Out-of-plane magnetic vortices and central peaks: A Comment

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Costa and Costa [Phys. Rev B **54**, 994 (1996)] studied vortices in a two-dimensional easy-plane anisotropic ferromagnetic model. They found different vortex behaviors depending on whether the anisotropy parameter λ is less than or greater than a critical value λ_c, reproducing well-known results [Phys.Rev.B **39** 11840 (1989)]. They claim that the out-of-plane dynamic correlation function $S^{zz}(\mathbf{q},\omega)$ exhibits a central peak only for $\lambda > \lambda_c$, where the static vortices are of the out-of-plane form, but not for $\lambda < \lambda_c$, where the static vortices are planar. However, their data are physically inaccurate for such a conclusion.

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Recently Costa and Costa (CC) [1] simulated the two-dimensional anisotropic Heisenberg model, with classical nearest neighbor spin Hamiltonian on a square lattice, $H = -J\sum_{(i,j)}(S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z)$. Static vortex structures were found by a relaxation procedure, and dynamic correlations were calculated by Monte Carlo–spin dynamics simulation. We point out that the results of the static calculations are well-known, and second, that the dynamic correlation functions presented there appear to be physically unreliable for their conclusions.

Using simulated annealing, CC found that the minimum energy vortex structure remains planar for $\lambda < \lambda_c$, where $\lambda_c \approx 0.709$, whereas, for $\lambda > \lambda_c$, the structure has a nonzero radially-dependent out-of-plane form, $S^z(r)$. The existence of this crossover at a critical anisotropy λ_c is a well-known result. To our knowledge, the possibility of two types of vortex solutions (in-plane and out-of-plane) was first pointed out by Takeno and Homma [2] and further analyzed by Hikami and Tsuneto [3]. The crossover from in-plane to out-of-plane vortices for $\lambda > \lambda_c$ was discussed by Wysin *et al.* [4] and by Gouvêa *et al.* [5], and different values of λ_c were found depending on the type of lattice ($\lambda_c \approx 0.72, 0.86, 0.62$ for square, honeycomb and triangular lattices, respectively). Wysin [6] made an analysis of the core region of a vortex on a discrete lattice and was able to make a more precise estimate of λ_c (≈ 0.7044 for square lattice) by analytical means. Zaspel *et al.* [7] used this method to show that λ_c increases in the presence of a magnetic vacancy. A particular normal mode of oscillation of the vortex, which softens at λ_c, is responsible for this vortex instability [6,8]. CC found λ_c slightly higher because of this lengthening of time scales near λ_c, where they did not wait long enough for equilibration, similar to the over-estimated values found earlier in Refs. [4,5].

For $T > T_{KT}$, the Berezinskii-Kosterlitz-Thouless vortex-unbinding temperature [9], the vortex ideal gas phenomenology of Mertens *et al.* [10] predicts central peaks (CP) in the dynamic correlation functions of in-plane and out-of-plane spin components [$S^{xx}(\mathbf{q},\omega)$ and $S^{zz}(\mathbf{q},\omega)$]. One Mertens *et al.* prediction is that the static out-of-plane vortex structure for $\lambda > \lambda_c$ as well as the dynamic vortex structure due to vortex motion for any $0 \le \lambda < 1$ is expected to contribute to a CP in S^{zz}. CC used a combination of cluster Monte Carlo (MC) [11] and spin dynamics, for a 64×64 system, averaging S^{xx} and S^{zz} over 200 MC initial conditions. The transition temperature for $\lambda = 0$ is known to be $T_{KT}/J \approx 0.70$ based on finite size scaling calculations [12], and decreases monotonically as λ approaches one. CC studied $\lambda = 0.5, 0.8$, at temperatures $T/J = 0.6, 0.8$. For both of these anisotropies, $0.6 < T_{KT}/J < 0.8$.

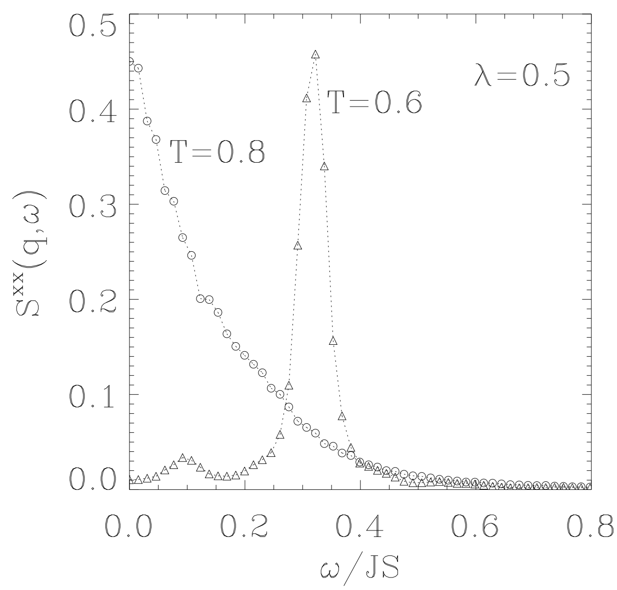

FIG. 1. Simulation of S^{xx} for $\lambda < \lambda_c$ at temperatures below and above T_{KT}, for wavevector ($3\pi/32$,0) on a 64x64 lattice. Results for $\lambda > \lambda_c$ are similar. Dotted lines are guides.

CC reported that a CP in $S^{zz}(\mathbf{q},\omega)$ appears only for $\lambda > \lambda_c$, where the static vortex structure is out-of-plane. However, the S^{xx} and S^{zz} data presented by CC appear to be inadequate to support any conclusion, for two reasons. First, the CC data for both S^{xx} and S^{zz} do not reproduce the sharp spinwave peaks expected for temperatures below T_{KT} [12]. In the low-T phase, spinwaves dominate and should have narrow linewidths $\Delta\omega_q$ with some weak dependence on λ, possibly decreasing with λ in step with the λ-dependent dispersion relation ω_q. Second, the CC data for S^{xx} do not show the drastic appearence of a CP that is expected when crossing T_{KT}. Any numerical simulation may be vulnerable to systematical or programming errors, whose ultimate source we cannot possibly determine here. In this case, however, one source of these problems could be the inadequately short time of integration used in the spin-dynamics simulation, as we describe below.

Lacking an exact theory for $\Delta\omega_q$, we can compare the CC results to those of Evertz and Landau (EL) [12], and to our own simulations. We repeated the MC-spin-dynamics simulation as described in Ref. [13], with the addition of the Wolff cluster algorithm [11] applied to the in-plane spin components, averaging S^{xx} and S^{zz} over 400 MC initial states. Each of the 400 initial states used were separated by 200 steps consisting of a Metropolis sweep followed by Wolff single-cluster move, all following 5000 equilibration steps (e.g, 85,000 total steps). We used a fourth order Runge Kutta scheme with step $dt = 0.04$ for the time integration out to $t_{max} = 410/JS$, in order to reach a frequency resolution down to $\delta\omega/JS = 2\pi JS/t_{max} = 0.015$. In Figs. 1 and 2 we show the raw data without the application of an unnecessary smoothing window [12].

For $L = 64$, $\lambda = 0$, $T/J = 0.6$, and wavevectors near $\mathbf{q}a = (3\pi/32, 0)$, the EL data and our own data for S^{zz} have spinwave half-widths $\Delta\omega_q/JS \approx 0.03$. The CC data for this same case, but with $\lambda = 0.5$, exhibit much broader spinwave peaks, with $\Delta\omega_q/JS \approx 0.2$. In the same case but for $\lambda = 0.8$, the half-width of the CC data has reduced slightly to about $\Delta\omega_q/JS \approx 0.15$, while our data exhibits $\Delta\omega_q/JS \approx 0.015$. Clearly, $t_{max} > 410/JS$ is necessary to resolve this peak.

For low-T S^{xx} data, we obtain, consistently with EL, a weak and oscillatory intensity *below* the spinwave frequency, and intensity rapidly aproaching zero *above* ω_q. It is impossible to tell if such a feature appears in the CC data. The low-T CC data, especially for S^{zz}, exhibit unphysical oscillations *above* ω_q and extremely long high-ω tails, rather than rapidly approaching zero. This spread out noise effectively reduces the sharpness of the KT transition and appearence of the CP in S^{xx} when crossing T_{KT}, compared to what we find (Fig. 1).

CC used 1200 time steps of size $0.025/JS$ to get a maximum time of only $t_{max} = 30/JS$, leading to a frequency resolution $\delta\omega/JS = 0.21$, which is much larger than the physical spinwave width at these low wavevectors. This is an inadequate resolution to study the low frequency form of the low-wavevector spinwaves or for studying the CP properties. CC applied a cutoff function to the data,

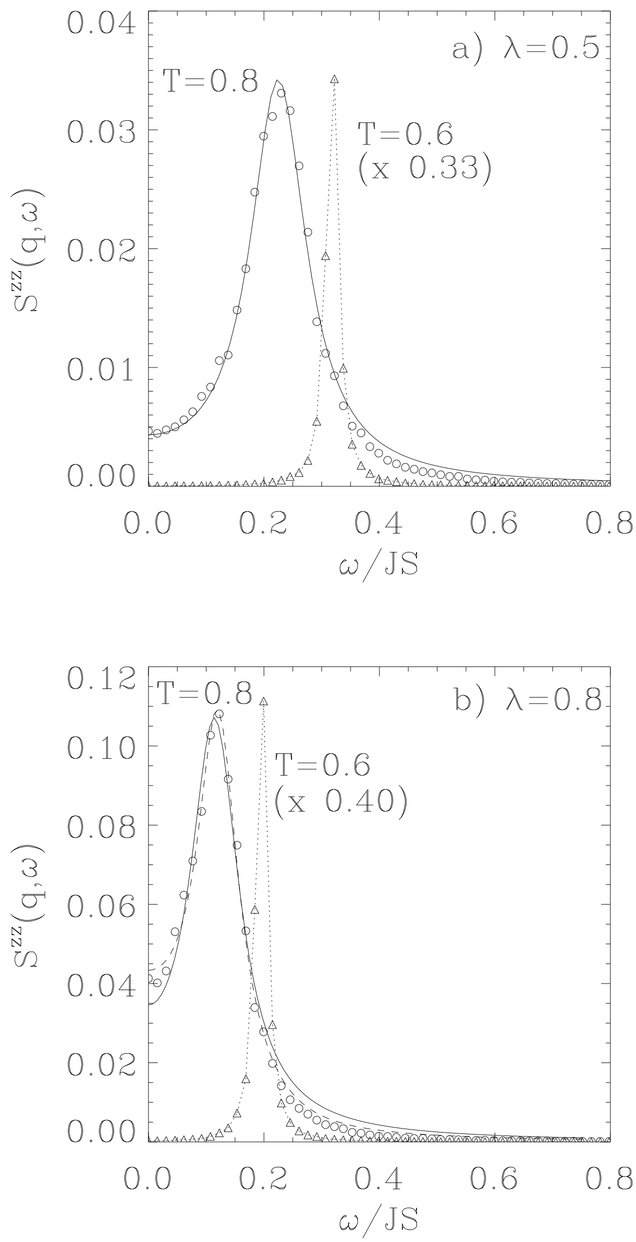

FIG. 2. Simulation of out-of-plane structure function for a) $\lambda < \lambda_c$ and b) $\lambda > \lambda_c$ at temperatures below and above T_{KT}, wavevector ($3\pi/32$,0) on a 64x64 lattice. Dotted lines are guides to the eye. Solid lines are fits to Lorentzian spinwaves, and the dashed line is a fit to Lorentzian spinwaves plus a Gaussian CP component. T=0.6 data has been scaled by the indicated factors.

but it is clear that this process cannot improve the frequency resolution. This limited resolution may also be responsible for the unphysical oscillations above the spinwave frequency.

There is no controversy that a CP emerges in S^{xx} above T_{KT}, although it is possible that sources other than vortices may be responsible. The more difficult question is whether a CP develops in S^{zz}, and if so, whether vortices are responsible. It is possible that heavily damped spinwaves with low ω_q and large $\Delta\omega_q$ can make S^{zz} appear to have a CP. Therefore we show fits of our S^{zz} data for $T > T_{KT}$ to the sum of symmetrically located Lorentzians (damped spin waves) at $\pm\omega_q$. This form fits well near ω_q, however, it has particular trouble in the high-ω tail of the spinwave peak, lying well above the data there. It suggests that at this high temperature, Lorentzian functions are not adequate to describe the spinwave lineshape, or additionally, a different spinwave component in combination with a CP component is needed. Other fits, including an additional Gaussian CP, produce some improvement near $\omega = 0$ for $\lambda > \lambda_c$, but still do not describe well the high-frequency tail. From our data it appears likely that there is indeed a CP in S^{zz} for $\lambda > \lambda_c$. For $\lambda < \lambda_c$, in the absence of knowing the precise CP and spinwave lineshapes, we cannot rule out a weak CP in S^{zz}. More precise data and more information about the shapes of the CP and spinwave contributions are needed in order to decide this question. For both $\lambda < \lambda_c$ and $\lambda > \lambda_c$, it is clear that the CC data are inadequate for this purpose.

The ideal gas theory is approximate: it assumes ballistic motion, it ignores vortex-vortex and vortex-spinwave interactions, and it assumes an infinite free-vortex lifetime, although there is evidence that typical vortex lifetimes are short [14], and that over this lifetime a typical vortex moves on the order of one lattice constant. Therefore it is good to consider alternative explanations even for the CP in S^{xx}. CC have suggested that creation-annihilation processes may contribute to CP intensity. But in the absence of a detailed creation-annihilation theory it is impossible to account for the relative contributions to S^{xx} and S^{zz} due to vortex motions compared to those due to local vortex number fluctuations.

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