Vortex contribution to the defect-induced alternating magnetization in 2D antiferromagnets

Alessandro Cuccoli
Dipartimento di Fisica, Università di Firenze e Unità CNISM, via G. Sansone 1, I-50019 Sesto Fiorentino (FI), Italy

Ruggero Vaia
Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, via Madonna del Piano 10, I-50019 Sesto Fiorentino (FI), Italy

E-mail: cuccoli@fi.infn.it

Abstract. Quantum Monte Carlo (MC) simulations of the 2D S=1/2 Heisenberg antiferromagnet (AFM) with a vacancy and an applied magnetic field [1] showed that the characteristic decay length of the alternating magnetization around the defect displays an unexpected maximum in the neighborhood of the Berezinskii-Kosterlitz-Thouless (BKT) transition temperature. Given the role played in the BKT transition by vortex excitations, we investigated their contribution to the alternating-order behaviour, showing that isolated vortices modulate the parameters entering the effective model introduced in [1]: the temperature dependence of the vortex population allows us to explain the observed behaviour of the alternating-order decay length. We support such conclusions with MC simulations of the classical AFM, which also reveal some differences between the quantum and the classical model.

Magnetic properties of antiferromagnetic systems are well known[2, 3] to be strongly affected by the possible insertion of non-magnetic impurities in the lattice, and this is especially true when the low dimensionality of the system forbids the onset of ordering in the perfectly translation-invariant model at any finite temperature. Among the most intriguing phenomena pertaining to such systems there is the appearance of a finite staggered magnetization, localized around the defect, in response to the application of an external uniform field[3, 4]. If the starting reference model is the isotropic Heisenberg antiferromagnet, the applied field, in addition of inducing the staggered magnetization, makes the system behave as an effective easy-plane magnet: the choice of a two-dimensional lattice thus makes things even more interesting, as a Berezinskii-Kosterlitz-Thouless (BKT) behaviour sets in, with its low-temperature quasi-long-range ordered phase, where power-law decaying correlations suggest for a possible strong response of the system to external perturbations. Such a model was recently considered in Ref. [1], where an approximate energy functional was derived to describe the low-temperature behaviour of the alternating magnetization; in the same paper an explicit solution for the induced alternating order was eventually given, showing its almost exponential decay as a function of the distance from the defect, with a characteristic decay length \( \lambda \) independent of temperature and of the microscopic details of the model. Such conclusions were substantially confirmed in the same paper by Quantum Monte Carlo simulations of the two-dimensional \( S = 1/2 \) antiferromagnet with a
vacancy, but for an unexpected feature: after staying constant in a wide range of temperature, \( \lambda \) begins to grow when the BKT transition temperature is approached, and only when temperature is further raised well above \( T_{\text{BKT}} \) it decreases, as expected, toward zero, as a consequence of increasing thermal fluctuations. The proximity of the observed counterintuitive behaviour of \( \lambda \) to \( T_{\text{BKT}} \) led us [5] to identify vortices (V) and antivortices (AV), i.e., the non-linear excitations contributing to the BKT transition, as a possible origin of the increase of \( \lambda \) around \( T_{\text{BKT}} \). Here we discuss how they may affect the decay of the induced magnetization; our conclusions are supported by Monte Carlo simulations of the two-dimensional classical AFM with a vacancy, which also show some significant differences from the behaviour of the quantum model.

We consider a classical Heisenberg antiferromagnet with spins of length \( |S_i| = S \) lying on a bipartite lattice with \( N \) sites and subjected to a magnetic field:

\[
\mathcal{H} = \frac{J}{2} \sum_{\langle ij \rangle} (S_i \cdot S_j)^2 - H \sum_i S_i^z .
\] (1)

The quantity \( JS^2 \) is the natural energy unit of the system, so that in what follows we will employ the dimensionless temperature \( t \equiv T/JS^2 \) and field \( h \equiv H/JS \); moreover, all lengths will be measured in units of the lattice spacing. Given such definitions, we can safely rewrite the dimensionless version of Eq. (1) in terms of unit spins \( |s_i| = 1 \) and split it in a ‘perpendicular’ and a ‘parallel’ part, \( \mathcal{H} = \mathcal{H}^\perp + \mathcal{H}^\parallel \), with

\[
\mathcal{H}^\perp = \frac{1}{2} \sum_{\langle ij \rangle} (s_i^x + s_j^x)^2 ,
\] (2)

\[
\mathcal{H}^\parallel = \frac{1}{2} \sum_{\langle ij \rangle} (s_i^x + s_j^x)^2 - h \sum_i s_i^z ,
\] (3)

being \( s_i^\perp = (s_i^x, s_i^y) \).

Below the saturation field \( h_s = 2z \) (\( z \) is the lattice coordination number, i.e., \( z = 4 \) in our model), the classical minimum-energy configuration is the canted one,

\[
s_i^z = \sin \delta_0 \equiv \frac{h}{h_s} , \quad s_i^\perp = \pm \cos \delta_0 \left( \cos \varphi_0, \sin \varphi_0 \right) ,
\] (4)

where the sign \( \pm \) refers to the two different sublattices, and the arbitrarily chosen azimuthal angle \( \varphi_0 \) selects one of the infinite degenerate minima connected to each other by a uniform rotation around the \( z \) axis. For small field, configurations where the spins lie on the \( xy \) plane are clearly favoured, i.e., the field acts as an effective easy-plane anisotropy, as can be seen by rewriting the spin components after explicitly allowing for a canting angle \( \delta \), minimizing with respect to it, and neglecting afterwards any residual dependence on \( \delta \propto (h/h_s) \) (see Refs. [1, 5] for details). Indeed, by the outlined procedure, the low-field effective description of the system can be summarized by

\[
\mathcal{H}^\parallel = \frac{1}{2} \sum_{\langle ij \rangle} (s_i^x + s_j^x)^2 + \frac{A_u}{2} \sum_i (s_i^z)^2 ,
\] (5)

where the effective anisotropy parameter

\[
A_u = \frac{h^2}{2z}
\] (6)

has been defined; substituting the spin components \( s_i^z \) with the alternating magnetization variables \( \sigma_i = \pm s_i^z \) the continuum approximation can be easily devised, finally getting the
energy functional [1]

$$H^\parallel = \frac{1}{2} \int d^D r [\rho_s (\nabla \sigma_r)^2 + A_u \sigma_r^2] . \tag{7}$$

The dimensionless spin stiffness $\rho_s$ represents for the quantum model a phenomenological parameter embodying most of the renormalizations due to zero-point quantum fluctuations, while $\rho_s = 1$ for the classical model at the same level of approximation, i.e., neglecting thermal renormalization. When a vacancy is introduced in the lattice, from the effective energy functional (7) it follows [1] that the induced local alternating magnetization behaves as:

$$\langle \sigma_r \rangle = \frac{h}{2\pi \rho_s} K_0 \left( \frac{r}{\lambda} \right) , \quad \lambda = \sqrt{\frac{\rho_s}{A_u}} , \tag{8}$$

$r$ being the vector joining the defect to the lattice site, and $K_0(x)$ the modified Bessel function; $K_0(x) \sim x^{-1/2} e^{-x}$ for large $x$.

When we allow for vortex excitations, Eqs. (5) and (7) can still be retained as effective Hamiltonians, but the anisotropy constant $A_u = \frac{h^2}{2z}$ must be replaced by [5]

$$A = \frac{h^2}{2z(1 - \mathcal{L})} - 2z \mathcal{L} , \quad \mathcal{L}(t) \simeq \frac{2\pi}{z} \frac{\ln r_v(t)}{R_v^2(t)} , \tag{9}$$

where $R_v(t)$ is the average distance between V-AV pairs, while $r_v(t)$ is the typical size of a pair; $r_v(t) \simeq 1$ up to $t_{BKT}$, where pairs begin to decouple, and $\to 1$ at very high temperature, where V-AV excitations fill the whole lattice: as a consequence $A$ and, by Eq. (8), the decay length $\lambda$, are thus expected to be significantly modified by the presence of vortices only around the BKT transition; when only uniform configurations (i.e. no V-AV excitations) are considered we obviously have $\mathcal{L} = 0$ and Eq. (6) is recovered.

With the proviso given above about the choice of the effective parameters, the approximation scheme just outlined applies equally to classical and quantum models. Therefore, in order to

Figure 1. Induced staggered magnetization as a function of the distance $r$ from the defect for $h=0.4$ and different temperatures: $t=0.2$ (red square), $t=0.4$ (blue up triangle), $t=0.5$ (purple diamond), $t=0.6$ (green left triangles), $t=0.7$ (black circle); the last temperature is well above $t_{BKT} \simeq 0.55$ [6].
test our predictions about the role played by vortex-like non-linear excitations, and gain a better quantitative understanding of the phenomenon, we resorted to Monte Carlo simulations of the classical isotropic Heisenberg antiferromagnet with a vacancy and a small applied uniform magnetic field; periodic boundary conditions were applied and lattice sizes up to 128x128 were considered; a mix of Metropolis and conical over-relaxed moves (i.e. microcanonical moves where each spin is rotated maintaining constant the angle it forms with the local effective field) was employed[7].

Typical data about the average alternating magnetization as a function of the distance from the defect are given in Fig. 1 for \( h = 0.4 \) and different temperatures below and above \( t_{BKT}(h = 0.4) \simeq 0.55 \)[6]; at all temperatures simulation data can well be fitted (continuous lines in the figure) by Eq. (8), which is thus confirmed to give a really good quantitative description also for the classical model. A more refined scan in temperature was done around \( t_{BKT} \): the fitted values of \( \lambda \) are reported in Fig. 2 as a function of temperature for two different values of the applied field. The expected “bump” around the critical temperature is clearly observed, in agreement with our V-AV hypothesis; at variance with the quantum model, also a linear increase of \( \lambda \) at very low temperature is observed, which we interpret as due to thermal renormalization of the spin stiffness and effective anisotropy, an effect probably negligible in the quantum \( S = 1/2 \) model, where thermal fluctuations at low temperatures only represent a small correction to the strong renormalization due to zero-point quantum fluctuations already embodied in the definition of the effective spin-stiffness and perpendicular susceptibility at \( t = 0 \).

References