Two-dimensional quantum spin-$\frac{1}{2}$ Heisenberg model with competing interactions

J. Ricardo de Sousa[1] and N. S. Branco[2]
[1]*Departamento de Física, Universidade Federal do Amazonas, 69077-000, Manaus, AM-Brazil*
[2]*Departamentio de Física, Universidade Federal de Santa Catarina 88040-900, Florianópolis, SC-Brazil*
(Received 19 April 2005; revised manuscript received 6 July 2005; published 21 October 2005)

We study the quantum spin-$\frac{1}{2}$ Heisenberg model in two dimensions, interacting through a nearest-neighbor antiferromagnetic exchange (J) and a ferromagnetic dipolarlike interaction (J_d), using double-time Green's function, decoupled within the random phase approximation. We obtain the dependence of k_BT_c/J_d as a function of frustration parameter δ, where T_c is the ferromagnetic (F) transition temperature and δ is the ratio between the strengths of the exchange and dipolar interaction (i.e., $\delta=J/J_d$). The transition temperature between the F and paramagnetic phases decreases with δ, as expected, but goes to zero at a finite value of this parameter, namely, $\delta=\delta_c=\pi/8$. At $T=0$ (quantum phase transition), we analyze the critical parameter $\delta_c(p)$ for the general case of an exchange interaction in the form $J_{ij}=J_d/r_{ij}^p$, where ferromagnetic and antiferromagnetic phases are present.

DOI: 10.1103/PhysRevB.72.134421 PACS number(s): 75.10.Jm, 05.50.+q

I. INTRODUCTION

Considerable attention during the last decade has been devoted to the investigation of systems with long-range interactions. In particular, the interest in films and quasi-two-dimensional systems have attracted attention mainly due to their technological applications as, for example, in electronics, data storage, catalysis in the case of metal-on-metal films, biotechnology, and pharmacology in the case of molecular films. The magnetic size unit and its thermal stability are essential points to be considered in order to obtain a good performance in magneto-optical recording.[1] The magnetic properties of these films depend on the subtle interplay between the long-range antiferromagnetic dipolar interaction, the short-range rotational invariant exchange, and the magnetic surface anisotropy. The presence of antiferromagnetic domains (AF) was observed in epitaxial thin films by the polarization-dependent x-ray magnetic linear dichroism spectra microscopy.[2] A possible intrinsic mechanism leading to AF domains is the competition between anisotropy and dipolar interaction.[3]

In two-dimensional lattices and for spins with rotational symmetry, long-range order does not occur at any finite temperature, for quantum and classical models with short-range interactions.[4] That is the case when only short-range exchange interactions are present, for the *XY* and Heisenberg models, for example. For all real systems there is a long-range dipolar interaction, with the important property that it breaks the symmetry between out-of-plane orientation of the spins and the in-plane orientation of the spins in the ordered state. The presence of dipolar interactions in systems with rotational symmetry (exchange) may stabilize long-range order at finite temperatures, for both classical and quantum models.[5]

The competition between long-range antiferromagnetic dipolar and short-range ferromagnetic exchange interactions in two-dimensional uniaxial (Ising) spin systems is responsible for a very rich phenomenological scenario concerning both their equilibrium statistical mechanics[6–9] and nonequilibrium dynamic properties.[1,10–15] By means of Monte Carlo simulations and analytical calculations of the ground state, MacIsaac *et al.*[6] studied the two-dimensional spin-$\frac{1}{2}$ Ising model with ferromagnetic exchange and antiferromagnetic dipolar interactions, and have shown that for $\delta \equiv J/J_d < 0.425$, J and J_d being the strength of exchange and dipolar interactions, respectively, the antiferromagnetic state is stable. For $\delta > 0.425$ the AF state becomes unstable with respect to the formation of striped domain structures, i.e., to state configurations with spins aligned along a particular axis forming a ferromagnetic stripe of constant width h, forming a superlattice in the direction perpendicular to the stripes. Monte Carlo results[8] at low temperatures give further support to this proposal, at least for intermediate values of δ.

There are few numerical results concerning the equilibrium statistical mechanics of quantum models with competitive exchange and dipolar interactions in two-dimensional lattices.[14,15] The two-dimensional antiferromagnetic (AF) Heisenberg model has been investigated by many authors to explain, for example, the magnetic mechanism of high T_c superconductivity.[16,17] Antiferromagnetic fluctuations are believed to play an important role in the superconductivity of the cuprates,[17] such as La_2CuO_4, which is well described by a quasi-two-dimensional quantum spin-$\frac{1}{2}$ Heisenberg AF model. Chandra and Doucot[18] have studied the square-lattice Heisenberg model at $T=0$ with next-nearest-exchange coupling and suggested that the AF order is destroyed due to the competition between the nearest and next-nearest-exchange interactions. Although frustration effects are very effective to destroy the AF order in general, they may not be effective in high T_c materials, considering the extended nature of the holes which destroy the AF order. A good example of quasi-two-dimensional AF materials in which the dipolar interaction (with presence of frustration) is comparable to the exchange coupling are the so-called high-T_c superconductors $R\mathrm{Ba}_2\mathrm{Cu}_3\mathrm{O}_{7-x}$ (where R stands for rare earth).[19]

From a theoretical point of view, the double-time Green's function (GF) theory[20] is both a convenient and an effective theoretical framework for interpretation and forecasting of

various characteristics of matter at all temperatures. The development of approximation schemes for the GF approach has focused on decoupling their equations of motion. This decoupling is usually chosen for convenience or for reasons which are essentially *ad hoc*. The consistency of the basic decoupling approximation with relevant operator identities is not always assured. Several first-order decoupling have been proposed in the literature: first, the random phase approximation (RPA) was applied to the quantum spin-$\frac{1}{2}$ Heisenberg ferromagnetic,[20] and extended to include a long-range interaction $J(r)$, which depends on the distance r between spins as an inverse power law $J(r)=J/r^p$, where $p>d$ (dimension).[21–23] This RPA decoupling predicts the absence of magnetic order in finite temperature and low-dimensionality ($d=1,2$) for $p>2d$, in accordance with the generalized Mermin and Wagner theorem.[24] The quantitative results of the phase diagram in the $(T-p)$ plane in the $d<p<2d$ region obtained by RPA (Ref. 23) are in accordance with quantum Monte Carlo simulations.[25]

The aim of this work is to investigate the results of the competition between the exchange and dipolar interactions in the two-dimensional quantum spin-$\frac{1}{2}$ Heisenberg model. In Sec. II, the model is presented and treated by the double-time GF technique in the RPA decoupling. In Sec. III, we analyze the phase diagram in the $T-\delta$ plane. Conclusions and remarks are summarized in Sec. IV.

II. MODEL AND GREEN'S FUNCTION METHOD

In order to study the consequences of both quantum effects and frustration, we propose here a spin model to describe the destruction of the F order, represented by the following Hamiltonian:

$$\mathcal{H}=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j-J_d\sum_{(i,j)}\frac{\mathbf{S}_i\cdot\mathbf{S}_j}{r_{ij}^3}, \tag{1}$$

where $\mathbf{S}_i=(S_i^x,S_i^y,S_i^z)$ is the spin-$\frac{1}{2}$ operator at site i. The first term J is the strength of the exchange interaction, and the sum is over all nearest-neighbor pairs $\langle i,j\rangle$ on a square lattice. The second term, $J_d=(g\mu_B)^2/a^3$ (g is the Landé factor, μ_B the Bohr magneton, a the lattice constant), represents a long-ranged dipole-dipole interaction and the sum is over all possible pairs of atoms on the square lattice. The dipolar interaction tends to align the spins in the F system at low temperatures ($T<T_c$), while the exchange interaction (antiferromagnetic, $J>0$) tends to destroy the long-range ferromagnetic order. Consequently the ground state of a system determined by the dipolar interaction alone differs from the ground state of a system determined by the exchange interaction alone. In the absence of the dipolar interaction (i.e., $J_d=0$), the isotropic Heisenberg model is regained and in two-dimensional lattices it does not present long-range order at $T>0$ (i.e., $T_c=0$). When both interactions are present the system is inherently *frustrated*.

The double-time Green's function $\langle\langle A(t);B(0)\rangle\rangle$ is defined by[20]

$$\langle\langle A(t);B(0)\rangle\rangle=-i\theta(t)\langle[A(t),B(0)]\rangle, \tag{2}$$

where $\theta(t)$ is the step function, $[A,B]$ is the commutator of operators A and B, and $\langle\cdots\rangle$ denotes an average with respect to the canonical density matrix of the system at temperature T. The time-Fourier transform of Eq. (2) $\langle\langle A;B\rangle\rangle_E$, satisfies the following equation of motion:

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

and $\langle\langle[A,\mathcal{H}];B\rangle\rangle_E$ obeys an equation similar to Eq. (3), with a higher-order Green's function appearing on the right-hand side. In this way, an infinite set of coupled equations is generated. Therefore, an approximation (decoupling) is used to obtain the Green's function.

The correlation function $\langle BA(t)\rangle$ is obtained by the spectral representation theory, which gives

$$\langle BA(t)\rangle=\int_{-\infty}^{\infty}J(w)e^{-iwt}dw$$

$$=\int_{-\infty}^{\infty}\frac{i\{G(w+i\varepsilon)-G(w-i\varepsilon)\}e^{-iwt}dw}{e^{\beta w}-1}, \tag{4}$$

where $G(E)=\langle\langle A;B\rangle\rangle_E$ and $\varepsilon\to 0$. Note that Eq. (4) is the required spectral representation for the time correlation function, where $J(w)$ is the spectral intensity of the function $\langle BA(t)\rangle$ (in fact, its Fourier transform[20]).

With $A=S_g^+$ and $B=S_l^-$, where the spin operators are defined by the usual commutation rules, we obtain from Eq. (3)

$$E\langle\langle S_g^+;S_l^-\rangle\rangle_E=\frac{m}{\pi}\delta_{gl}+2\sum_{j\neq l}J_{jl}\{\langle\langle S_j^zS_g^+;S_l^-\rangle\rangle_E-\langle\langle S_g^zS_j^+;S_l^-\rangle\rangle_E\}, \tag{5}$$

where $m=\langle S_g^z\rangle$ is the magnetization per spin, $J_{jl}=-J$ for nearest-neighbor sites and $J_{jl}=J_d/r_{jl}^3$ for the dipolar interaction (with $\delta=J/J_d$).

The key problem of a first-order decoupling procedure is essentially to express the Green's function $\langle\langle S_a^zS_b^+;S_l^-\rangle\rangle_E$ in terms of lower-order Green's functions, which enables one to solve the infinite chain of equations of motion in an approximate way, and that can be expressed in the following form:

$$\langle\langle S_a^zS_b^+;S_l^-\rangle\rangle_E\simeq m\langle\langle S_b^+;S_l^-\rangle\rangle_E. \tag{6}$$

Using the decoupling (6) in Eq. (5), we obtain

$$EG_{gl}(E)=\frac{m}{\pi}\delta_{gl}+2m\sum_{j\neq l}J_{jg}\{G_{gl}(E)-G_{jl}(E)\}, \tag{7}$$

where $G_{gl}(E)\equiv\langle\langle S_g^+;S_l^-\rangle\rangle_E$.

The method of calculation we use is the same as Nakano and Takahashi,[23] and we shall not reproduce the details. Following their notation, we obtain from Eq. (7) the Fourier transform of the Green's function $G_K(E)=\mathcal{F}\{G_{gl}(E)\}$, defined by

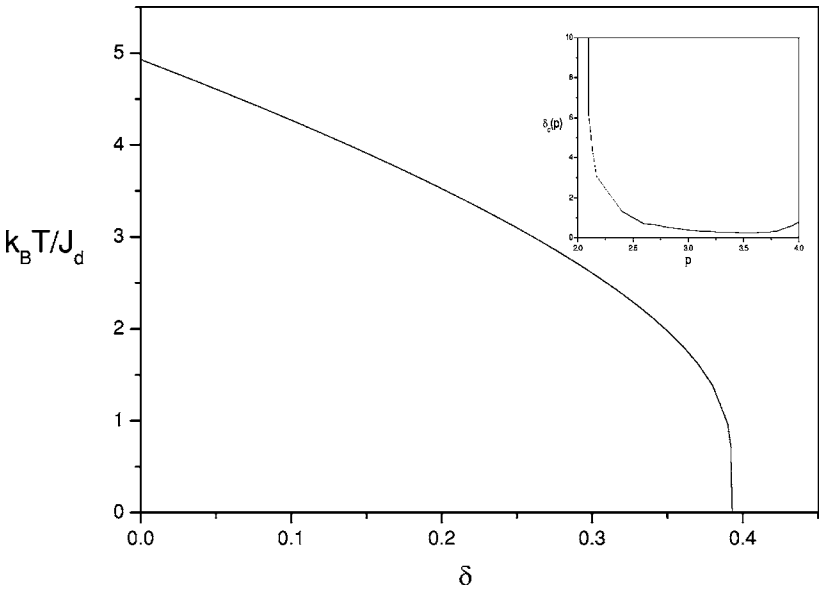

FIG. 1. Dependence of the reduced critical temperature k_BT_c/J_d on the parameter δ for the quantum spin-$\frac{1}{2}$ Heisenberg model with ferromagnetic and dipolar interactions with $p=3$. The inset is the behavior of $\delta_c(p)$ as a function of the parameter p.

$$G_K(E) = \sum_{g,l} G_{gl}(E) e^{-i\mathbf{k}(\mathbf{r}_g - \mathbf{r}_l)}, \tag{8}$$

and, in this way, we find

$$G_K(E) = \frac{m}{\pi(E - E_k)}, \tag{9}$$

where the magnon energy E_k is

$$E_k = 2m(J_o - J_k), \tag{10}$$

with

$$J_k = \sum_{(g,l)} J_{gl} e^{-i\mathbf{k}(\mathbf{r}_g - \mathbf{r}_l)}. \tag{11}$$

Using the low-$\mathbf{k}$ expression in two dimensions (as in Ref. 23) for $p=3$ [recall that the ferromagnetic interaction is assumed to decay with the distance between spins, r, as $J(r) = J/r^p$] we obtain

$$E_k = 2mJ_d k(\pi^2/8 - \delta k). \tag{12}$$

Using Eqs. (4), (8), and (9), we obtain the correlation function $\langle S^- S^+ \rangle$; for spin $S=1/2$ we have $\langle S^- S^+ \rangle = 1/2 - m$ and, therefore, the magnetization is written in the form

$$m = \frac{1}{2}\left[\frac{1}{N} \sum_k \coth(\beta E_k/2) \right]^{-1}. \tag{13}$$

III. RESULTS AND DISCUSSION

In the limit $m \to 0$, we find, from Eqs. (12) and (13), the critical temperature (T_c), which is given by

$$\frac{k_B T_c}{J_d} = \left[\frac{2}{N} \sum_k \frac{1}{k(\pi^2/8 - \delta k)} \right]^{-1}. \tag{14}$$

In the thermodynamic limit ($N \to \infty$) one must replace the sum $\frac{1}{N}\Sigma_k \psi(\mathbf{k})$ by an integral $1/(2\pi)^d \int_{1\mathrm{BZ}} \psi(\mathbf{k}) d^d\mathbf{k}$ in the d-dimensional $\mathbf{k}$ space, where 1BZ denotes the first Brillouin zone. Then, the integral (14) is obtained by using the expansion (12), and the critical temperature is given by

$$\frac{k_B T_c}{J_d} = \frac{4\pi\delta}{\ln\left(\frac{\delta_c}{\delta_c - \delta}\right)}. \tag{15}$$

Note that the critical temperature vanishes at δ_c, which, within the present approximation, is given by $\delta_c = \pi/8 \simeq 0.39$.

Numerical results for T_c are shown in Fig. 1. The parameter δ is a measure of the strengthen of the frustration; therefore, long-range order decreases as δ increases. Consequently, $T_c(\delta)$ goes to zero at the critical value $\delta = \delta_c = \pi/8$. When the interactions have the general form J_d/r^p, the existence of a finite-temperature phase transition occurs for $2 < p < 4$ in two dimensions. By numerically performing the sum in Eq. (13) for $2 < p < 4$ (see Ref. 23 for the general dispersion relation), we obtain the critical parameter $\delta_c(p)$ as a function of p at $T=0$ (see the inset of Fig. 1), where above the curve the ordered phase is antiferromagnetic, while below it the long-range order is ferromagnetic. We note that $\delta_c(p)$ increases as p decreases, and when p approaches $p=2$ we have a divergence (T_c also diverge) in $\delta_c(p=2)$ and around $p \simeq 3.6$ a minimum point appears. The point $p=4$ corresponds to the Kosterlitz-Thouless phase transition,[23] and with the presence of the AF nearest-neighbor interaction the critical temperature vanishes at $\delta_c(p=4) \simeq 0.793$. For $p > 4$, the critical frustration parameter, $\delta_c(p)$, is zero, as physically expected.

IV. CONCLUSIONS

We study the phase diagram of the quantum spin-$\frac{1}{2}$ Heisenberg model with competing interactions (i.e., presence of AF exchange and dipolar interactions). The influence of the frustration is analyzed through the variation of the pa-

rameter $\delta=J/J_d$. We observe that $T_c(\delta)$ is null when we reach the critical value $\delta_c=\pi/8$. We also analyzed the case of the general dependence of the long-range interaction in the form $J_{ij}=J_d/r_{ij}^p$, and verified that T_c tends to zero at the critical parameter $\delta_c(p)$. The dependence of $\delta_c(p)$ on p $(2<p<4)$ presents a divergence at $p=2$ ($p\leqslant 2$ being the nonextensive regime) and a minimum point around $p\simeq 3.6$, with finite value at $p=4$ (Kosterlitz-Thouless transition). Although quantitative results are not expected to be very precise, within the approximation we applied, we believe that we obtain reliable qualitative results for the whole range of the parameters of the Hamiltonian. In particular, our results agree with previous ones, when available.

ACKNOWLEDGMENTS

We would like to thank CNPq, FAPESC/FUNCITEC, and FAPEAM (Brazilian agencies) for partial financial support.

[1] K. De Bell, A. B. MacIsaac, and J. P. Whitehead, Rev. Mod. Phys. **72**, 225 (2000), and references therein.
[2] A. Scholl, J. Stöhr, J. Lüning, J. W. Seo, J. Fompeyrine, H. Siegwart, J. -P. Loequt, F. Nolting, S. Anders, E. E. Fullerton, M. R. Scheinfein, and H. A. Padmore, Science **287**, 1014 (2000).
[3] D. S. Deng, X. F. Jin, and Ruibao Tao, Phys. Rev. B **65**, 132406 (2002).
[4] N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).
[5] S. V. Maleev, Sov. Phys. JETP **43**, 1240 (1976).
[6] A. B. MacIsaac, J. P. Whitehead, M. C. Robinson, and K. De Bell, Phys. Rev. B **51**, 16033 (1995).
[7] A. Kashuba and V. L. Pokrovsky, Phys. Rev. Lett. **70**, 3155 (1993).
[8] P. M. Gleiser, F. A. Tamarit, and S. A. Cannas, Physica D **168-169**, 73 (2002).
[9] A. Magni and G. Vertey, Phys. Rev. B **61**, 3203 (2000).
[10] L. C. Sampaio, M. P. de Albuquerque, and F. S. de Menezes, Phys. Rev. B **54**, 6465 (1996).
[11] J. H. Toloza, F. A. Tamarit, and S. A. Cannas, Phys. Rev. B **58**, R8885 (1998).
[12] D. A. Stariolo and S. A. Cannas, Phys. Rev. B **60**, 3013 (1999).
[13] P. M. Gleiser, F. A. Tamarit, S. A. Cannas, and M. A. Montemuiro, Phys. Rev. B **68**, 134401 (2003).
[14] A. M. Abu-Labdeh, J. P. Whitehead, K. De Bell, and A. B. MacIsaac, Phys. Rev. B **65**, 024434 (2001).
[15] D. S. Deng, X. F. Jin, and R. Tao, Phys. Rev. B **69**, 172403 (2004).
[16] A. Aharony, R. J. Birgereau, A. Coniglio, M. A. Castner, and H. E. Stanley, Phys. Rev. Lett. **60**, 1330 (1988); K. B. Lyons, P. A. Fleury, L. F. Schneemeyer, and J. V. Waszczak, *ibid.* **60**, 732 (1988); J. M. Tranquada, W. H. Li, H. A. Mook, B. C. Sales, and Z. Fisk, *ibid.* **60**, 2781 (1988).
[17] Y. Endoh *et al.* Phys. Rev. B **37**, 7443 (1988); A. P. Kampf, Phys. Rep. **249**, 219 (1994); B. Keimer *et al.* Phys. Rev. B **46**, 14034 (1992).
[18] P. Chandra and B. Doucot, Phys. Rev. B **38**, 9335 (1988).
[19] T. W. Clinton, J. W. Lynn, J. Z. Liu, Y. X. Jia, and R. N. Shelton, J. Appl. Phys. **70**, 5751 (1991); D. M. Paul, H. A. Mook, A. W. Hewat, B. C. Sales, L. A. Boatner, J. R. Thompson, and M. Mostoller, Phys. Rev. B **37**, 2341 (1988); H. A. Mook, D. M. Paul, B. C. Sales, L. A. Boatner, and L. Cussen, *ibid.* **38**, 12008 (1988); J. W. Lynn, T. W. Clinton, W. -H. Li, R. W. Erwin, J. Z. Liu, K. Vandervoort, and R. N. Shelton, Phys. Rev. Lett. **63**, 2606 (1989).
[20] D. N. Zubarev, Usp. Fiz. Nauk **71**, 71 (1960); see also S. V. Tayablikov, *Methods in the Quantum Theory of Magnetism* (Plenum, New York, 1967).
[21] M. Hamedoun, Y. Cherriet, A. Hourmatallah, and N. Benzakour, Phys. Rev. B **63**, 172402 (2001).
[22] A. Cavallo, F. Cosenza, and L. De Cesare, Phys. Rev. B **66**, 174439 (2002).
[23] H. Nakano and M. Takahashi, Phys. Rev. B **52**, 6606 (1995).
[24] P. Bruno, Phys. Rev. Lett. **87**, 137203 (2001).
[25] O. N. Vassiliev, I. V. Rojdestvenski, and M. G. Cottam, Physica A **294**, 139 (2001).