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The quantum easy-plane ferro- and antiferromagnet

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The Berezinskii-Kosterlitz-Thouless (BKT) phase transition is peculiar of two-dimensional magnetic systems with easy-plane anisotropy. Their prototype is the classical planar (or XY) model, that neglects the role of the out-of-plane spin component. The latter is accounted for in the (easy-plane) XXZ model, that has been studied on a square two-dimensional lattice. From Monte Carlo simulation for the classical XXZ model the classical transition temperature $T_{\rm BKT}^{\rm (cl)}$ turns out to be considerably lower than that of the planar model. The quantum XXZ model is approached by the *pure-quantum self-consistent harmonic approximation*, which leads to the investigation of an effective classical model. Quantum fluctuations reduce the effective exchange interaction, resulting in a lower BKT transition temperature $T_{\rm BKT}$.

1 The quantum XXZ model

The two-dimensional ferromagnetic (FM) and antiferromagnetic (AFM) XXZ models are described by the general Hamiltonian

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

where the negative (positive) sign refers to the FM (AFM) case. 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 $\mathcal{SU}(2)$ 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, $|\hat{\boldsymbol{S}}_{\mathbf{i}}|^2 = S(S+1)$.

In the AFM case the lattice is such that it can be considered as two interpenetrating identical sublattices (the 'positive' 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, lattices with frustration are not considered here.

If $(-)^{\mathbf{i}} = \pm 1$ denotes the sign of the sublattice containing the site $\mathbf{i}$, the canonical transformation

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

transforms the AFM XXZ model into the FM XXZ model, but with a negative $\lambda \in (-1, 0]$, so that it is apparent that the AFM and the FM cases can be treated simultaneously considering only the FM one with $\lambda \in (-1, 1)$, as done in the following. The order parameter $\langle \hat{\boldsymbol{S}}_{\mathbf{i}} \rangle$ describes both the FM magnetization and the AFM staggered magnetization. For $\lambda = 0$ the above Hamiltonian describes the $XX0$ model, often called 'quantum XY model'; of course, the AFM $XX0$ model is equivalent to its FM counterpart.

2 The classical XXZ model

The Hamiltonian (1) has a classical counterpart, that can be obtained by replacing each spin operator $\hat{\boldsymbol{S}}_{\mathbf{i}}$ with a classical vector $\boldsymbol{S}_{\mathbf{i}}$ of a suitable length $\widetilde{S}$ [a]In terms of unit vectors $\boldsymbol{s}_{\mathbf{i}} = \boldsymbol{S}_{\mathbf{i}}/\widetilde{S}$ the Hamiltonian of the classical XXZ model reads then

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

with the exchange energy $\varepsilon = J\widetilde{S}^2$. It is convenient to make use of the dimensionless temperature $t = T/\varepsilon$.

At variance with the quantum system, in the classical one the FM and the AFM cases are fully equivalent as far as the static properties are concerned, since the classical expression of thermal averages is invariant under independent reflections of the spin components (*i.e.* under the transformation $\lambda \to -\lambda$).

The minimum configuration of the classical Hamiltonian corresponds to the ordered state, where all the spins are aligned in an arbitrary direction in the xy-plane. In the AFM picture this state is the Néel state: the two sublattices are ordered ferromagnetically in the xy plane, but in opposite directions. However,

[a]The choice of $\widetilde{S}$ is not trivial; *e.g.* the values S or $\sqrt{S(S+1)}$ are both reasonable.

Table 1: BKT transition temperatures of the classical XXZ model [11].

λ	0	0.5	0.9	0.95
$t_{\rm BKT}^{\rm (cl)}$	0.695 ± 0.005	0.683 ± 0.005	0.59 ± 0.01	0.55 ± 0.01

this configuration is unstable against thermal fluctuations: as a consequence of the Mermin-Wagner theorem [1] the classical XXZ model in two dimensions cannot have finite magnetization at nonzero temperature.

If one neglects the z-components of the spins, the so-called *planar* (or '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, $\mathcal{H} = -\frac{1}{2}\varepsilon \sum_{\mathbf{i},\mathbf{d}} \cos(\varphi_{\mathbf{i}} - \varphi_{\mathbf{i}+\mathbf{d}})$. This is the prototype system that undergoes the Berezinskii-Kosterlitz-Thouless (BKT) phase transition [2,3,4] which occurs at the temperature $t_{\rm BKT} = T_{\rm BKT}/\varepsilon \simeq 0.89$ (this value has been calculated by Monte Carlo simulations [5,6]). The order parameter $\langle \boldsymbol{s}_{\mathbf{i}} \rangle$, is vanishing at any temperature, and the mechanism underlying the transition is the unbinding of vortex pairs [3,7]. For $t < t_{\rm BKT}$ the correlation function $\langle \cos(\varphi_{\mathbf{i}} - \varphi_{\mathbf{j}}) \rangle \sim |\mathbf{i} - \mathbf{j}|^{-\eta(t)}$ displays a power-law decay, whereas for $t > t_{\rm BKT}$ the decay is exponential; the correlation length ξ and the susceptibility χ have an exponential divergence for $t \to {t_{\rm BKT}}^{+}$,

$$\xi \ , \ \chi \ \sim \ e^{a(t - t_{\rm BKT})^{-1/2}} \ , \tag{3}$$

and stay infinite for all temperatures $t \leq t_{\rm BKT}$, so that an entire line of critical points appears in the phase diagram. The specific heat does not display any divergence, but only a maximum located slightly above the transition temperature (at $t \simeq 1.1\, t_{\rm BKT}$ in the pure planar model [5,6]).

With the inclusion of the third components of the spins, *i.e.* for the generic XXZ model (2), the system symmetry remains unchanged and a BKT transition is still expected at a finite temperature $t_{\rm BKT}(\lambda)$, which vanishes logarithmically [8,9,10] as $t_{\rm BKT} \sim -1/\ln(1 - |\lambda|)$ in the isotropic limit $|\lambda| \to 1$.

We have recently performed Monte Carlo simulations for the classical XXZ model that provide useful data [11] for the XXZ model on the square lattice, at anisotropy values $\lambda = 0$, 0.5, 0.95, and 0.99, with lattice sizes from 32×32 up to 256×256. These observations have lead to identify the transition as BKT, and to locate the corresponding critical temperatures as reported in Table 1. In order to investigate the divergence of ξ and χ in approaching $t_{\rm BKT}$ only outcomes of those simulations not affected by appreciable finite-size effects have been used, *i.e.* the data obtained for lattice sizes $L \geq 6\,\xi$. In order

to ascertain the BKT character of the transition the data were fitted by the chi-square minimization criterion using Eq. (3), which turns out to reproduce the data better than the power law

$$\xi \ , \ \chi \ \sim \ (t - t_c)^{-\nu} \ , \tag{4}$$

typical of second-order phase transitions. In Fig. 1 BKT and power-law fits to the data for $\lambda = 0$ are reported.

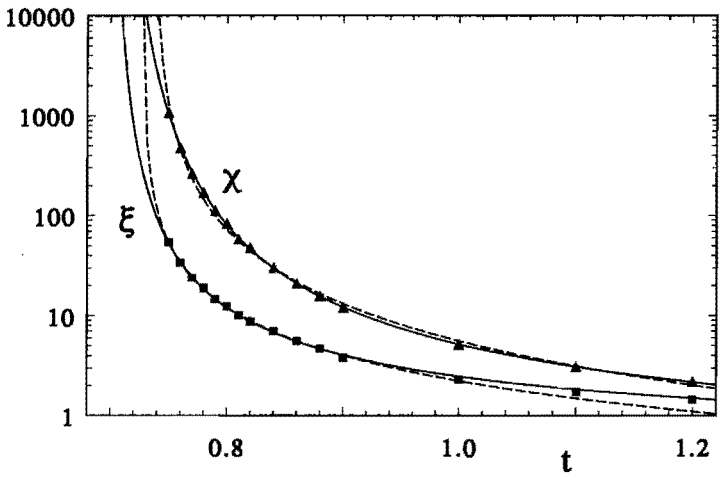

Figure 1: Monte Carlo data for the in-plane susceptibility χ (triangles) and correlation length ξ (squares) at $\lambda = 0$ plotted as function of temperature. The full line and dashed line are the best BKT [Eq. (3)] and power-law [Eq. (4)] fitting functions, respectively.

3 Quantum correction to the BKT transition temperature

The *pure-quantum self-consistent harmonic approximation* (PQSCHA) [12] reduces the thermodynamics of the quantum XXZ model to the study of an *effective* classical problem, that embodies the contribution of the pure-quantum part of the fluctuations (treated in a harmonic approximation) through its temperature-dependent renormalized interaction parameters.

In Refs. [13,14] one finds 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 [15], and the identification of the classical counterpart of the transformed Hamiltonian by the prescription of *Weyl ordering* [16]. It is just the Weyl ordered form of the Villain-transformed

spin operators that leads [17] to the identification $\widetilde{S} = S + \frac{1}{2}$. Eventually, the following effective Hamiltonian is found:

$$\mathcal{H}_{\rm eff} = \frac{\varepsilon}{2} j_{\rm eff} \sum_{\mathbf{i},\mathbf{d}} \left(s^x_{\mathbf{i}} s^x_{\mathbf{i}+\mathbf{d}} + s^y_{\mathbf{i}} s^y_{\mathbf{i}+\mathbf{d}} + \lambda_{\rm eff} s^z_{\mathbf{i}} s^z_{\mathbf{i}+\mathbf{d}} \right) + N\varepsilon\, G(t) \ . \qquad (5)$$

Within the PQSCHA [12], quantum effects are embodied in

$$j_{\rm eff}(S,\lambda,t) \ = \ (1-\tfrac{1}{2}D_\perp)^2 \ e^{-\frac{1}{2}\mathcal{D}_\parallel} \ , \qquad (6)$$

$$\lambda_{\rm eff}(S,\lambda,t) \ = \ \lambda \ (1-\tfrac{1}{2}D_\perp)^{-1} \ e^{\frac{1}{2}\mathcal{D}_\parallel} \ , \qquad (7)$$

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

$$D_\perp \ = \ \frac{1}{2\widetilde{S}} \frac{1}{N} \sum_{\mathbf{k}} \frac{b_{\mathbf{k}}}{a_{\mathbf{k}}} \left(\coth f_{\mathbf{k}} - f_{\mathbf{k}}^{-1} \right) \ , \qquad (8)$$

$$\mathcal{D}_\parallel \ = \ \frac{1}{2\widetilde{S}} \frac{1}{N} \sum_{\mathbf{k}} (1-\gamma_{\mathbf{k}}) \frac{a_{\mathbf{k}}}{b_{\mathbf{k}}} \left(\coth f_{\mathbf{k}} - f_{\mathbf{k}}^{-1} \right) \ , \qquad (9)$$

represent, within the PQSCHA, the *pure-quantum* part of the square fluctuations [12,17] of $\hat{s}^z_{\mathbf{i}}$ and of $(\hat{\varphi}_{\mathbf{i}} - \hat{\varphi}_{\mathbf{j}})$ ($\mathbf{i}$, $\mathbf{j}$ nearest-neighbors), respectively. They decrease with t and S, and vanish both for $t \to \infty$ or $S \to \infty$. The other quantities are $a^2_{\mathbf{k}} = z\, e^{-\mathcal{D}_\parallel/2} \ (1+\lambda_{\rm eff}\, \gamma_{\mathbf{k}})$, $b^2_{\mathbf{k}} = z(1-\frac{1}{2}D_\perp)^2 \ e^{-\mathcal{D}_\parallel/2} \ (1-\gamma_{\mathbf{k}})$, $f_{\mathbf{k}} = a_{\mathbf{k}} b_{\mathbf{k}} / (2\widetilde{S}t)$, $\gamma_{\mathbf{k}} = z^{-1} \sum_{\mathbf{d}} \cos(\mathbf{k}\cdot\mathbf{d})$, and $\mathbf{k}$ is a wavevector varying in the first Brillouin zone.

Therefore, the exchange energy is reduced 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. 2, and 3, 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. (8) and (9), get the main contribution from the high-frequency part of the effective magnon spectrum $\omega_{\mathbf{k}} = (J\widetilde{S}/\hbar) a_{\mathbf{k}} b_{\mathbf{k}}$, 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 $f_{\mathbf{k}} \to 0$); 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 $\mathcal{D}_\parallel$.

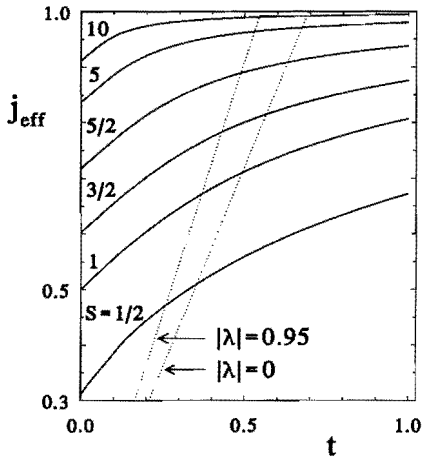

Figure 2: The effective exchange coupling $j_{\rm eff}(S,\lambda=-0.5,t)$ for the (AFM) XXZ model *vs.* temperature and for different spin S. The dotted lines represent $t/t^{\rm (cl)}_{\rm BKT}(\lambda)$ for $\lambda = 0$ and 0.95.

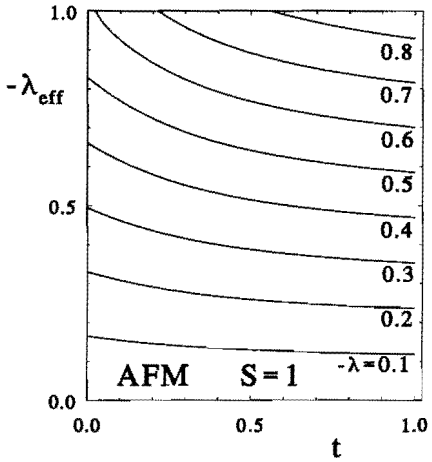

Figure 3: The effective anisotropy parameter $\lambda_{\rm eff}$ for the $S = 1$ AFM XXZ model *vs.* temperature, at different values of λ. For high values of λ the curves reach the isotropic value $\lambda_{\rm eff} = -1$.

Using the PQSCHA formalism [12] the quantum average of any observable $\hat{\mathcal{O}}$ is reduced to a classical expression as

$$\left\langle \hat{\mathcal{O}} \right\rangle = \left\langle \tilde{\mathcal{O}} \right\rangle_{\rm eff} = \mathcal{Z}^{-1} \left(\prod_{\mathbf{i}} \int ds_{\mathbf{i}} \right) \tilde{\mathcal{O}}\, e^{-\beta \mathcal{H}_{\rm eff}} \ ,$$

where $\tilde{\mathcal{O}}$ is obtained by Gaussian smearing, on the scale of the pure-quantum fluctuations, of the Weyl symbol $\mathcal{O}$ associated to $\hat{\mathcal{O}}$ [12,17]. In this way one can easily realize that the in-plane correlations $\langle \hat{S}^x_{\mathbf{i}} \hat{S}^x_{\mathbf{j}} \rangle$ have the same asymptotic behaviour as $\langle s^x_{\mathbf{i}} s^x_{\mathbf{j}} \rangle_{\rm eff}$, so that the correlation length ξ is just that obtained for the effective classical model, and its divergence signals the occurrence of the BKT transition in the quantum system. The transition temperature $t_{\rm BKT}(S,\lambda)$ can then be estimated from the knowledge of the corresponding classical one $t^{\rm (cl)}_{\rm BKT}(\lambda)$, with a self-consistency arising from the dependence on t and λ of the renormalized interaction parameters, Eqs. (6) and (7):

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

It is easy to solve graphically this equation for the $XX0$ model [14], since $\lambda_{\rm eff} = 0$

for $\lambda = 0$. However, it can be solved also for $\lambda \neq 0$, using a rough fit of $t_{\rm BKT}^{\rm (cl)}(\lambda)$ from the available values of Table 1, reported as squares in Fig. 4. Then Eq. (10), rewritten as $j_{\rm eff} = t_{\rm BKT}/t_{\rm BKT}^{\rm (cl)}$, can be solved by recursion. The results are reported for different values of S in Fig. 4, where also the recent quantum Monte Carlo results [18,19] for $S = \frac{1}{2}$ are reported, showing fair agreement with ours for $\lambda = 0$ and 0.5. For $\lambda = 0$ and $S = \frac{1}{2}$ other independent results are available, namely those found by high temperature expansions [20] (0.39) and by real-space renormalization group techniques [21] (0.40).

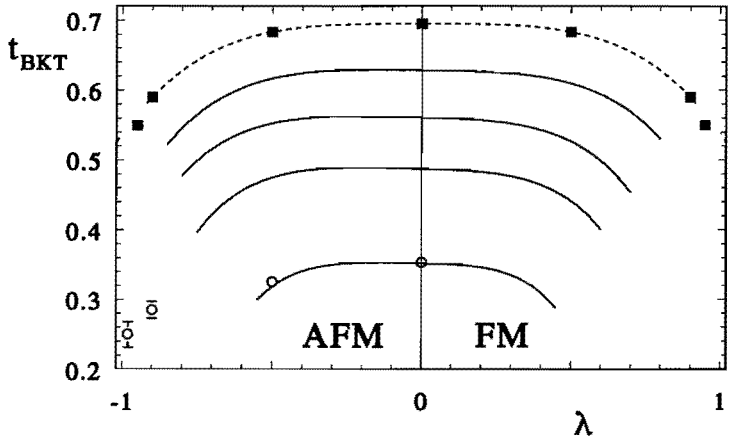

Figure 4: The critical temperature $t_{\rm BKT}$ of the XXZ model *vs.* the anisotropy parameter λ, for different spin S. The circles report quantum Monte Carlo simulation results [19].

When $|\lambda|$ is risen enough, one sees from Fig. 3 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 when $\lambda/\lambda_{\rm c}(S) \geq 1$ (For the AFM one finds $-\lambda_{\rm c} = 0.58$, 0.75, 0.85, 0.90, 0.92, for $S = \frac{1}{2}$, 1, $\frac{3}{2}$, 2, $\frac{5}{2}$, respectively; those for the FM are slightly lower). However, this situation has to be considered with care, because the derivation of the effective Hamiltonian relies on the validity of the Villain transformation [15], 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 the renormalization scheme, since out-of-plane fluctuations become so strong that the assumed easy-plane character becomes meaningless. The break-down does not occur for $\lambda/\lambda_{\rm c} \ll 1$, of course, and therefore it does not affect the results reported in Fig. 4.

The suppression of the BKT transition by 'effective isotropization' is there-

fore unlikely to be a physical phenomenon. This is suggested also by the cited quantum Monte Carlo simulations of the S-$\frac{1}{2}$ XXZ antiferromagnet [19]: 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, one could 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 symmetrically way, so that one expects 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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