



Critical properties of the frustrated quasi-two dimensional XY-like antiferromagnet

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ABSTRACT

We study, using a self-consistent harmonic approximation, the quasi-two-dimensional frustrated Heisenberg antiferromagnet with easy-plane single ion anisotropy. Besides the transition temperature from the high-temperature paramagnetic phase to the low-temperature ordered phase, we also obtain, at zero temperature, the critical single ion anisotropy parameter D_c that separates the low D region from the large D quantum paramagnetic phase. We have found disordered phases at zero temperature that could be possible candidates for spin liquids states.

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1. Introduction

Frustrated quantum antiferromagnets on the square lattice have been the subject of intense research over the last decades, with particular interest in the spin $S=1/2$ case relevant for the cuprates, whereas interest in higher spin values increased with the discovery of the pnictides [1]. As by now it is well known that the antiferromagnetic Heisenberg model on the square lattice has long-range order in the ground state even for $S=1/2$. It is also known that this long range order can be destroyed by frustration caused, for instance, by next nearest neighbor antiferromagnetic interactions [2–10].

On the other side, spin liquid is a hot topic in condensed matter physics since the discovery of high- T_c superconductivity. A spin liquid is a disordered state, but not all disordered states are a spin liquid [4]. So, a first step in the research of spin liquids is to look for disordered states. In this context, the antiferromagnetic Heisenberg model (AFHM) with competing interactions has been widely studied, but the same is not true for the XY model.

Several new magnetic materials characterized by competing interactions have been synthesized, but a detailed theoretical understanding of the ground state properties of simple models displaying both frustration and quantum fluctuations is still missing [11], and interpretations of the experimental results often relies on simple perturbative or semiclassical methods.

When $J_2/J_1 < 1/2$, where J_1 is the nearest-neighbor and J_2 the next-nearest neighbor interaction, the classical ground state has a Néel order. However when $J_2/J_1 > 1/2$, the ground state consists of

two independent sublattices with antiferromagnetic order. The classical ground state energy does not depend on the relative orientations of both sublattices. However, quantum fluctuations lift this degeneracy and select a collinear order state, where the neighboring spins align ferromagnetically along one axis of the square lattice and antiferromagnetically along the other [3,4].

Additional terms, as for instance single ion anisotropy, are possible when $S > 1/2$ and can lead to new physical features, such as a quantum phase transition to a large D phase. Study of these models are not only of an academic interest since materials with $S=1$ and single ion anisotropy have been synthesized recently [12]. The system is more complex as there are now two mechanisms by which we can vary the quantum fluctuations and get disordered phases. One mechanism is the anisotropy; the other is the competing interactions to the bare model where we can vary the relative strengths of the exchange interactions. The combined effect of competing interactions J_1 , J_2 and J_3 and single ion anisotropy may lead (or not lead) to frustrations, depending on their mutual values. In real magnetic material, single-ion anisotropy plays a major role in determining the magnetic behavior of the system [12,13].

In this paper we will study a quasi-two-dimensional Heisenberg antiferromagnet with an easy-plane single ion anisotropy described by the following Hamiltonian:

$$H = \frac{J_1}{2} \sum_{r,a} (S_r^x S_{r+a}^x + S_r^y S_{r+a}^y + \lambda S_r^z S_{r+a}^z) + D \sum_r (S_r^z)^2 \\ + \frac{J_2}{2} \sum_{r,d} (S_r^x S_{r+d}^x + S_r^y S_{r+d}^y + \lambda S_r^z S_{r+d}^z) \\ + \frac{J_3}{2} \sum_{r,\delta} (S_r^x S_{r+\delta}^x + S_r^y S_{r+\delta}^y + \lambda S_r^z S_{r+\delta}^z). \quad (1)$$

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Here J_1 is the nearest-neighbor, J_2 the next-nearest neighbor exchanges interactions, both in the XY-plane, and J_3 the inter-plane coupling. We take $S=1$, but our calculations can be applied for any $S > 1/2$. The main physical motivation for our study is to find phases which do not carry a magnetic moment, and therefore are candidate for a spin liquid state.

The spectrum of the Hamiltonian (1) changes drastically as D varies from very small to very large values. A strong anisotropy favors a quantum paramagnetic ground state, which is separated from the ordered state by a quantum critical point. This phase consists of a unique ground state with total magnetization $S_{total}^z = 0$, separated by a gap from the first excited states, which lie in the sectors $S_{total}^z = \pm 1$. The primary excitations is a gaped $S=1$ exciton with an infinite lifetime at low energies.

As it is well known, the isotropic 2D AFHM is ordered only at zero temperatures, while in the XY model a Kosterlitz–Thouless (KT) phase transition occurs when $J_3=0$, resulting from the unbinding of vortex–antivortex pairs. Therefore it is interesting to calculate the KT transition temperature T_{KT} for the XY model with competing interactions. For $J_3=0$ the critical behavior of the quantum XY model is of the KT-type, as in the classical case. Quantum fluctuations change the quantitative behavior of the model, but the qualitative picture of the classical system persists [14]. When $J_3 > 0$, we have the usual order-disorder phase transition.

For $J_3=0$, there is no spontaneous magnetization for $T > 0$. However, for $T < T_{KT}$ there is a quasi long-range order and the spin-spin correlation functions shows a power law decrease with distance (with an exponent proportional to T as $T \rightarrow 0$). A new property appearing below the phase-transition temperature is the stiffness ρ introduced by Berezinskii [15], by analogy with superfluid helium. At the KT temperature ρ drops to zero. Of course, for $J_3 > 0$, the magnetization is non null, but it is related to ρ , and thus goes to zero at the same point where ρ vanishes.

2. Self-consistent Harmonic approximation

Simple approaches which yield an analytical description are very useful for practical purposes. For an XY-like model such as Hamiltonian Eq. (1), a very convenient theory is the self consistent harmonic approximation (SCHA), which replaces the Hamiltonian by an effective one with temperature-dependent renormalized parameters [14,16,17]. Although it is a semiclassical theory it has the advantage of being the only spin wave theory which gives the KT-transition. We write the spins components in the Hamiltonian (1) in terms of the Villain representation [18]

$$S_r^+ = e^{i\varphi_r} \sqrt{(S+1/2)^2 - (S_r^z + 1/2)^2}, \quad S_r^- = \sqrt{(S+1/2)^2 - (S_r^z - 1/2)^2} e^{-i\varphi_r}. \quad (2)$$

where φ is the operator corresponding to the azimuthal angle of the spin around the z axis. Taking Eq. (2) into Eq. (1), writing $\varphi = \phi + \pi$ for the near-neighbor term (antiferromagnetic order), and expanding the cosine term we obtain:

$$H_1 = \frac{J_1}{2} \sum_{r,a} [\rho_1 \tilde{S}^2 (\phi_r^2 - \phi_r \phi_{r+a}) + \lambda S_r^z S_{r+a}^z] + D \sum_r (S_r^z)^2 \quad (3)$$

where $\tilde{S}^2 = S(S+1)$, and the stiffness ρ_1 for the near-neighbor spins is given by [14]

$$\rho_1 = \left\langle \left[1 - \left(\frac{S_r^z}{\tilde{S}} \right)^2 \right] \right\rangle \langle \cos(\phi_r - \phi_{r+a}) \rangle. \quad (4)$$

Here we are supposing that $|\phi_{r+a} - \phi_r| < \pi$. This is true for $T < T_{KT}$, but not for $T > T_{KT}$ where the dissociation of vortices

disorder the system. Therefore our calculation is valid only at low temperatures, i. e. $T < J$ [15].

Taking the Fourier transform we get

$$H_1 = 2J_1 \sum_q [\rho_1 \tilde{S}^2 (1 - \gamma_q) \phi_q \phi_{-q} + (1 + d + \lambda \gamma_q) S_q^z S_{-q}^z] \quad (5)$$

where

$$\gamma_q = \frac{1}{2}(\cos q_x + \cos q_y), \quad \text{and} \quad d = D/2J_1.$$

A procedure similar can be used for the other terms. We remark that for the next-near-neighbor, in the Néel phase, the spins are in the same direction and we take $\varphi = \phi$. Doing all the calculations we arrive at the final result for the Néel phase

$$H = \sum_q [\tilde{S}^2 a(q) \phi_q \phi_{-q} + b(q) S_q^z S_{-q}^z] \quad (6)$$

with

$$a(q) = 2J_1 \left[\rho_1 (1 - \gamma_q) - \eta \rho_2 (1 - \xi_q) + \frac{\alpha \rho_3}{2} (1 - \cos q_z) \right] \quad (7)$$

$$b(q) = 2J_1 \left[1 + d - \eta + \frac{\alpha}{2} + \lambda (\gamma_q + \eta \xi_q + \frac{\alpha}{2} \cos q_z) \right] \quad (8)$$

The stiffness constants, renormalized by quantum fluctuations, are given by

$$\rho_i = \left\langle \left[1 - \left(\frac{S_i^z}{\tilde{S}} \right)^2 \right] \right\rangle \exp \left[- \sum_q g_i(q) \langle \phi_q \phi_{-q} \rangle \right] \quad (9)$$

where

$$g_1 = (1 - \gamma_q), \quad g_2 = (1 - \xi_q), \quad g_3 = (1 - \cos q_z). \quad (10)$$

$$\xi_q = \cos q_x \cos q_y, \quad \eta = J_1/J_2, \quad \text{and} \quad \alpha = J_3/J_1. \quad (11)$$

By introducing the canonical transformation

$$\phi_q = \left(\frac{b(q)}{a(q)} \right)^{1/4} (a_q^+ + a_{-q}), \quad S_q^z = i \left(\frac{a(q)}{b(q)} \right)^{1/4} (a_q^+ - a_{-q}) \quad (12)$$

where a_q^+ and a_q are the boson-creation and annihilation operators, respectively, we can write Eq. (6) as

$$H = \sum_q \omega_q (a_q^+ a_q + 1/2) \quad (13)$$

where

$$\omega_q = 2\tilde{S} \sqrt{a(q)b(q)}. \quad (14)$$

Using Eq. (12), the static correlations can be calculated, and the result is

$$\langle (S_r^z)^2 \rangle = \frac{\tilde{S}}{2\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi d^3 q \sqrt{\frac{a(q)}{b(q)}} \cot h \left(\frac{\beta \omega_q}{2} \right) \quad (15)$$

$$\langle \phi_q \phi_{-q} \rangle = \frac{1}{2\tilde{S}} \sqrt{\frac{b(q)}{a(q)}} \cot h \left(\frac{\beta \omega_q}{2} \right). \quad (16)$$

In the collinear phase, Eqs. (7) and (8) are substituted by

$$a(q) = J_1 \rho_1 (\cos q_y - \cos q_x) + 2J_2 \rho_2 (1 - \cos q_x \cos q_y) + J_3 \rho_3 (1 - \cos q_z). \quad (17)$$

$$b(q) = J_1 \lambda (\cos q_x + \cos q_y) + D + 2J_2 (1 + \lambda \cos q_x \cos q_y) + J_3 (1 + \lambda \cos q_z). \quad (18)$$

The other equations remain the same. The critical temperature T_C and the critical anisotropy parameter D_C can be evaluated where the stiffness drops to zero. We remark, once more, that for $\alpha=0$, T_C is the Kosterlitz–Thouless transition temperature T_{KT} .

In the classical model, the action associated to a pair vortex–antivortex is [19]

$$S_0 = 4\pi J_1(1-2\eta)\ln(r/a) \quad (19)$$

where r is the distance separating the two vortices and a is the lattice parameter. Therefore, the KT transition is given by

$$T_{KT} = (\pi/2)J_1(1-2\eta). \quad (20)$$

When $\eta = 1/2$, $T_{KT} = 0$, indicating that vortex solutions are allowed in the classical vacuum at $T = 0$. Since vortices also exist in the semi-classical model, we can speculate that disordered states, even in the quantum case, are constituted of free vortices.

The main motivation of this work was to study the critical properties of the Hamiltonian Eq. (1), but we have also calculated the following thermodynamic quantities: internal energy, specific heat, entropy and free energy. In the SCHA we can perform the calculation, as mentioned before, only at temperatures below the critical temperature. The calculations were done using the following standard expressions:

$$U = \frac{1}{(2\pi)^d} \int n_k \omega_k d^d k \text{ internal energy.} \quad (21)$$

$$C = \frac{\partial U}{\partial T} \text{ specific heat.} \quad (22)$$

$$S = -\frac{1}{(2\pi)^d} \int d^d k [n_k \ln(n_k) - (1+n_k) \ln(1+n_k)] \text{ entropy} \quad (23)$$

$$F = T \int \frac{d^d k}{(2\pi)^d} \ln(1 - e^{-\frac{\omega_k}{T}}) \text{ free energy.} \quad (24)$$

Here, d is the dimension, $n_k = 1/[\exp(\omega_k/T) - 1]$, and we have taken the Boltzmann constant $k_B = 1$. We remark that in these equations ω_k is temperature dependent and therefore our results are different from the ones for a non interacting boson gas.

For the standard Bose gas where $\omega_q \propto q^2$, for small q , we have a divergence at $q = 0$ in two dimensions. However for the model studied here $\omega_q \propto q$ for small q , and the above equations can be used in two dimensions.

3. Results

In Fig. 1 we show the critical parameter D_C/J_1 as a function of η , for $\lambda = 0$ and $\alpha = 0$. The parameter D_C vanishes at the points

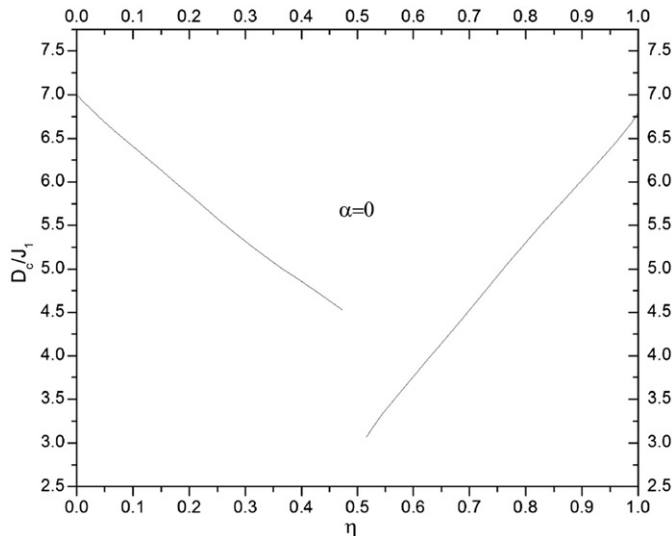


Fig. 1. Critical anisotropy parameter D_C/J_1 as a function of η for $\lambda = 0$ and $\alpha = 0$.

$\eta_{1C} = 0.49$ and $\eta_{2C} = 0.52$. There are two ordered phases separated by the magnetically disordered phase. These values are quite different from the ones calculated for $S = 1/2$ Heisenberg antiferromagnet [4]. Here, the range of the paramagnetic phase is very narrow. The discontinuity of the curve is an artifact of the SCHA. In Fig. 2, we present the same data for $\lambda = 1$. Now $\eta_{1C} = 0.49$ and $\eta_{2C} = 0.51$, the paramagnetic phase is slight smaller. We have found $D_C/J_1 = 7.32$ for $\eta = 0$, $\alpha = 0$, $\lambda = 1$. This value agrees reasonably well with the result 6.38 obtained by Wong et al. [20] using the coupled-cluster expansions. When we increase the value of α , the size of the disordered phase decreases, and it disappears for $\alpha = 1$. This result is expected since the effect of quantum fluctuations is smaller in 3D. Fig. 3 shows the case $\alpha = 1$, $\lambda = 0$, and as we can see the value of D_C is larger compared to the value for $\alpha = 0$. In Fig. 4 we show the critical temperature T_C/J_1 as a function of frustration η , for $\alpha = 0$ and $\lambda = 0$ and two different values of the anisotropy D/J_1 . In Fig. 5 we show the critical temperature T_C/J_1 as a function of D/J_1 , in the Néel phase, for $\alpha = 0$, $\lambda = 0$, and three values of η . In Fig. 6 we show T_C/J_1 as a function of D/J_1 , in the same phase for $\eta = 0.4$, $\lambda = 0$, and two values of α . We remark that the hump in the critical line, at small T , has been observed in

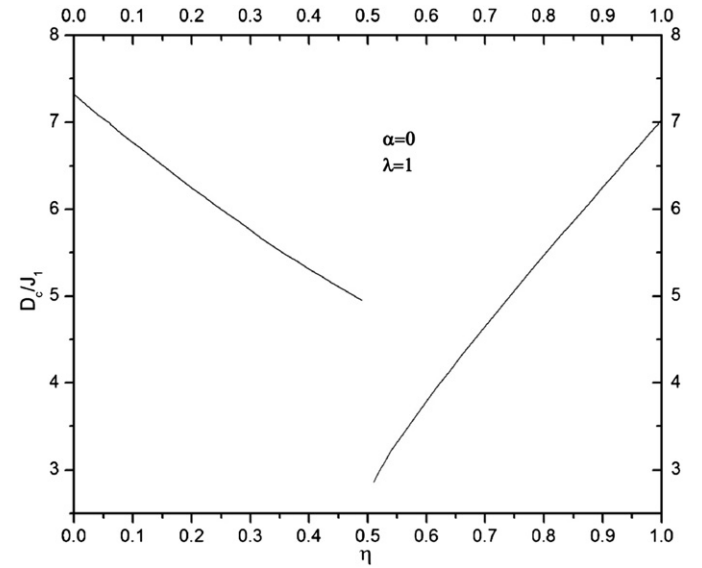


Fig. 2. Critical anisotropy parameter D_C/J_1 as a function of η for $\lambda = 1$ and $\alpha = 0$.

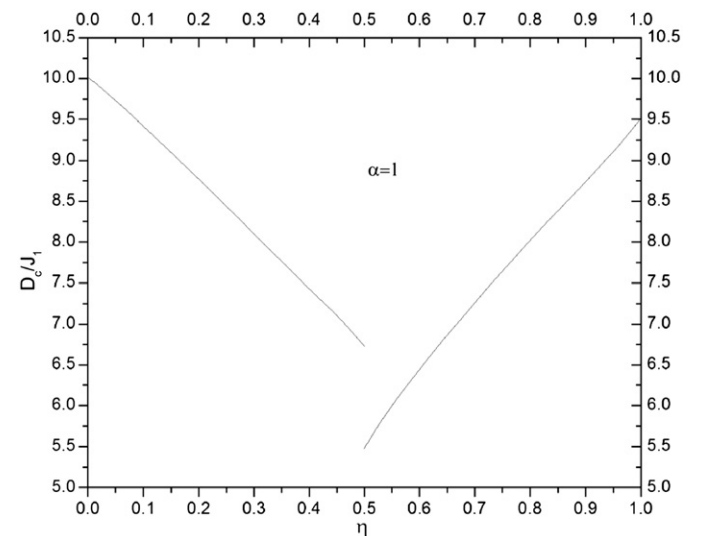


Fig. 3. Critical anisotropy parameter D_C/J_1 as a function of η for $\lambda = 0$ and $\alpha = 1$.

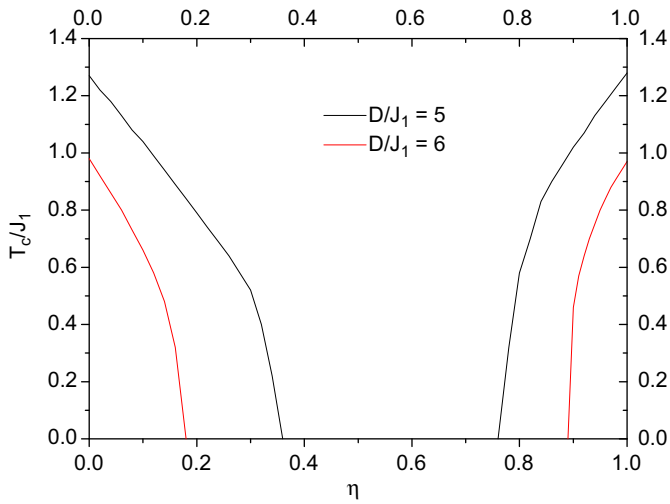


Fig. 4. Critical temperature T_c/J_1 as a function of η , for $\alpha=0, \lambda=0$ and 2 values of D/J_1 .

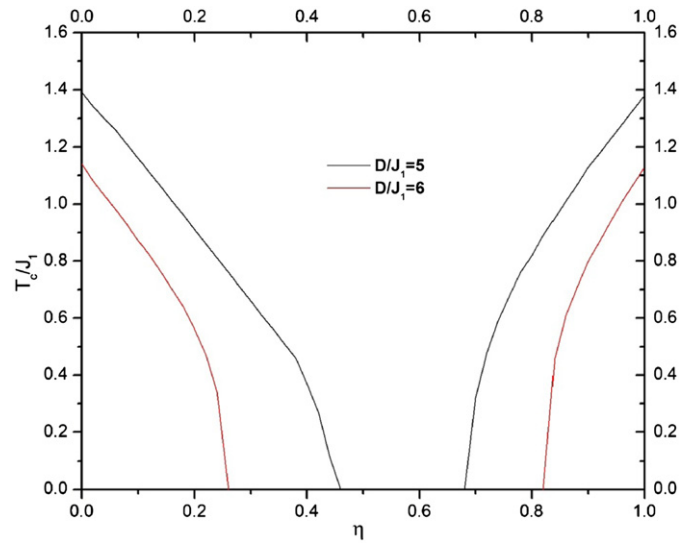


Fig. 7. Critical temperature T_c/J_1 as a function of η , for $\alpha=0, \lambda=1$ and 2 values of D/J_1 .

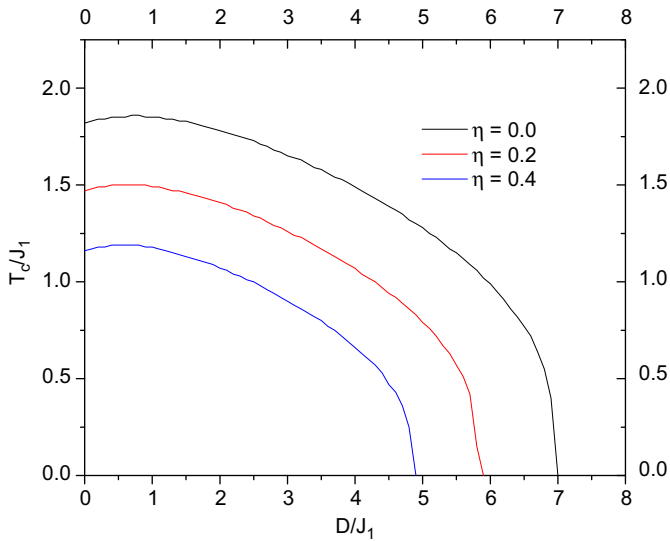


Fig. 5. Critical temperature T_c/J_1 as a function of D/J_1 in the Néel phase for $\alpha=0, \lambda=0$, and 3 values of η .

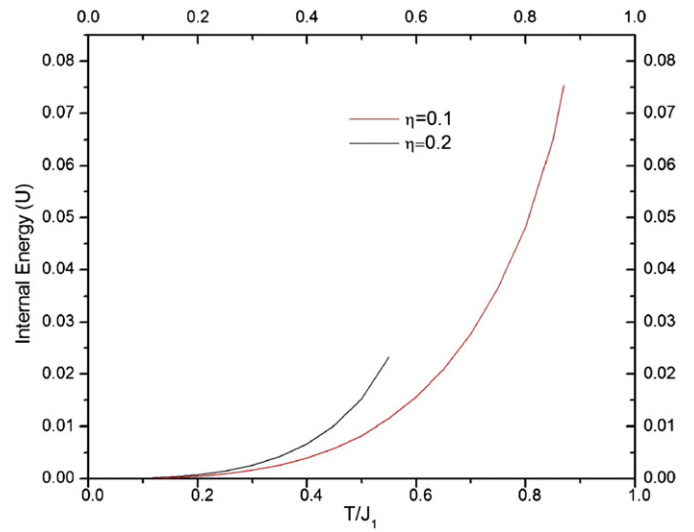


Fig. 8. Internal energy as function of temperature T/J_1 , for $\alpha=0, \lambda=1, D/J_1=6.0$ and 2 values of η .

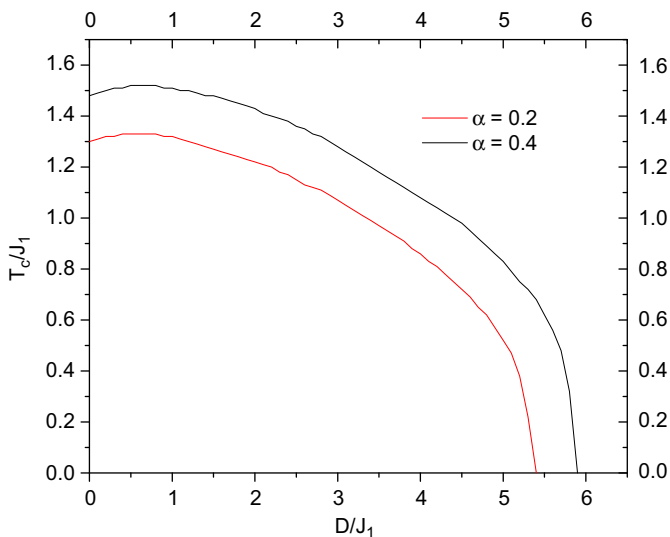


Fig. 6. Critical temperature T_c/J_1 as a function of D/J_1 in the Néel phase, $\eta=0, \lambda=0$, and 2 values of α .

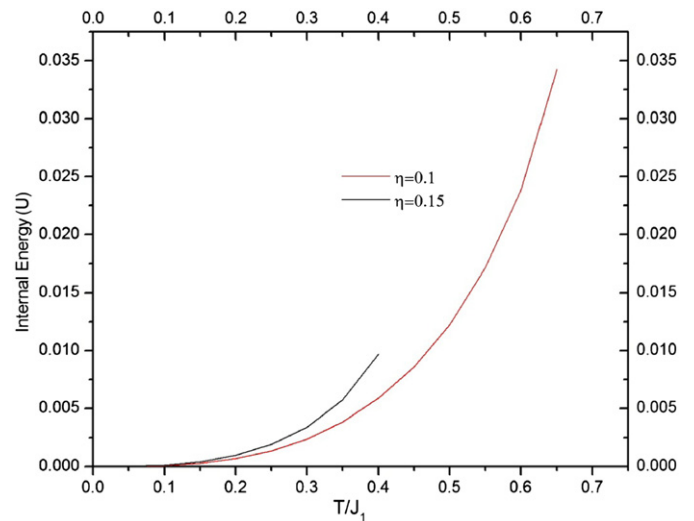


Fig. 9. Internal energy as function of temperature T/J_1 , for $\alpha=0, \lambda=0, D/J_1=6.0$ and 2 values of η .

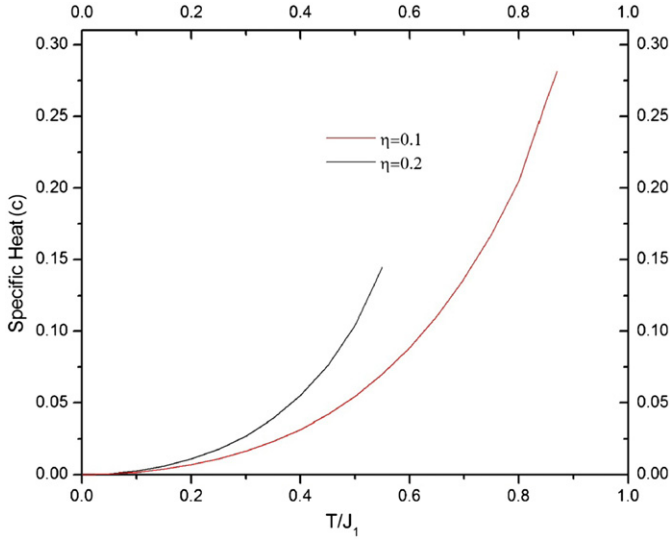


Fig. 10. Specific heat as function of temperature T/J_1 for $\alpha=0$, $\lambda=1$, $D/J_1=6.0$ and 2 values of η .

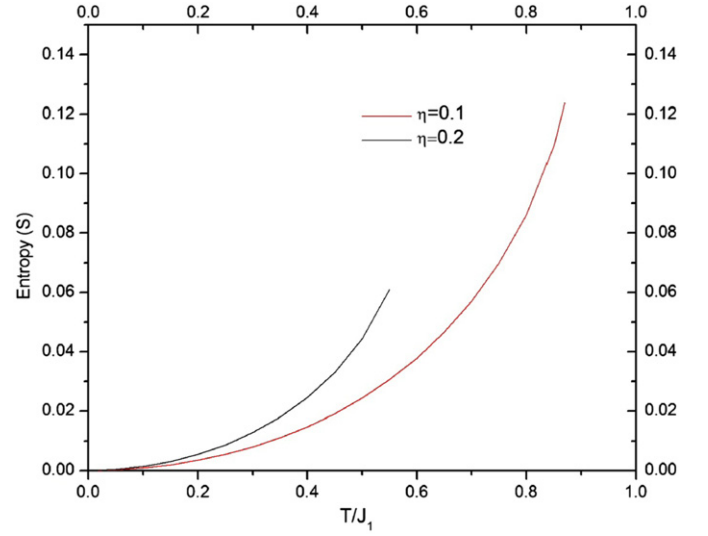


Fig. 12. Entropy as function of temperature T/J_1 , for $\alpha=0$, $\lambda=1$, $D/J_1=6.0$ and 2 values of η .

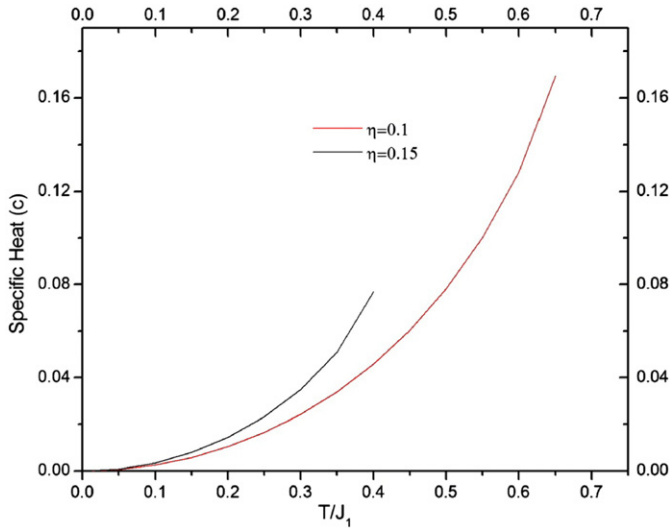


Fig. 11. Specific heat as function of temperature T/J_1 , for $\alpha=0$, $\lambda=0$, $D/J_1=6.0$ and 2 values of η .

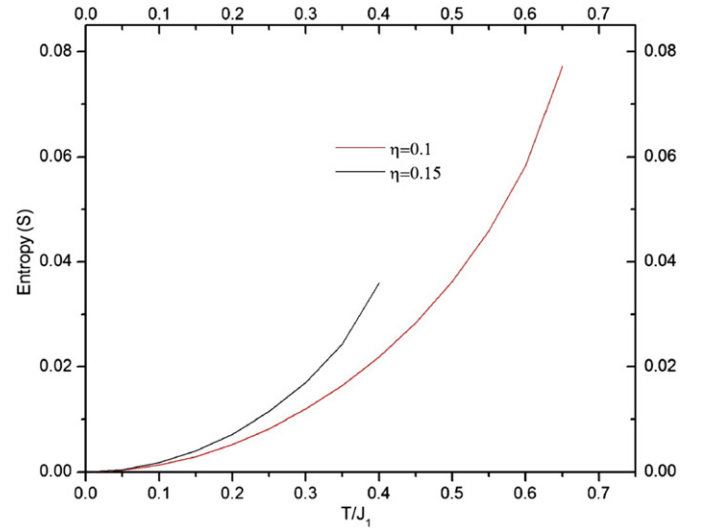


Fig. 13. Entropy as function of temperature T/J_1 , for $\alpha=0$, $\lambda=0$, $D/J_1=6.0$ and 2 values of η .

previous calculations [13,22]. In the classical case when we increase D , fluctuations out of the XY plane are suppressed, and in the limit $D \rightarrow \infty$ we have what is called the plane rotor model with a KT temperature greater than the one for the former model. This is, T_{KT} increase with D [21]. In the quantum case, large D leads to quantum fluctuations out of the XY plane and therefore to a decrease of T_{KT} . We believe this competition is responsible for the broad maximum for small values of D .

In Fig. 7 we show T_C/J_1 as a function of η , for $\alpha=0$, $\lambda=1$ and 2 values of D/J_1 . As expected, the region of the paramagnetic phase increases with D .

In Figs. 8 and 9 we show the internal energy as a function of the temperature for $\alpha=0$, $\lambda=1(0)$ and $D/J_1=6$. In Figs. 10 and 11 we show the specific heat as a function of the temperature for $\alpha=0$, $\lambda=1(0)$ and $D/J_1=6$. In Figs. 12 and 13 we show the entropy as function of the temperature for $\alpha=0$, $\lambda=1(0)$ and $D/J_1=6$. As expected the entropy increases with temperature as we go to the disordered phase. In Figs. 14 and 15 we show the free energy

as a function of the temperature for $\alpha=0$, $\lambda=1(0)$ and $D/J_1=6$. As expected the free energy decreases with temperature.

For the classical 2D, J_1-J_2 XY model it has been shown [19] that the transition from the collinear to the paramagnetic phase is in the same universality class than the XY-Ising models. The SCHA cannot distinguish between this kind of transition and a pure KT transition.

Without frustration, magnetic order for $\alpha=1$ appears below a temperature scale Θ_{cw} set by the interaction strength J_1 . By contrast, in geometrically frustrated systems nothing sharp is observed at this region: instead, the paramagnetic phase extends to temperatures $T \ll \Theta_{cw}$. Ordering may appear at a low temperature T_C , but a large value for the ratio Θ_{cw}/T_C is a signature of frustration [4].

To summarize, in this paper we have studied the quasi-two-dimensional frustrated Heisenberg antiferromagnet with easy-plane single ion anisotropy. We have calculated the transition temperature from the high-temperature paramagnetic phase to

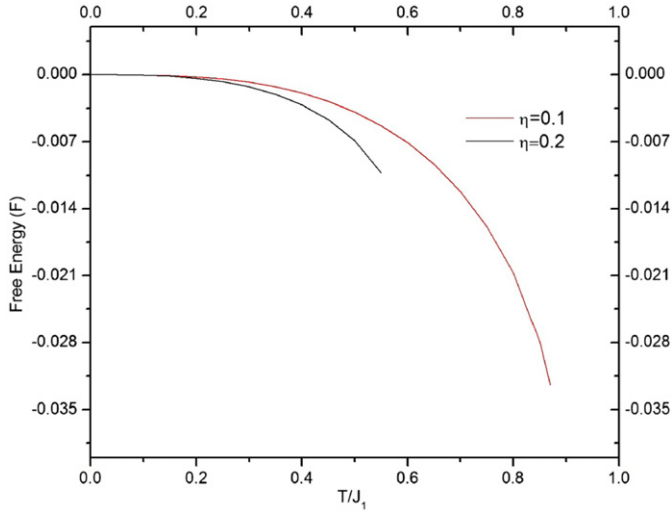


Fig. 14. Free energy as function of temperature T/J_1 , for $\alpha=0$, $\lambda=1$, $D/J_1=6.0$ and 2 values of η .

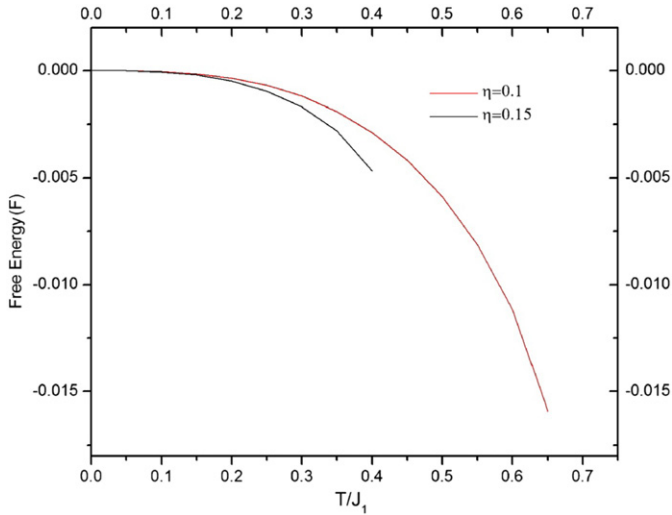


Fig. 15. Free energy as function of temperature T/J_1 , for $\alpha=0$, $\lambda=0$, $D/J_1=6.0$ and 2 values of η .

the low-temperature phase, and the critical single ion anisotropy parameter D_c , that separates the low D region from the large D quantum paramagnetic phase, at zero temperature. We have two

mechanisms that lead to disorder: the single ion anisotropy, whose strength is measured by D , and the competing interaction measured mainly by J_2/J_1 .

The disordered phases at $T=0$ found in our calculations could be a spin liquid state, and therefore presents a new candidate for experimentalists looking for this state.

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