INTRINSIC AND FIELD-INDUCED XY-LIKE BEHAVIOUR IN TWO-DIMENSIONAL QUANTUM ANTIFERROMAGNETS*

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I study the thermodynamic properties of $S = 1/2$ two-dimensional quantum antiferromagnets with easy-plane anisotropy, both in the case of intrinsic anisotropy (XXZ model in zero field) and in the case of field-induced anisotropy (Heisenberg antiferromagnet in a uniform magnetic field), making use of the continuous-time Quantum Monte Carlo method. For the model with intrinsic anisotropy I single out the characteristic features of the Heisenberg-to-XY crossover anticipating the Berezhinskii–Kosterlitz–Thouless (BKT) transition. Then I show how these features are reproduced in the case of a field-induced anisotropy and BKT transition. Implications for the experimental realization and detection of a disordered two-dimensional XY-like phase in real antiferromagnets are discussed.

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The Berezhinskii–Kosterlitz–Thouless (BKT) critical behaviour has been observed in many two-dimensional physical systems, such as superfluid or superconducting films [1] and Josephson junction arrays [2]. In the context of magnetism, where the BKT theory was originally formulated as referred to the classical $2d$-XY model, such a behaviour is expected in layered magnets in which the isotropic Heisenberg spin–spin coupling is perturbed by an easy-plane anisotropy [3]. Nevertheless in most layered compounds whose spin–spin interaction is known to have an easy plane, the entity of the anisotropy is very small, representing a perturbation of order $10^{-2} \div 10^{-4}$ with respect to the dominant isotropic coupling, and therefore a test of the Kosterlitz–Thouless predictions seems to be hardly feasible. Moreover, the existence

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of a residual inter-layer coupling, driving the system towards $3d$ long-range order, masks the purely $2d$ transition. Therefore a more realistic point in light of experiments would be to detect clear signatures of the anisotropy away from the transition, marking the onset of an XY-like behaviour.

The purposes of this work are two-fold. First of all I show that even a tiny easy-plane anisotropy (as small as 10^{-3}), comparable to those experimentally observed in real compounds, is able to lead to clear deviations from the isotropic Heisenberg behaviour in a $S = 1/2$ $2d$ quantum antiferromagnet (AFM), for what concerns the thermodynamic behaviour of out-of-the-easy-plane susceptibilities. Then I illustrate how the application of a uniform magnetic field to an isotropic two-dimensional quantum antiferromagnet, inducing an easy-plane anisotropy and a BKT transition, leads to analogous signatures; this shows that a field-induced XY-like behaviour can be realized and detected in real AFMs.

I consider the $S = 1/2$ two-dimensional XXZ quantum antiferromagnet on the square lattice in a uniform magnetic field, whose Hamiltonian reads:

$$\hat{\mathcal{H}} = J \sum_{\boldsymbol{i},\boldsymbol{d}} \left(\hat{S}^x_{\boldsymbol{i}} \hat{S}^x_{\boldsymbol{i}+\boldsymbol{d}} + \hat{S}^y_{\boldsymbol{i}} \hat{S}^y_{\boldsymbol{i}+\boldsymbol{d}} + \lambda \hat{S}^z_{\boldsymbol{i}} \hat{S}^z_{\boldsymbol{i}+\boldsymbol{d}} \right) - h \sum_{\boldsymbol{i}} \hat{S}^z_{\boldsymbol{i}} \,, \tag{1}$$

where $\boldsymbol{i} = (i_1, i_2)$ runs over the sites of a square lattice, $\boldsymbol{d}$ connects each site to its four nearest neighbours, $J > 0$ is the antiferromagnetic exchange integrals and $\lambda < 1$ represents the easy-plane anisotropy parameter. The spin operators $\hat{S}^\alpha_{\boldsymbol{i}}$ $(\alpha = x, y, z)$ are such that $|\hat{\boldsymbol{S}}|^2 = S(S+1)$ with $S = 1/2$ and obey $[\hat{S}^\alpha_{\boldsymbol{i}}, \hat{S}^\beta_{\boldsymbol{j}}] = i\varepsilon_{\alpha\beta\gamma}\delta_{\boldsymbol{ij}}\hat{S}^\gamma_{\boldsymbol{i}}$.

I first consider the anisotropic model in zero field. Previous Quantum Monte Carlo (QMC) simulations [4] have shown evidence for a BKT critical behaviour in this model, suggesting the existence of a finite-temperature transition, for anisotropies as small as $\lambda = 0.98$. Making use of the QMC method based on the loop algorithm in continuous imaginary time [5], I am able to enforce this evidence by considering non-diverging quantities whose thermodynamic behaviour has not been discussed by Ref. [4].

Relevant non-critical signatures of the anisotropy are in fact found in the uniform susceptibility perpendicular to the easy-plane, χ_0^{zz}. In Fig. 1(a) the uniform susceptibility is presented for the case $\lambda = 0.999$; as we see, it shows a remarkable deviation from the isotropic behaviour, exhibiting a minimum at a temperature T^* well above the estimated BKT critical temperature. The mechanism leading to the appearance of the minimum becomes clear when considering what happens to, *e.g.*, the staggered susceptibility χ_s^{zz} (Fig. 1(b)) and correlation length measured along the same direction; both quantities exhibit a maximum at roughly the same temperature T^*, which manifests suppression of antiferromagnetic fluctuations and correlations along the hard-axis z at and below T^*; at the same time it becomes easier to magnetise the system by applying a uniform field along z, and therefore the uniform susceptibility begins to increase. The temperature T^* is then seen as the upper bound of a temperature region where the spin fluctuations lose the full rotational symmetry of the Heisenberg model and tend to be confined to the easy-plane, thus marking a Heisenberg-to-XY crossover. Remarkably, we are still far from criticality, so that this behaviour can be unambiguously observed in real layered magnets, as indeed happens in the weakly easy-plane anisotropic layered antiferromagnet $Sr_2CuO_2Cl_2$ [7], which shows a minimum in the uniform susceptibility at $T^* \approx 330$ K, well above the transition temperature $T_N = 256$ K.

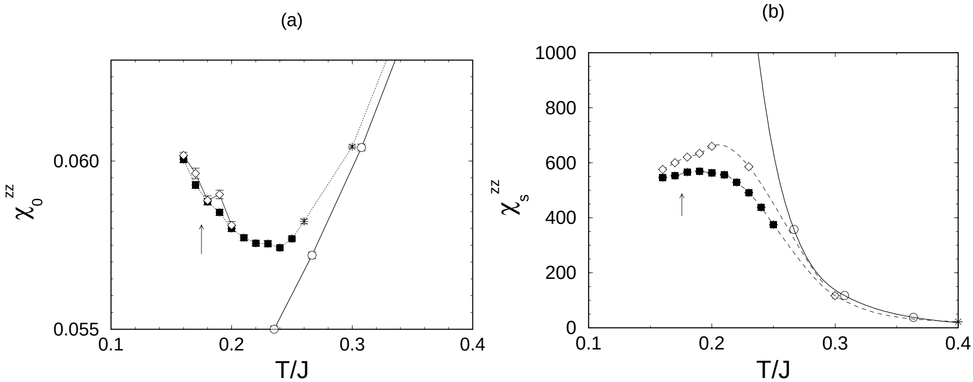

Fig. 1. Uniform (a) and staggered (b) susceptibility along the hard axis (z) in the two-dimensional easy-plane $S = 1/2$ quantum antiferromagnet ($\lambda = 0.999$), for different lattice sizes: $L = 64$ (stars), 128 (squares), 200 (open diamonds); the arrows indicate the BKT critical temperature. Open circles are QMC data for the isotropic model (from Ref. [6]).

Further quantum simulations have been performed for the model described by the Hamiltonian (1) with $\lambda = 1$ and in a field. My simulations are based on the worm algorithm, originally exposed in Ref. [8], but reformulated as a generalisation of the loop algorithm. At variance with the loop algorithm, the worm algorithm allows to include a magnetic field of arbitrary intensity without any loss of efficiency.

In the realistic case of low fields $h = 0.05$, 0.1 and 0.2, I observe analogous signatures of the field-induced anisotropy in the thermodynamic behaviour of the uniform and staggered susceptibility along the z axis (Fig. 2) as in the case of the intrinsic anisotropy: again the transition is anticipated by the suppression of out-of-plane antiferromagnetic fluctuations and correlations. This latter effect is well separated from the onset of the critical regime: this means that, applying an intense uniform field to a real layered AFM, the field-induced XY-like behaviour can be indeed observed in a temperature region where the inter-layer coupling does not play any role, *i.e.* where the system really behaves as a two-dimensional magnet. Uniform susceptibility, which is a conventional observable for magnetic systems, allows to clearly detect the temperature range over which the XY-like phase extends. Further measurements in this regime, *e.g.* focused on spin dynamics, come to be very appealing.

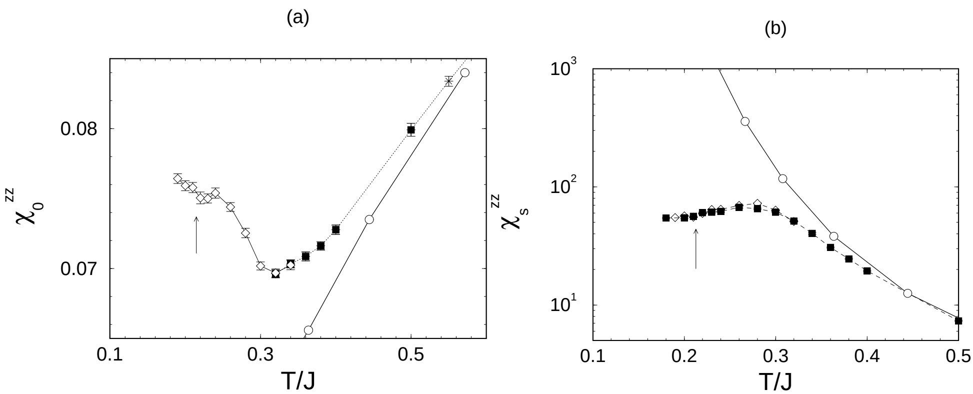

Fig. 2. Uniform (a) and staggered (b) susceptibility along the z axis in the two-dimensional $S = 1/2$ Heisenberg antiferromagnet in a uniform field $h = 0.2$, for different lattice sizes: $L = 32$ (stars), 64 (squares), 96 (open diamonds); the arrows indicate the BKT critical temperature. Open circles are QMC data for the isotropic model [6].

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