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Quantum correction to the BKT transition for 2D easy-plane antiferromagnets

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We consider the quantum antiferromagnet with easy-plane exchange anisotropy, namely the antiferromagnetic XXZ model, on the square lattice. Its classical counterpart, compared to the planar model shows a reduction of the critical temperature $T_{\rm BKT}$ of the Berezinskii-Kosterlitz-Thouless phase transition, that is a consequence of the thermal out-of-plane fluctuations. For the quantum system we use the pure-quantum self-consistent harmonic approximation to calculate how much the effective exchange interaction is weakened as an effect of the pure-quantum part of the fluctuations. One can then predict the further reduction of $T_{\rm BKT}$ with respect to the corresponding classical system. The theory works well in a wide range of values of the easy-plane anisotropy. In the extreme case of the spin-$\frac{1}{2}$ model, the result is compatible with the estimate of $T_{\rm BKT}$ obtained by previous quantum Monte Carlo simulations. When the anisotropy is weak the theory leads to an unphysical 'isotropization' due to the use of the Villain spin-boson transformation.

The two-dimensional antiferromagnetic XXZ model is described by the general Hamiltonian

$$\hat{\mathcal{H}} = \tfrac{1}{2}J\sum_{\mathbf{i},\mathbf{d}}\left(\hat{S}^x_{\mathbf{i}}\hat{S}^x_{\mathbf{i+d}} + \hat{S}^y_{\mathbf{i}}\hat{S}^y_{\mathbf{i+d}} + \lambda\,\hat{S}^z_{\mathbf{i}}\hat{S}^z_{\mathbf{i+d}}\right)\,, \qquad (1)$$

where the index $\mathbf{i}\equiv(i_1,i_2)$ runs over the sites of a two-dimensional lattice, and $\mathbf{d}\equiv(d_1,d_2)$ represents the displacements of the z nearest-neighbors of each site.

The sum describes an exchange interaction $J>0$ between nearest-neighbor spins, with an easy-plane anisotropy $\lambda\in[0,1)$. The quantum mechanical operators $\hat{\boldsymbol{S}}_{\mathbf{i}}$ satisfy the $SU(2)$ commutation relations $[\hat{S}^\alpha_{\mathbf{i}},\hat{S}^\beta_{\mathbf{j}}]=\delta_{\mathbf{ij}}\epsilon^{\alpha\beta\gamma}\hat{S}^\gamma$ and belong to the spin-S representation, $|\hat{\boldsymbol{S}}_{\mathbf{i}}|^2=S(S{+}1)$.

The lattice is such that it can be considered as two interpenetrating identical sublattices (the 'positive' sublattice and the 'negative' one), in such a way that the nearest neighbors of any site in a sublattice belong to the other one; in other words, we do not consider lattices with frustrated bonds.

For $\lambda=0$ the above Hamiltonian describes the $XX0$ model, often (improperly) called 'quantum XY model'; it is to be noticed that the $XX0$ model is equivalent to its ferromagnetic counterpart. Indeed, the canonical transformation

$$\left(\hat{S}^x_{\mathbf{i}},\hat{S}^y_{\mathbf{i}},\hat{S}^z_{\mathbf{i}}\right) \quad\longrightarrow\quad \left((-)^{\mathbf{i}}\hat{S}^x,(-)^{\mathbf{i}}\hat{S}^y,\hat{S}^z\right)\,,$$

where $(-)^{\mathbf{i}}=\pm1$ is the sign of the sublattice containing the site $\mathbf{i}$, transforms the antiferromagnetic $XX0$ model into the ferromagnetic $XX0$ model. More generally, for the XXZ model this canonical transformation is equivalent to put $J\to-J$ and $\lambda\to-\lambda$.

The classical counterpart of the Hamiltonian (1) is obtained by associating to each spin operator $\hat{\boldsymbol{S}}_{\mathbf{i}}$ a classical vector $\boldsymbol{S}_{\mathbf{i}}$ of given length $\widetilde{S}$. In terms of unit vectors $\boldsymbol{s}_{\mathbf{i}}=\boldsymbol{S}_{\mathbf{i}}/\widetilde{S}$,

$$\mathcal{H} = \tfrac{1}{2}\varepsilon\sum_{\mathbf{i},\mathbf{d}}\left(s^x_{\mathbf{i}}s^x_{\mathbf{i+d}} + s^y_{\mathbf{i}}s^y_{\mathbf{i+d}} + \lambda\,s^z_{\mathbf{i}}s^z_{\mathbf{i+d}}\right)\,, \qquad (2)$$

with the exchange energy $\varepsilon=J\widetilde{S}^2$; in the following we will only use the dimensionless temperature $t=T/\varepsilon$. The choice of $\widetilde{S}$ is not trivial, since values as S or $\sqrt{S(S+1)}$ are both reasonable: a different answer, $\widetilde{S}=S+\frac{1}{2}$, arises by applying the *pure-quantum self-consistent harmonic approximation* (PQSCHA) to the quantum Hamiltonian (1), as we will show below. The minimum 'configuration' of the classical Hamiltonian corresponds to the Neél state: the two sublattices are ordered ferromagnetically in the xy plane, but in opposite directions.

At difference with the quantum case, in the classical case the ferromagnetic and the antiferromagnetic cases are fully equivalent (*i.e.*, $J\to-J$), as far as the static properties are concerned.

In the approximation of dominating easy-plane anisotropy the z-components of the spins are neglected and the so-called *planar* model (frequently 'classical XY model') is obtained. Since the spins are reduced to two-component vectors in the xy plane, $\boldsymbol{s}_i=(\cos\varphi_{\mathbf{i}},\sin\varphi_{\mathbf{i}})$, its Hamiltonian can be written in terms of the azimuthal angles, $\mathcal{H}=\frac{1}{2}\varepsilon\sum_{\mathbf{i},\mathbf{d}}\cos(\varphi_{\mathbf{i}}-\varphi_{\mathbf{i+d}})$. This is the prototype system that undergoes the Berezinskii-Kosterlitz-Thouless (BKT) phase transition [1–3] occurring at the temperature $t_{\rm BKT} = T_{\rm BKT}/\varepsilon \simeq 0.89$, that has been calculated by Monte Carlo simulations [4,5]. The antiferromagnetic order parameter $\langle(-)^{\bf i}\, {\boldsymbol s}_{\bf i}\rangle$, is vanishing at any temperature, and the mechanism underlying the transition is the unbinding of vortex pairs [2,6]. For $t < t_{\rm BKT}$ the correlation function $\langle(-)^{\bf i-j}\cos(\varphi_{\bf i}-\varphi_{\bf j})\rangle$ displays a power law decay, $\sim |{\bf i}-{\bf j}|^{-\eta(t)}$, whereas for $t > t_{\rm BKT}$ the behavior is exponential; moreover, the susceptibility has an exponential divergence for $t \to t_{\rm BKT}{}^+$.

With the inclusion of the out-of-plane components $s^z_{\bf i}$ of the spins still a BKT transition is expected at a finite temperature $T_{\rm BKT}(\lambda)$, which vanishes logarithmically [7,8] in the isotropic limit $\lambda \to 1$. Monte Carlo simulations for the classical XXZ model that provide useful data have been published in Ref. [9]; the simulations are performed on the square lattice for $\lambda = 0$, 0.5, 0.95, and 0.99. These observations have lead to identify the transition in the classical XXZ model as BKT, and the corresponding transition temperatures were located at the temperatures reported in Fig. 3.

The quantum system (1) preserves the rotational symmetry around the z-axis; therefore, from universality arguments, it displays the qualitative features of a BKT system as its classical analogue, with quantitative modifications of the critical parameters arising from quantum fluctuations.

The aim of this work is to apply a recent theoretical approach, the *pure-quantum self-consistent harmonic approximation* (PQSCHA) [10], in the treatment of the quantum antiferromagnetic XXZ model (1). By means of the PQSCHA, the thermodynamics of the quantum model is indeed reduced to the study of an *effective* classical problem, that embodies the contribution of quantum fluctuations (which are treated exactly up to the harmonic level) in its temperature-dependent renormalized interaction parameters. The ferromagnetic system has been already treated by PQSCHA [11]. In Ref. [12] one also finds – for the ferromagnetic case – an outline of the derivation of the effective Hamiltonian $\mathcal{H}_{\rm eff}$ in terms of classical spins, a procedure that involves the *Villain transformation* from quantum spin to bosonic variables [13], and the identification of the classical counterpart of the transformed Hamiltonian by the prescription of *Weyl ordering* [14]. It is just the Weyl ordered form of the Villain transformed spin operators that leads to the identification $\widetilde{S} = S + \frac{1}{2}$ [15].

Eventually, the PQSCHA recipe gives the following effective Hamiltonian for the antiferromagnetic XXZ model [16]:

$$\mathcal{H}_{\rm eff} = \frac{\varepsilon}{2} j_{\rm eff} \sum_{\bf i,d} \Big(s^x_{\bf i} s^x_{\bf i+d} + s^y_{\bf i} s^y_{\bf i+d} + \lambda_{\rm eff} s^z_{\bf i} s^z_{\bf i+d} \Big) + + N\varepsilon\, G(t) \ . \quad (3)$$

As in Eq. (2), $\{{\boldsymbol s}_{\bf i}\}$ are classical normalized spin variables. Within the PQSCHA [10], quantum effects are embodied in the following dimensionless interaction parameters

$$j_{\rm eff}(S,\lambda,t) = (1-\tfrac{1}{2}D_\perp)^2\ e^{-\frac{1}{2}\mathcal{D}_\parallel} \ , \quad (4)$$

$$\lambda_{\rm eff}(S,\lambda,t) = \lambda\ (1-\tfrac{1}{2}D_\perp)^{-1}\ e^{\frac{1}{2}\mathcal{D}_\parallel} \ , \quad (5)$$

while $G(t)$ is an additive renormalization that does not enter the calculation of operator averages. The self-consistent renormalization parameters

$$D_\perp = \frac{1}{2\widetilde{S}}\frac{1}{N}\sum_{\bf k}\frac{b_{\bf k}}{a_{\bf k}}\Big(\coth f_{\bf k} - f_{\bf k}^{-1}\Big) \ , \quad (6)$$

$$\mathcal{D}_\parallel = \frac{1}{2\widetilde{S}}\frac{1}{N}\sum_{\bf k}(1-\gamma_{\bf k})\frac{a_{\bf k}}{b_{\bf k}}\Big(\coth f_{\bf k} - f_{\bf k}^{-1}\Big) \ , \quad (7)$$

represent, within the PQSCHA, the *pure-quantum* part of the square fluctuations [10,15] of the z-components of the spins and of the relative azimuthal angle of nearest-neighbor spins, respectively, and are decreasing functions of t and S, vanishing both for $t \to \infty$ or $S \to \infty$. They depend on t, S, and λ through the quantities

$$a^2_{\bf k} = z\, e^{-\frac{1}{2}\mathcal{D}_\parallel}\ (1+\lambda_{\rm eff}\gamma_{\bf k}) \ , \quad (8)$$

$$b^2_{\bf k} = z(1-\tfrac{1}{2}D_\perp)^2\ e^{-\frac{1}{2}\mathcal{D}_\parallel}\ (1-\gamma_{\bf k}) \ , \quad (9)$$

$f_{\bf k} = a_{\bf k}b_{\bf k}/(2\widetilde{S}t)$, $\gamma_{\bf k} = z^{-1}\sum_{\bf d}\cos({\bf k}\cdot{\bf d})$, and ${\bf k}$ is a wavevector varying in the first Brillouin zone. Therefore, the exchange-energy is renormalized by the factor $j_{\rm eff}$, and the easy-plane anisotropy is weakened ($\lambda_{\rm eff} \geq \lambda$), due to the cooperative effect of in-plane and out-of-plane pure-quantum fluctuations. Their typical temperature behavior in the case of the square lattice is reported in Figs. 1, and 2, respectively. For $S \to \infty$, i.e. in the classical limit, $j_{\rm eff} \to 1$ and $\lambda_{\rm eff} \to \lambda$. We notice that the integrals of the pure-quantum fluctuation parameters, Eqs. (6) and (7), get the main contribution from the high-frequency part of the effective magnon spectrum $\omega_{\bf k} = (J\widetilde{S}/\hbar)a_{\bf k}b_{\bf k}$, just because the pure-quantum part of the square fluctuations is obtained by subtracting from the full (harmonically approximated) expression the corresponding classical part (*i.e.* the leading behavior for $f_{\bf k} \to 0$); on the other hand those effects due to the presence of nonlinear excitations (vortices) would mainly affect the low-frequency part, i.e. they are essentially 'classical' and therefore they cannot sensitively change $D_\perp$ and $\mathcal{D}_\parallel$.

Using the PQSCHA formalism [10] one can calculate averages and correlations by means of classical expressions involving the Boltzmann factor corresponding to the effective Hamiltonian. In the present case the classical average with the effective Hamiltonian is defined as

$$\langle\cdots\rangle_{\rm eff} = \mathcal{Z}^{-1}\Big(\prod\nolimits_{\bf i}\int d{\boldsymbol s}_{\bf i}\Big)\ (\cdots)\, e^{-\beta\mathcal{H}_{\rm eff}} \ .$$

In order to obtain the PQSCHA thermal average of a quantum observable, the dots are to be replaced by a phase-space function that is obtained by Gaussian smearing, on the scale of the pure-quantum fluctuations, of the Weyl symbol associated with the same observable [10,15]. In this way we find expressions for the in-plane correlations

$$\langle \hat{S}_{\mathbf{i}}^x \hat{S}_{\mathbf{j}}^x \rangle = \widetilde{S}^2 \, (1 - \tfrac{1}{2} D_\perp)^2 \, e^{-\frac{1}{2}\mathcal{D}_\parallel} e^{D_{\mathbf{ij}}^{\parallel}} \, \langle s_{\mathbf{i}}^x s_{\mathbf{j}}^x \rangle_{\rm eff} \ ,$$

where the renormalization parameters $D_{\mathbf{ij}}^{\parallel}$ [16] for the relative azimuthal fluctuations between sites $\mathbf{i}$ and $\mathbf{j}$ are such that $D_{\mathbf{ij}}^{\parallel} \to 0$ for $|\mathbf{i}-\mathbf{j}| \to \infty$. Therefore, the asymptotic behavior and the correlation length are just those obtained for the effective classical model. It follows that the divergence of the in-plane correlation length related to the classical correlation function $\langle s_{\mathbf{i}}^x s_{\mathbf{j}}^x \rangle_{\rm eff}$ signals the occurrence of the BKT transition in the quantum system. The quantum transition temperature $t_{\rm BKT}(S,\lambda)$ can then be estimated from the knowledge of the corresponding classical one $t_{\rm BKT}^{\rm (cl)}(\lambda)$, with a self-consistency arising from the dependence on t and λ of the renormalized interaction parameters, Eqs. (4) and (5):

$$\frac{t_{\rm BKT}(S,\lambda)}{j_{\rm eff}(S,\lambda,t_{\rm BKT})} = t_{\rm BKT}^{\rm (cl)}\Big(\lambda_{\rm eff}(S,\lambda,t_{\rm BKT})\Big) \ . \qquad (10)$$

It is rather easy to solve this equation for the $XX0$ model [11], since $\lambda_{\rm eff} = 0$ for $\lambda = 0$. In order to solve it for $\lambda \neq 0$ we have made a rough fit of $t_{\rm BKT}^{\rm (cl)}(\lambda)$ using the available values [9] reported as squares in Fig. 3. The fit, as shown in the figure, is considered only for $\lambda < 0.8$, in such a way that we do not run into the zone where $t_{\rm BKT}^{\rm (cl)} \sim [-\ln(1{-}\lambda)]^{-1}$ vanishes logarithmically [7]. Then Eq. (10), rewritten as $j_{\rm eff} = t_{\rm BKT}/t_{\rm BKT}^{\rm (cl)}$, can be solved graphically in Fig. 1 in a recursive way: one estimates the transition temperature using $t_{\rm BKT}^{\rm (cl)}(\lambda)$ and then the value of $\lambda_{\rm eff}$ at this temperature is taken for redoing the procedure, and so on. The results obtained in this way are also reported for different values of S in Fig. 3.

For the $XX0$ model there is a possible comparison with other data in the extreme case of $S = \frac{1}{2}$. Our result is $t_{\rm BKT} = 0.36$ and compares very well with the values found by high temperature expansions [17] (0.39), by real-space renormalization group techniques [18] (0.40), and by recent quantum Monte Carlo simulations [19,20] (0.35).

When λ is risen enough, we see from Fig. 2 that it may happen that $\lambda_{\rm eff}(S,\lambda,t) \geq 1$. When $\lambda_{\rm eff} = 1$ is reached the effective Hamiltonian becomes isotropic, and the theory therefore predicts the disappearance of the BKT transition at sufficiently high values of $\lambda \geq \lambda_c(S)$ (Some values are $\lambda_c = 0.58, 0.75, 0.85, 0.90, 0.92$, for $S = \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}$, respectively). However, this situation has to be considered with care, because the derivation of the effective Hamiltonian relies on the validity of the Villain transformation [13], which is meaningful only for easy-plane systems. Indeed, the possible break-down of the quantum BKT scenario for sufficiently small anisotropy occurs together with the break-down of our renormalization scheme, since the out-of-plane fluctuations become so strong that the assumed dominant easy-plane character becomes meaningless. The break-down does not occur for $\lambda \ll \lambda_c$, of course, and therefore does not affect teh results reported in Fig. 3.

The suppression of the BKT transition by 'effective isotropization' is therefore unlikely to be physical, as confirmed also by quantum Monte Carlo simulations of the S-$\frac{1}{2}$ XXZ antiferromagnet [21]: at $\lambda = 0.90$ and 0.98 the BKT behavior is still observed, with substantially high transition temperatures, $t_{\rm BKT} = 0.285$ and 0.25, respectively. In order to reach this regime by means of the PQSCHA, we should resort to a different spin-boson transformation, as the Holstein-Primakoff one [22], which is useful also in the isotropic case since it treats the spin fluctuations in a symmetrical way, so that we expect to obtain $\lambda_{\rm eff} < 1$ for any $\lambda < 1$. On the other hand, the calculation of $\mathcal{H}_{\rm eff}$ becomes much more complicated: work is in progress along this line.

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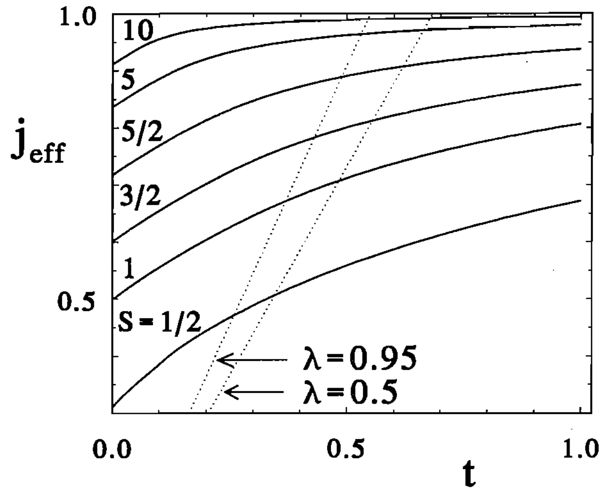

FIG. 1. The effective exchange coupling $j_{\rm eff}(S,\lambda=0.5,t)$ for the $XX0$ antiferromagnetic model *vs.* temperature $t=T/\varepsilon$ and for different values of the spin S (solid lines). The energy scale is $\varepsilon=J\widetilde{S}^2=J(S+\frac{1}{2})^2$. The dotted lines are the curves $t/t^{\rm (cl)}_{\rm BKT}(\lambda)$ for $\lambda=0.5$ and 0.95. See the text for the discussion about the use of such curves for graphically solving Eq. (10).

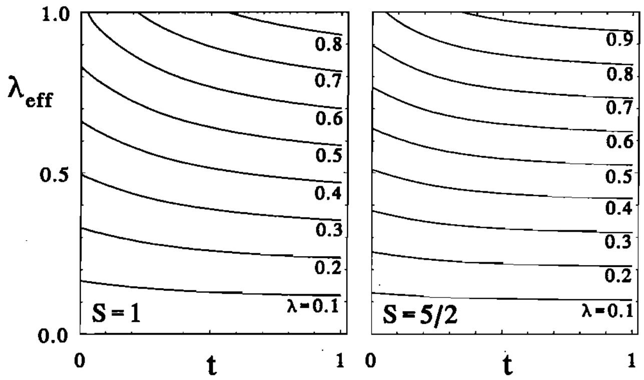

FIG. 2. The effective anisotropy parameter $\lambda_{\rm eff}$ for the $XX0$ antiferromagnetic model *vs.* temperature and for spin $S=1$ and $S=5/2$, at different values of λ. For high values of λ the curves reach the isotropic value $\lambda_{\rm eff}=1$.

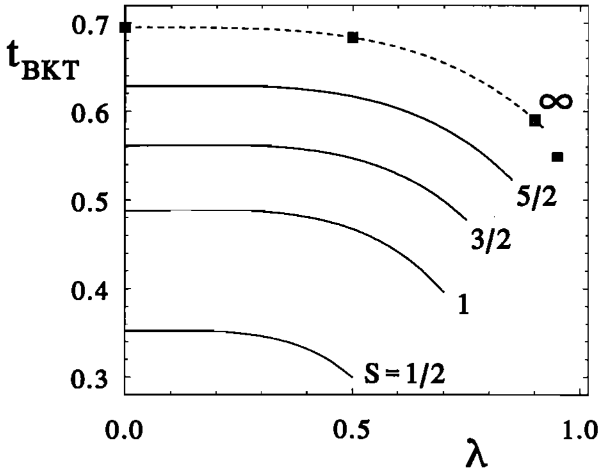

FIG. 3. The critical temperature $t_{\rm BKT}$ of the XXZ antiferromagnetic model *vs.* the value of the anisotropy λ and for different values of the spin S. The classical values (squares) from Ref. [9] are 0.695 ± 0.005, 0.683 ± 0.005, 0.59 ± 0.01, 0.55 ± 0.01, for $\lambda=0$, 0.5, 0.9, and 0.95, respectively. Note that $t_{\rm BKT}(S,\lambda)$ decreases when λ is increased, and the theory would lead to the disappearance of the transition by a mechanism of 'isotropization'. See comments in text.