $T/J=0.89$. For this and lower temperatures, there is no numerical solution to our equations because $\omega^x_{\vec{q}}$ becomes an imaginary number for $q\to 0$. The divergence of Δ, and thus of χ_x, suggests a phase transition and we can take $T_c/J=0.89$ as a rough estimate for the transition temperature for the 2D square XY model since it is known that the Green's function technique does not work well in the vicinity of T_c. Obviously, this is not an order-disorder transition since $\langle S^x\rangle=0$ for all T. For the classical model, as mentioned before, we have the well-known Kosterlitz-Thouless topological transition.[22] The quantum 2D easy-plane Heisenberg ferro- and antiferromagnetic models have been studied by Cuccoli *et al.*[26] and, more recently, by Capriotti *et al.*[27] by using the so-called pure-quantum self-consistent harmonic approximations to obtain the transition temperature and spin-correlation length for several spin values and in a wide range of the anisotropy parameter. For $S=1$ and anisotropy corresponding to the XY model, they obtained[27] $T_c/J\approx 1.08$, which is not too far from our result.

The spin correlations obtained for the 2D model are shown in Fig. 5. We can see from this figure that, as in the 1D case, the correlation C_1^z is negative for all T and, also, that the other correlations C_0^z, C_1^x, and C_2^z have a similar behavior as a function of the reduced temperature as found in 1D. We only notice that, here, the reduction of C_0^z as T decreases is more pronounced than in the 1D case: this means that the spins are more concentrated on the XY plane in the 2D case.

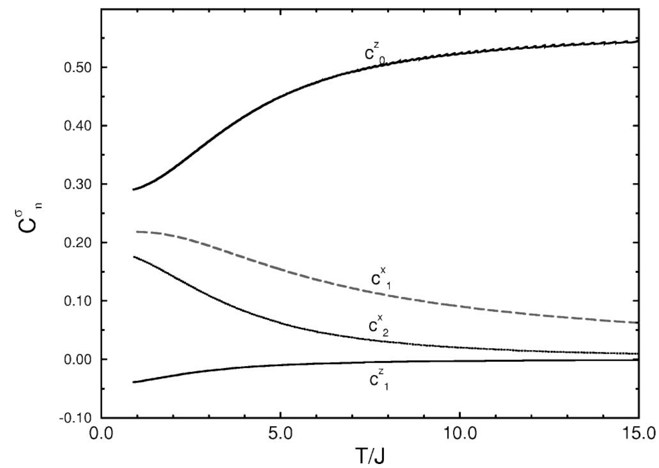

FIG. 5. Temperature dependence of the four correlation functions for the 2D XY model with $S=1$, as explained in the text.

V. CONCLUSION

We have studied the XY ferromagnet with spin $S=1$ in one and two dimensions using the two-time Green's function method and performing a decoupling proposed by Kondo and Yamaji.[4] We have calculated static spin-spin correlation functions for spins located one and two sites apart for the whole range of temperatures.

At $T=0$, our results for the 1D case agree very well to the ones obtained using the SCHA (Ref. 21) theory. For the 2D model, we have also obtained a transition temperature which is in fair agreement to Monte Carlo calculations.

ACKNOWLEDGMENTS

This work was partially supported by CNPq (Conselho Nacional para o Desenvolvimento da Pesquisa).

[1] N. N. Bogolyubov and S. V. Tyablikov, Dokl. Akad. Nauk. (SSSR) **126**, 53 (1959) [Sov. Phys. Dokl. **4**, 589 (1959)]; S. V. Tyablikov, Ukr. Mat. Zh. **11**, 287 (1959).

[2] S. V. Tyablikov, in *Methods in the Quantum Theory of Magnetism* (Plenum, New York, 1967).

[3] L. Siurakshina, D. Ihle, and R. Hayn, Phys. Rev. B **61**, 14 601 (2000).

[4] J. Kondo and K. Yamaji, Prog. Theor. Phys. **47**, 807 (1972).

[5] R. H. Knapp and D. ter Haar, J. Stat. Phys. **1**, 149 (1969).

[6] H. Shimahara and S. Takada, J. Phys. Soc. Jpn. **60**, 2394 (1991).

[7] S. A. Scales and H. A. Gersch, Phys. Rev. Lett. **28**, 917 (1972); J. Stat. Phys. **7**, 95 (1973).

[8] M. Takahashi, Phys. Rev. B **40**, 2494 (1989).

[9] J. C. Bonner and M. E. Fisher, Phys. Rev. **135**, A640 (1964).

[10] K. Yamaji and J. Kondo, Phys. Lett. **45A**, 317 (1973).

[11] M. Uchinami, S. Takada, and F. Takano, J. Phys. Soc. Jpn. **47**, 1047 (1979).

[12] S. Katsura, T. Horiguchi, and M. Suzuki, Physica (Amsterdam) **46**, 67 (1970).

[13] S. Winterfeld and D. Ihle, Phys. Rev. B **56**, 5535 (1997); **59**, 6010 (1999).

[14] S. Q. Bao, Hu. Zhao, J. L. Shen, and G. Z. Yang, Phys. Rev. B **53**, 735 (1996).

[15] T. Kawabe, Prog. Theor. Phys. **81**, 976 (1989).

[16] Y. Fukumoto and A. Oguchi, J. Phys. Soc. Jpn. **65**, 264 (1996).

[17] Z. H. Dong and S. Feng, Mod. Phys. Lett. B **12**, 677 (1998).

[18] Y. Song, H. Q. Lin, and J. L. Shen, Phys. Rev. B **58**, 9166 (1998).

[19] D. Ihle, C. Schindelin, A. Weisse, and H. Fehske, Phys. Rev. B **60**, 9240 (1999).

[20] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961); S. Katsura, Phys. Rev. **127**, 1508 (1962).

[21] J. Villain, J. Phys. (France) **35**, 27 (1974).

[22] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973); J. M. Kosterlitz, *ibid.* **7**, 1046 (1974).

[23] M. E. Gouvêa, G. M. Wysin, A. R. Bishop, F. G. Mertens, Phys. Rev. B **39**, 11 840 (1989); A. R. Pereira, A. S. T. Pires, M. E. Gouvêa, and B. V. Costa, Z. Phys. B: Condens. Matter **89**, 109 (1992); A. S. T. Pires and M. E. Gouvêa, Phys. Rev. B **48**, 12 698 (1993).

[24] J. Villain, J. Phys. (France) **36**, 581 (1975).

[25] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).

[26] A. Cuccoli, V. Tognetti, P. Verrucchi, and R. Vaia, J. Appl. Phys. **75**, 5814 (1994).

[27] L. Capriotti, A. Cuccoli, V. Tognetti, R. Vaia, and P. Verrucchi, Physica D **119**, 68 (1998).