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L Capriotti A Cuccoli V Tognetti R Vaia and P Verrucchi

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Thermodynamics of two-dimensional XXZ easy-plane quantum Heisenberg magnets

Luca Capriotti, Alessandro Cuccoli, Valerio Tognetti
Dipartimento di Fisica dell'Università di Firenze and Istituto Nazionale di Fisica della Materia - INFM, largo E. Fermi 2, I-50125 Firenze, Italy

Ruggero Vaia
Istituto di Elettronica Quantistica del Consiglio Nazionale delle Ricerche, via Panciatichi 56/30, I-50127 Firenze, Italy

Paola Verrucchi
ISIS Facility, Rutherford Appleton Laboratory, Chilton, Oxfordshire OX11 0QX, U.K.

We consider the quantum easy-plane (XXZ) magnet on the square lattice. In the classical case the system exhibits the Berezinskii-Kosterlitz-Thouless transition. Simulations, both for ferro- and antiferromagnets, using the method of the effective classical Hamiltonian, are made for different spin values and refer to the specific heat, the static spin correlation functions and correlation lengths in a broad range of temperatures, below and above the transition. The effects of quantum fluctuations are quantitatively evaluated and discussed.

The two-dimensional (2-d) XXZ model is described by the general Hamiltonian

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

where the index $\mathbf{i}\equiv(i_1,i_2)$ runs over the sites of a square lattice with nn displacements $\mathbf{d}$. The spin operators satisfy $|\hat{\mathbf{S}}_{\mathbf{i}}|^2=S(S+1)$. This hamiltonian describes a ferromagnetic (FM) interaction for $J>0$ or an antiferromagnetic (AFM) one for $J<0$, with an easy-plane anisotropy $\lambda\in[0,1)$.

The Hamiltonian keeps its form, but with $(J,\lambda)\to(-J,-\lambda)$, by performing the canonical transformation $(\hat{S}^x_{\mathbf{i}},\hat{S}^y_{\mathbf{i}},\hat{S}^z_{\mathbf{i}})\to((-)^{i_1+i_2}\hat{S}^x_{\mathbf{i}},(-)^{i_1+i_2}\hat{S}^y_{\mathbf{i}},\hat{S}^z_{\mathbf{i}})$. Therefore it is sufficient to consider the FM model only, with $\lambda\in(-1,1)$, to treat simultaneously both FM and AFM. This also explicitly shows that the XX0 ($\lambda=0$) AFM and FM models are equivalent.

The classical counterpart of the Hamiltonian (1) is

$$\mathcal{H} = -\tfrac{1}{2}J\widetilde{S}^2\sum_{\mathbf{i},\mathbf{d}} \Big(s^x_{\mathbf{i}}s^x_{\mathbf{i}+\mathbf{d}} + s^y_{\mathbf{i}}s^y_{\mathbf{i}+\mathbf{d}} + \lambda\,s^z_{\mathbf{i}}s^z_{\mathbf{i}+\mathbf{d}}\Big)~, \qquad (2)$$

where $\mathbf{s}_{\mathbf{i}}=\mathbf{S}_{\mathbf{i}}/\widetilde{S}$ is a unit vector. In the following we will use the dimensionless temperature $t=T/J\widetilde{S}^2$. At variance with the quantum case, as far as the static properties are concerned, the classical ferromagnetic and antiferromagnetic model are fully equivalent, since the corresponding classical integrals are invariant under the transformation $\mathbf{s}_{\mathbf{i}}\to(-)^{i_1+i_2}\mathbf{s}_{\mathbf{i}}$.

For any value of $|\lambda|<1$ the classical model described by the Hamiltonian (1) undergoes a Berezinskii-Kosterlitz-Thouless (BKT) phase transition [1,2] at a finite temperature $t_{\rm BKT}=T_{\rm BKT}/J\widetilde{S}^2$ alike the planar, or classical XY, model. In the latter, the out of plane fluctuations are completely suppressed, and the spins are reduced to two-component vectors in the xy plane.

The distinctive feature of a BKT transition is the vanishing of the order parameter at any temperature, the transition being signalled by the exponential divergence of the in-plane susceptibility and spin fluctuations correlation length at $t_{\rm BKT}$, accompanied by the change in the behaviour of the spin-spin correlation function, which decays exponentially in the completely disordered region, i.e. for temperature above $t_{\rm BKT}$, and as a power law below it. The physical mechanism driving the transition is the unbinding of vortex pairs, which gives rise also to the appearance of a maximum in the specific heat at a temperature slightly higher than $t_{\rm BKT}$.

Monte Carlo simulations of the classical systems [3–6] confirm that the planar and XXZ model have the same qualitative behaviour, but the value of the transition temperature $t_{\rm BKT}\simeq0.89$ [7,8] of the planar model lowers to $t_{\rm BKT}\simeq0.70$ [5,6] of the XX0 model as a consequence of the inclusion of the out-of-plane spin fluctuations, and decreases further as λ increases, vanishing logarithmically [9,10] as the isotropic limit $\lambda\to1$ is approached.

Experiments and quantum Monte Carlo simulations indicate that the qualitative features of a BKT transition are preserved in the quantum system, with quantitative modifications of the critical parameters arising from quantum fluctuations. Such arguments suggest that the theoretical approach we recently introduced [11], named *pure-quantum self-consistent harmonic approximation* (PQSCHA) can be very effective in estimating the quantitative modification of the features of the BKT transition in the XXZ model due to quantum effects, as it allows to recast the study of the quantum thermodynamics of a model to that one of an effective classical model with suitable renormalized parameters. The effectiveness of such approach has been confirmed by the PQSCHA estimates of the critical temperature for strongly easy-plane quantum ferro- and antiferromagnet obtained by a simple scaling procedure and reported in Refs. [12–14]. In this paper we present a more comprehensive investigation of the properties of the quantum XXZ model, focusing our attention on some relevant thermodynamic quantities, as magnetic specific heat, spin-spin correlation functions and correlation length, which we have obtained by classical Monte Carlo simulations of the system described by the effective Hamiltonian; moreover, we will show as reliable estimates of the critical temperature, which well compare with quantum Monte Carlo data, can be obtained also in the quasi isotropic limit $\lambda \to 1$.

An outline of the derivation of the effective Hamiltonian $\mathcal{H}_{\rm eff}$ in terms of classical spins is given in Refs. [16,12–14]. The procedure which leads from $\hat{\mathcal{H}}$ to $\mathcal{H}_{\rm eff}$ involves a transformation from quantum spins to bosonic variables. The most suitable spin-boson transformation are the *Villain transformation* [17] in the strongly easy-plane case and the *Holstein-Primakoff* (HP) in the almost isotropic case ($\lambda \to 1$).

Eventually, the PQSCHA recipe gives the following effective Hamiltonian for the XXZ model [12,14,15]:

$$\mathcal{H}_{\rm eff} = -\frac{J\widetilde{S}^2}{2} j_{\rm eff} \sum_{i,d} \left(s_i^x s_{i+d}^x + s_i^y s_{i+d}^y + \lambda_{\rm eff} s_i^z s_{i+d}^z \right) + + NJ\widetilde{S}^2 G(t) \ . \quad (3)$$

As in Eq. (2), $\{s_i\}$ are classical normalised spin variables, and the spin length is determined unambigously by the theory to be $\widetilde{S} = S + \frac{1}{2}$. Within the PQSCHA [11] the contribution of pure-quantum fluctuations, which are treated at the self-consistent harmonic level, are embodied in the dimensionless interaction parameters $j_{\rm eff}$ and $\lambda_{\rm eff}$, while $G(t)$ is an additive renormalization that does not enter the calculation of operator averages. $j_{\rm eff}$ and $\lambda_{\rm eff}$ may be written [12,14,15] in terms of suitable renormalisation parameters, representing the pure-quantum part of the square fluctuations of the in-plane and out-of-plane spin components. The renormalization of the exchange-energy by the factor $j_{\rm eff} < 1$, and the weakening of the easy-plane anisotropy ($|\lambda_{\rm eff}| \geq |\lambda|$), are thus the result of the cooperative effect of in-plane and out-of-plane pure-quantum fluctuations. For $t \to \infty$ or $S \to \infty$, $j_{\rm eff} \to 1$ and $|\lambda_{\rm eff}| \to |\lambda|$) and the classical limit is recovered.

Using the PQSCHA formalism [11] 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

$$\langle \cdots \rangle_{\rm eff} = \mathcal{Z}^{-1} \left(\prod_i \int ds_i \right) (\cdots) \, e^{-\beta \mathcal{H}_{\rm eff}} \ .$$

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 [11,18].

For a 2-d spin system the classical-like averages $\langle \cdots \rangle_{\rm eff}$ can be obtained only numerically. At variance with previous work, where only the problem of the renormalization of the BKT transition temperature was addressed, for a given value of λ it is not possible to rely on a simple temperature rescaling of the results obtained for the classical system. Indeed, when we are interested to the complete thermodynamic behaviour of the quantum system, due to the temperature dependence of the renormalised anisotropy parameter $\lambda_{\rm eff}$, new simulation runs are needed for any value of temperature, anisotropy and spin. Monte Carlo simulations of the classical system described by the effective hamiltonian (3) were done in the whole relevant temperature range for $\lambda = 0, 0.5, 0.7, 0.9$ and $S = 1/2, 1, 3/2, 5/2$, and quantum internal energy, magnetic susceptibility and spin-spin correlation function were obtained by means of the proper PQSCHA expressions.

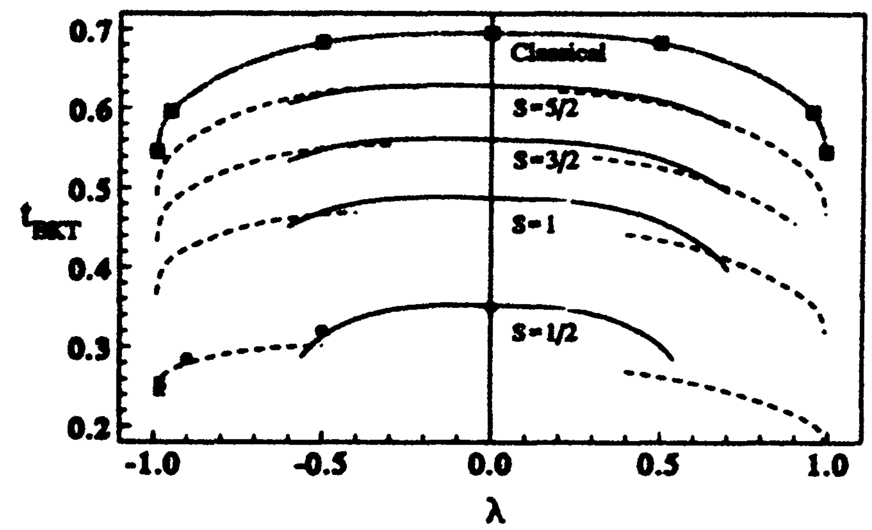

FIG. 1. Predicted transition temperature $T_{\rm BKT}/J\widetilde{S}^2$ of the quantum XXZ antiferro- ($\lambda < 0$) and ferromagnetic ($\lambda > 0$) model. The curves refer to increasing values of the spin going upwards; the symbols are the results of classical (squares) [5] and quantum (circles) [19–22] Monte Carlo simulations. Full line: Villain transformation; dashed line: Holstein-Primakoff; dot-dashed line: interpolated classical results.

Fig. 1 shows the BKT transition temperature of the quantum XXZ model as a function of λ and S, both for FM ($\lambda > 0$) and AFM ($\lambda < 0$) coupling, obtained by the simple scaling procedure described in Refs. [12,14]. The data for small values of $|\lambda|$ are those given by the effective hamiltonian constructed by using the Villain transformation; however, as observed previously, the latter become improper when the system looses its strongly easy-plane character. For almost isotropic system the HP transformation imposes itself as a better choice and it has been employed to construct the branches of the curves near $|\lambda| = 1$. In such a way we are able to cover the whole range of λ, getting estimates of the critical temperature in very good agreement with the available data of quantum Monte Carlo simulations for any value of λ even in the extreme quantum case of $S = 1/2$.

The magnetic specific heat has been obtained by numerical derivation of the internal energy for different values of the spin, from the classical model ($S = \infty$) up to spin $S = \frac{1}{2}$. In Fig. 2 the specific heat for $\lambda = 0$ is reported. Save the obvious effect that the specific heat in the quantum case approaches 0 as $t \to 0$, we see that the qualitative behaviour does not change as the system becomes more and more quantum, but the position of the maximum follows the decrease of $t_{\rm BKT}$, remaining about 10% higher. The agreement with quantum Monte Carlo data [19], available only for $S = 1/2$, should still be considered satisfactory, as the high values of the renormalization paramaters for such strongly quantum system puts it at the boundary of the range of applicability of the effective Hamiltonian method.

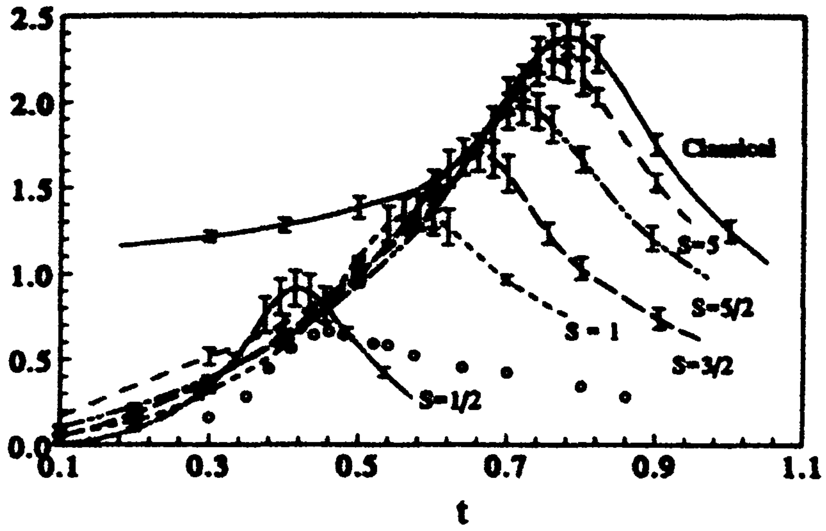

FIG. 2. Specific heat of the XX0 model. Dot-dashed line: $S = 1/2$; short-dashed line: $S = 1$; long-dashed line: $S = 3/2$; dot-dot-dashed line: $S = 5/2$; dashed line: $S = 5$; full-line: $S = \infty$ (classical); circles: $S = 1/2$ data from quantum Monte Carlo simulation [19].

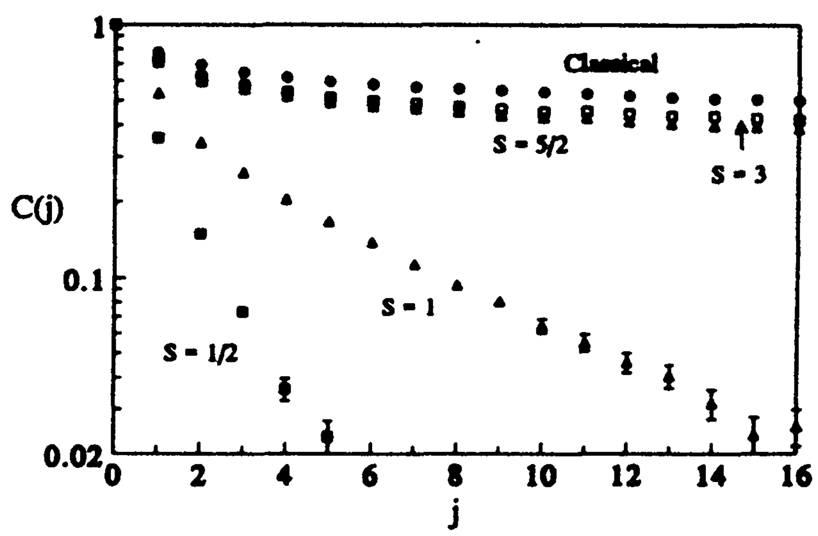

FIG. 3. In-plane normalized spin-spin correlation function $C(j)$ of the quantum XXZ antiferromagnetic model for $\lambda = 0.5$ at $t = 0.6$. Filled squares: $S = 1/2$; open triangles: $S = 1$; filled triangles: $S = 5/2$; open squares: $S = 3$; filled circles: $S = \infty$ (classical).

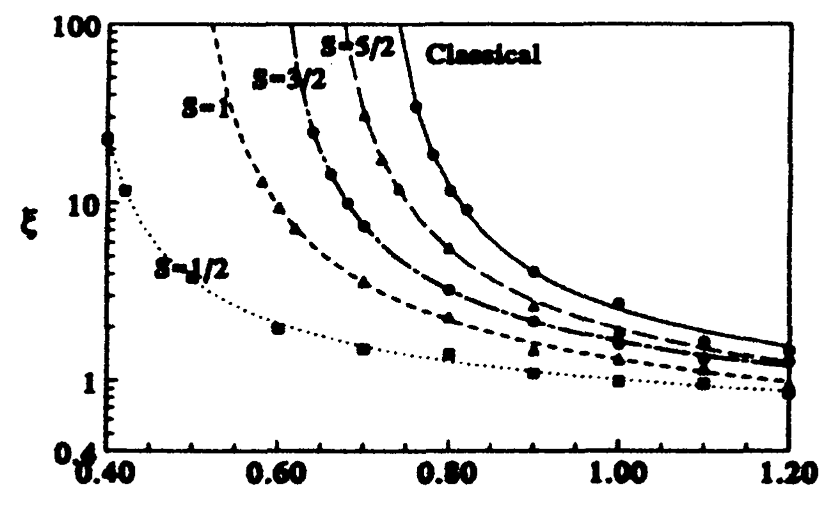

FIG. 4. Spin-fluctuations correlation length ξ of the quantum XXZ antiferromagnetic model for $\lambda = 0.5$ as a function of temperature. Filled squares: $S = 1/2$; open triangles: $S = 1$; open circles: $S = 3/2$; filled triangles: $S = 5/2$; filled circles: $S = \infty$ (classical).

In Fig. 3 the in-plane spin-spin correlation function $C(j)$ of the quantum 2-d antiferromagnet for $\lambda = 0.5$ and different values of the spin, are reported as a function of the spin separation j at a fixed temperature $t = 0.6$. From Fig. 1 follows that such temperature should be above $t_{\rm BKT}$ for $S > 3/2$, and this is confirmed by the behaviour of the correlation function: indeed, the log-linear plot clearly shows as $C(j)$ decays as a power law for $S = 5/2$ and higher, and exponentially for $S = 1$ and $S = 1/2$, i.e. for low spin the quantum fluctuations are strong enough to drive the system in the completely disordered region.

The correlation length ξ of spin fluctuations is another relevant quantity to investigate the BKT transition: in Fig. 4 we report ξ as a function of temperature again for the XXZ antiferromagnet and $\lambda = 0.5$. It is apparent that the quantum fluctuations destroy the correlations, as ξ at a given temperature decreases with S. At the same time, however, the divergence of ξ as $t \to t_{\rm BKT}$ is still well described by the BKT law $\xi \propto e^{b_\xi (t-t_{\rm BKT})^{-1/2}}$, and the best fits of the data appearing in Fig.4 give estimates of the transition temperature in agreement with those given in Fig. 1.

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