Quantum effects on the Berezinskii-Kosterlitz-Thouless transition in the ferromagnetic two-dimensional XXZ model

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The quantum easy-plane ferromagnetic two-dimensional XXZ model is approached by the pure-quantum self-consistent harmonic approximation that reduces it to an effective classical model. Quantum fluctuations weaken both the effective exchange, leading to a reduced Berezinskii-Kosterlitz-Thouless transition temperature with respect to the classical model, and the effective easy-plane anisotropy. The latter vanishes when the anisotropy is smaller than a cutoff value, leading to an instability that could be interpreted as a crossover to a strongly quantum regime where a picture of classical-like renormalized vortices is inadequate.

The two-dimensional (2D) classical XY (or planar) model is known to undergo the topological transition due to vortex-pair unbinding[1] that is usually referred to as the Berezinskii-Kosterlitz-Thouless (BKT) transition.[2–4] At difference with this classical model, the quantum one necessarily deals with three-component spins, even though the out-of-plane spin components could not explicitly appear (if $\lambda=0$) in the Hamiltonian:

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

The index $\mathbf{i}\equiv(i_1,i_2)$ runs over the sites of a two-dimensional Bravais lattice, and $\mathbf{d}\equiv(d_1,d_2)$ represents the displacements of the z nearest neighbors of each site. The quantum spin operators $\hat{\boldsymbol{S}}_{\mathbf{i}}$ satisfy the $\mathcal{SU}(2)$ commutation relations $[\hat{S}^\alpha_{\mathbf{i}},\hat{S}^\beta_{\mathbf{j}}]=i\,\delta_{\mathbf{ij}}\,\epsilon^{\alpha\beta\gamma}\hat{S}^\gamma_{\mathbf{i}}$ and belong to the spin-S representation, $|\hat{\boldsymbol{S}}_{\mathbf{i}}|^2=S(S{+}1)$. They interact through the exchange integral J, with an easy-plane exchange anisotropy λ ($0\le\lambda<1$). Adopting a clear and widely used terminology, we call the system described by the above Hamiltonian the quantum "XXZ model" (for $\lambda=0$, "$XX0$ model").

Its actual classical counterpart, obtained by considering Eq. (1) as a classical Hamiltonian with the spins taken as three-component vectors with some fixed length $\widetilde{S}$, is different from that of the classical XY model, since the z components of the spins are allowed to fluctuate:

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

where $|\boldsymbol{s}_{\mathbf{i}}|^2=1$. For convenience we use the energy scale $\varepsilon=J\widetilde{S}^2$ and define the reduced temperature $t\equiv k_BT/\varepsilon$.

In the classical 2D XXZ model a BKT transition is still expected[5,6] at a finite temperature $t_c(\lambda)$, which decreases weakly with λ, and eventually drops to zero logarithmically[5,6] in the isotropic limit, when the easy-plane anisotropy $\lambda\to1$. Early simulations[7] confirmed the theoretical asymptotic dependence of $t_c(\lambda\lesssim1)$. The BKT critical temperature of the classical $XX0$ model on the square lattice is $t_c(0)\simeq0.70$,[8] to be compared with that of the XY model, $t_c\simeq0.89$.[9,10]

However, the thermodynamic behavior of the quantum 2D XXZ model is still a rather controversial subject. The main point is whether the quantum model displays the same behavior of its classical counterpart, or the transition itself is (or can be) destroyed by quantum fluctuations. Many approaches have been used to answer this question, at least in the $XX0$ case; for instance, real-space renormalization group,[11,12] high-temperature expansions,[13] quantum Monte Carlo[14–18] (QMC).

Since the quantum system (1) preserves the rotational symmetry around the z axis, by universality arguments it should undergo a BKT transition,[2–4] with only quantitative modifications of the critical temperature and prefactors due to quantum fluctuations. For the extreme case of the spin-$\frac{1}{2}$ 2D $XX0$ model this has been recently stated by Ding and Makivić,[17,18] who performed extensive quantum Monte Carlo simulations showing the signatures of the BKT phase transition at $T_c/J\simeq0.35$. They conclude that quantum effects modify the quantitative prefactors, but not the universality class of the transition.

In this work we face the quantum 2D XXZ model by the *pure-quantum self-consistent harmonic approximation* (PQSCHA),[19] an approach we recently proposed that extends the effective potential method[20,21] to general nonstandard Hamiltonians (i.e., without a separated quadratic kinetic part) in order to eventually also treat quantum spin systems. By the PQSCHA the thermodynamics of the quantum model (1) can be reduced to an *effective* classical problem, where the quantum part of fluctuations is accounted for at the self-consistent harmonic level through temperature-dependent renormalized interaction parameters, thus embodying a full quantum treatment of spin waves. Even though the approach is essentially semiclassical, one has the great advantage of fully accounting for the role of nonlinear excitations like solitons[22] or vortices, whose character is essentially clas-

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sical and whose effects are extremely relevant for the thermodynamics of the system. Therefore, the PQSCHA is mainly useful in treating low-dimensional systems, where such nonlinear excitations exist and are at the origin of peculiar behavior, that the usual perturbative semiclassical theories are unable to describe. By the PQSCHA we can switch on the quantum effects in the 2D XXZ model starting from the classical limit, and evaluate their consequences on the critical behavior, showing that the BKT transition of the 2D XXZ model shifts towards lower temperature.

The derivation of the effective Hamiltonian of the 2D XXZ model[8] parallels the one made in an application[22] of the PQSCHA to the quasi-one-dimensional spin-1 easy-plane ferromagnet $CsNiF_3$, where we found excellent agreement with experimental and numerical data in a wide temperature range. As shown there, we use the Villain transformation[23] in order to represent spins in terms of canonically conjugate variables. This spin-boson transformation preserves the commutation rules, but neglects the so-called kinematic interaction due to the limited spectrum of $\hat{S}^z_{\mathbf{i}}$, so that it gives a better description when the spin system has a good easy-plane character and the spin states with large fluctuations of $\hat{S}^z_{\mathbf{i}}$ are less relevant to the thermodynamics. The rule of Weyl ordering, which is inherent in the PQSCHA,[19] leads to set $\widetilde{S} = S + \frac{1}{2}$, and the effective Hamiltonian reads

$$\mathcal{H}_{\mathrm{eff}} = -\frac{\varepsilon}{2} j_{\mathrm{eff}} \sum_{\mathbf{i},\mathbf{d}} \left(s^x_{\mathbf{i}} s^x_{\mathbf{i}+\mathbf{d}} + s^y_{\mathbf{i}} s^y_{\mathbf{i}+\mathbf{d}} + \lambda_{\mathrm{eff}} s^z_{\mathbf{i}} s^z_{\mathbf{i}+\mathbf{d}} \right) + N\varepsilon\, G(t) \; . \tag{3}$$

As in Eq. (2), $\{\boldsymbol{s}_{\mathbf{i}}\}$ are classical normalized spin variables. Within the PQSCHA,[19] quantum effects are embodied in the following dimensionless interaction parameters:

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

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

while

$$G(t) = \frac{t}{N}\sum_{\mathbf{k}} \ln\left(\frac{\sinh f_{\mathbf{k}}}{f_{\mathbf{k}}}\right) - \frac{t}{2}\ln(1-\tfrac{1}{2}D_\perp) - e^{-\frac{1}{2}\mathcal{D}_\parallel}\Big[2D_\perp + (1-D_\perp)\mathcal{D}_\parallel\Big] \tag{6}$$

is an additive renormalization that does not enter the calculation of operator averages. The self-consistent renormalization parameters

$$D_\perp = \frac{1}{N(2S+1)}\sum_{\mathbf{k}} \frac{b_{\mathbf{k}}}{a_{\mathbf{k}}}\left(\coth f_{\mathbf{k}} - f_{\mathbf{k}}^{-1}\right) \; , \tag{7}$$

$$\mathcal{D}_\parallel = \frac{1}{N(2S+1)}\sum_{\mathbf{k}} (1-\gamma_{\mathbf{k}})\frac{a_{\mathbf{k}}}{b_{\mathbf{k}}}\left(\coth f_{\mathbf{k}} - f_{\mathbf{k}}^{-1}\right) \; , \tag{8}$$

represent the *pure-quantum* square fluctuations[19,22] 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

$$a^2_{\mathbf{k}} = z\, e^{-\frac{1}{2}\mathcal{D}_\parallel}\, (1-\lambda_{\mathrm{eff}}\gamma_{\mathbf{k}}) \; , \tag{9}$$

$$b^2_{\mathbf{k}} = z(1-\tfrac{1}{2}D_\perp)^2\, e^{-\frac{1}{2}\mathcal{D}_\parallel}\, (1-\gamma_{\mathbf{k}}) \; , \tag{10}$$

$f_{\mathbf{k}} = a_{\mathbf{k}} b_{\mathbf{k}}/(2S+1)t$, $\gamma_{\mathbf{k}} = z^{-1}\sum_{\mathbf{d}}\cos(\mathbf{k}\cdot\mathbf{d})$, and $\mathbf{k}$ is a wave vector varying in the first Brillouin zone. Therefore, the exchange energy is renormalized by the factor j_{eff}, and the easy-plane anisotropy is weakened ($\lambda_{\mathrm{eff}} \geq \lambda$), due to the cooperative effect of in-plane and out-of-plane pure-quantum fluctuations. Their 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, $j_{\mathrm{eff}} \to 1$ and $\lambda_{\mathrm{eff}} \to \lambda$. We notice that the integrals of the pure-quantum fluctuation parameters, Eqs. (7) and (8), get the main contribution from the high-frequency part of the magnon spectrum $\omega_{\mathbf{k}} \sim a_{\mathbf{k}} b_{\mathbf{k}}$, since the classical asymptotic behavior for $f_{\mathbf{k}} \to 0$ is subtracted; on the other hand those effects due to the presence of nonlinear excitations (e.g., vortices) would mainly affect the low-frequency part, i.e., they are essentially classical and therefore they cannot sensitively change $D_\perp$ and $\mathcal{D}_\parallel$.

Proceeding as in Ref. 22, and defining the classical average with the effective Hamiltonian

$$\langle\cdots\rangle_{\mathrm{eff}} = \mathcal{Z}^{-1}\left(\prod\nolimits_{\mathbf{i}}\int d\boldsymbol{s}_{\mathbf{i}}\right)(\cdots)\, e^{-\beta\mathcal{H}_{\mathrm{eff}}} \; , \tag{11}$$

one can express averages by means of classical-like formulas involving the effective Hamiltonian. For instance, the in-plane correlations take the form

$$\langle \hat{S}^x_{\mathbf{i}} \hat{S}^x_{\mathbf{j}} \rangle = \widetilde{S}^2\, (1-\tfrac{1}{2}D_\perp)^2\, e^{-\frac{1}{2}\mathcal{D}_\parallel} e^{\mathcal{D}^\parallel_{\mathbf{ij}}}\, \langle s^x_{\mathbf{i}} s^x_{\mathbf{j}} \rangle_{\mathrm{eff}} \tag{12}$$

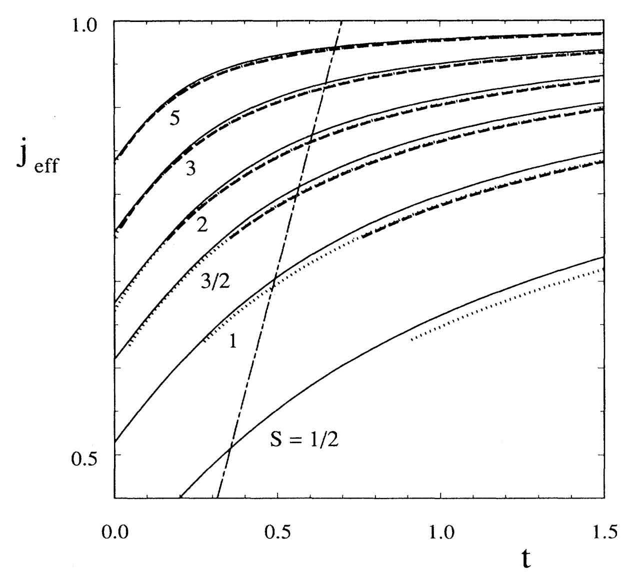

FIG. 1. The effective exchange coupling $j_{\mathrm{eff}}(t,S,\lambda)$ vs t, for different values of S; $\lambda = 0$ (solid lines); $\lambda = 0.7$ (dotted lines); $\lambda = 0.8$ (dashed lines). The energy unit is $\varepsilon = J\widetilde{S}^2 \equiv J(S+\frac{1}{2})^2$. The intersections of the solid lines with the straight dash-dotted line graphically solve Eq. (15). The curves for finite λ are cut off for $t < t_q(S,\lambda)$.

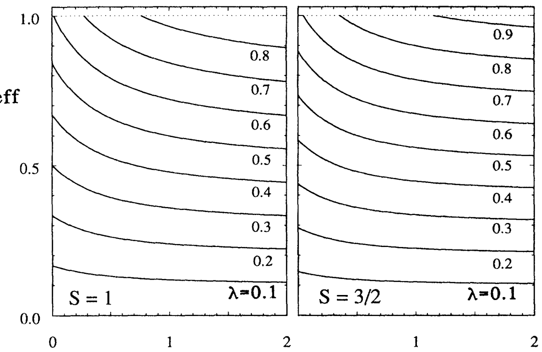

FIG. 2. $\lambda_{\rm eff}(t,S,\lambda)$ vs t, for $S=1$ and for $S=3/2$, at different values of λ. For high values of λ the curves reach the isotropic value $\lambda_{\rm eff}=1$, and identify the corresponding cutoff temperature t_q.

with

$$\mathcal{D}^{\parallel}_{\mathbf{ij}} = \frac{1}{N(2S+1)} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})} \, \frac{a_{\mathbf{k}}}{b_{\mathbf{k}}} \Big(\coth f_{\mathbf{k}} - f_{\mathbf{k}}^{-1} \Big) \ . \quad (13)$$

Since $\mathcal{D}^{\parallel}_{\mathbf{ij}}$ is bounded, the asymptotic behavior of the correlations in the transition region is just the same of the effective classical model, so that the critical behavior of the latter is preserved. It follows that the BKT temperature $t_c(S,\lambda)$ of the quantum system is connected with its classical counterpart $t_c^{(cl)}(\lambda)$ by the self-consistent relation

$$\frac{t_c(S,\lambda)}{j_{\rm eff}(t_c,S,\lambda)} = t_c^{(\rm cl)}\Big(\lambda_{\rm eff}(t_c,S,\lambda)\Big) \ . \quad (14)$$

The simplest situation occurs for $\lambda=0$, so that also $\lambda_{\rm eff}=0$ and one can use the value of the classical transition temperature quoted above, i.e., $t_c^{(\rm cl)}(0) \simeq 0.70$.[24] Equation (14) can be rewritten in this case as

$$\frac{t_c(S,0)}{t_c^{(\rm cl)}(0)} = j_{\rm eff}(t_c,S,0) \ . \quad (15)$$

This equation is solved graphically in Fig. 1, and the resulting values are reported in Table I. In the case of $S=\frac{1}{2}$ the solution extrapolates to $t_c(\frac{1}{2},0) \simeq 0.36$, a value that agrees with the quantum Monte Carlo result[17] (0.353 ± 0.003), and has to be compared with the values found by high-temperature expansions[13] (0.39) and by real-space renormalization group techniques[12] (0.40). However, this agreement is not enough to draw a definite conclusion about the extreme case of the spin-$\frac{1}{2}$ *XX0* model, because the present theory gives high values of the renormalization parameters, $D_\perp(t=t_c) \sim 0.3$ and $\mathcal{D}_\parallel(t=t_c) \sim 0.7$, signalizing the deeply quantum character of the system.[17]

Although the self-consistency of Eq. (14) is rather involute for $\lambda \neq 0$, one sees that $t_c(S,\lambda) \simeq t_c(S,0)$ for λ not close to 1. Indeed, reasoning as in the graphical solution made for $\lambda=0$, one can take into account two facts. First, as a consequence of the behavior of the classical transition temperature $t_c^{(\rm cl)}(\lambda)$ [discussed after Eq. (2)] the straight line of Fig. 1 does not rotate sensitively until $\lambda \to 1$, where it rapidly becomes vertical due to the logarithmic drop to zero of $t_c^{(\rm cl)}(\lambda)$. Second, it appears that $j_{\rm eff}(t,S,\lambda)$ depends very weakly on λ.

Another remarkable effect clearly appears in Fig. 2. Provided that λ is large enough, the curve $\lambda_{\rm eff}(t,S,\lambda)$ as a function of t can cross the value 1 (isotropic limit) at a finite cutoff temperature $t_q(S,\lambda)$. This means that out-of-plane fluctuations become so strong that the assumption of a dominant easy-plane character of the system[8,22] (justifying the use of the Villain transformation[23]) becomes inconsistent. When this happens, the effective Hamiltonian breaks down for temperatures $t < t_q$, since $a^2_{\mathbf{k}}$ becomes negative at small $\mathbf{k}$. Such instability could be only a consequence of the approximation used to study the system by a semiclassical method, but it could also be the signature (even if only qualitative) of a true physical effect, namely the *isotropization* of the effective-classical model. This phenomenon is related to the strength of quantum fluctuations, which make the system no more effectively easy plane. In particular it should be unable to support stable vortexlike excitations, nor, therefore, to display a standard BKT transition, if the effective isotropization sets in at a temperature higher than the critical one.

In fact, let us use the graphical solution procedure in order to estimate the expected quantum critical temperatures. In Fig. 1, the curves for $j_{\rm eff}(t,S,\lambda)$ are cut for $t < t_q(S,\lambda)$, making the solution impossible for values of λ larger than a cutoff value $\lambda_q(S)$. The relation that defines $\lambda_q(S)$ is $t_c(S,\lambda_q) = t_q(S,\lambda_q)$. For instance, at $\lambda=0.8$, the curves for $j_{\rm eff}$ (dashed lines in Fig. 1) corresponding to the four lowest spin values have a finite t_q, and are then cut for $t < t_q(S,\lambda)$. It appears that for $S=\frac{3}{2}$ there is still a temperature range where the effective system is easy plane and can show a BKT behavior, since there is still an (approximate) solution of Eq. (14), i.e., an intersection with the straight line, but for $S=1$ and $\frac{1}{2}$ the solution has already disappeared. Of course, such a breakdown cannot be observed in the *XX0* model. We find $\lambda_q(S) = 0.58, 0.75, 0.84, 0.89, 0.94, 0.97$, respectively, for $S=\frac{1}{2}, 1, \frac{3}{2}, 2, 3, 5$.

Our result could explain why clear experimental evidence of BKT behavior in quasi-two-dimensional ferromagnetic easy-plane materials has never, to our knowledge, been obtained: since the real compounds do not

TABLE I. Estimated BKT critical temperatures $t_c(S,\lambda)$ of the quantum *XXZ* model, for some values of S and $\lambda = 0$ and 0.5. The values in the last column ($S{=}\infty$) are the classical ones (Ref. 24).

S	1/2	1	3/2	2	3	5	∞
$t_c(S,0)$	0.36	0.49	0.57	0.61	0.65	0.68	0.70±0.01
$t_c(S,0.5)$	0.33	0.45	0.52	0.56	0.61	0.64	0.66±0.01

show very strong anisotropies, their values of λ are rather close to 1, so that quantum fluctuations could effectively destabilize the vortex picture. One of such materials, the spin-$\frac{1}{2}$ compound K_2CuF_4, for which $J = 11.36\,K$ and $\lambda \simeq 0.99$, has been studied experimentally[25] with the purpose of checking classical renormalization group analyses,[6] whose prediction is that its 3D ordering transition at $T = 6.25\,K$ (due to the small interlayer coupling $J' \simeq 6.8 \times 10^{-4}\,J$) sets in due to an incipient in-layer BKT transition that causes the correlation length to rise, enhancing the effect of interlayer coupling. However, these experiments do not permit us to assess unambiguously a BKT character.[26] For instance, magnetic susceptibility and correlation length data do not allow us to distinguish between a power-law and a BKT exponential behavior. In addition, Moussa and Villain[27] have successfully described the experimental outcomes for the spin dynamics of the same compound using an isotropic Hamiltonian. Actually, the interlayer coupling is an extra complication for a clear theoretical description of such a system. The recently developed ultrathin magnetic films are promising in this respect, even though finite-size effects are relevant also in macroscopic samples.[28]

The situation seems to be different for antiferromagnets: Quantum Monte Carlo calculations for the spin-$\frac{1}{2}$ 2D XXZ model indicate the existence of the BKT transition even down to $\lambda = 0.98$,[29] with $t_c(\frac{1}{2}, 0.98) \simeq 0.25$; in addition, experimental data for the quasi-2D easy-plane spin-1 compound $BaNi_2(PO_4)_2$ ($\lambda \sim 0.96$) have been successfully explained in terms of quasi-diffusive vortices,[30] also implying BKT behavior.

Summarizing, we have shown that the PQSCHA is well suited to investigate the properties of the strongly anisotropic quantum easy-plane 2D XXZ model, giving results that agree with those of simulations[17] and other theoretical approaches[12,13] also in the extreme quantum case $S = \frac{1}{2}$; the critical behavior of the quantum $XX0$ model may thus be considered rather well understood. When the anisotropy is small ($\lambda \to 1$), however, the situation is less clear. Considering the results of our calculations for the ferromagnetic XXZ model and the current status of the experimental work discussed above, we think that no firm conclusion can be presently reached, and the existence and the character of the transition in quantum weakly anisotropic quasi-two-dimensional systems has still to be regarded as an intriguing open problem, which deserves more accurate experimental and theoretical investigation.

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