Dynamic behavior of vortices in the classical two-dimensional anisotropic Heisenberg model

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We use Monte Carlo and spin-dynamics simulation to study the vortex dynamics in the two-dimensional anisotropic Heisenberg model. We calculated the lifetime of vortex-antivortex pairs, the time needed for a vortex to make a jump for one lattice spacing, the vortex density, the distance between pairs as a function of temperature, and the energy of the vortex core. Our results support the idea that a vortex does not move through the lattice for long distances and a creation-annihilation process is a more adequate picture to describe its ''dynamics.'' [S0163-1829(98)01514-8]

I. INTRODUCTION

The two-dimensional easy-plane anisotropic Heisenberg model (2D-XY model) provides a prototype for systems which exhibit topological excitations, such as superfluids films, Josephson-junction arrays, lipid layers, and others.[1–9] This model should not be confused with the plane rotator: Although they are in the same universality class, the spins in the plane rotator model have only two components. The plane rotator model does not exhibit any true long-range order. This lack of long-range order follows from the Mermin-Wagner theorem,[10,11] which asserts that a broken continuous symmetry prevents long-range order for continuous spin models in two dimensions. The plane rotator model however, does undergo a phase transition at a finite temperature T_{KT} from a high-temperature phase where the correlation function exhibits an exponential decay to a low-temperature phase with quasi-long-range order where the correlation function has a power-law decay.[12–14] This phase transition is believed to be driven by a vortex-antivortex unbinding mechanism. A vortex (antivortex) is a topological excitation in which spins on a closed path around the excitation core precess by 2π (-2π) in the same direction. Examples of unbound vortices and antivortices are shown in Figs. 1(a) and 1(b), respectively, for the plane rotator. An unbound vortex is a global excitation, while vortex-antivortex pairs are local (see Fig. 2). For the XY model the situation should be a bit more complicated due to the extra degree of freedom introduced by the S^z component. Some recent works[15–17] suggest that the XY model has a phase transition of the Kosterlitz-Thouless type just like the plane rotator model. We can expect the development of an out-of-plane structure as the temperature increases. In Fig. 3 we show two possible vortex spin configurations at a low but finite temperature. Figure 3(a) shows a coherent (ferromagnetic) arrangement, while Fig. 3(b) shows a random one. Below T_{KT} vortices and antivortices form a condensate of pairs superimposed on a background of spin-wave excitations. At T_{KT} pairs shielded by the background start to unbind. The Kosterlitz-Thouless temperature was independently calculated by Cuccoli *et al.*[15] and Evertz and Landau[16] to be $T_{\mathrm{KT}} \approx 0.700$ for the XY model on a square lattice. Although the static critical properties of the 2D-XY model are well understood (via plane rotator) the same is not true about its dynamical behavior. The dynamical structure factor $S(q,\omega)$ is of fundamental importance in the understanding of the spin dynamics. Some early theoretical works[18–20] studied the 2D-XY model at the region of low temperature ($T < T_{\mathrm{KT}}$) finding only spin-wave peaks in the

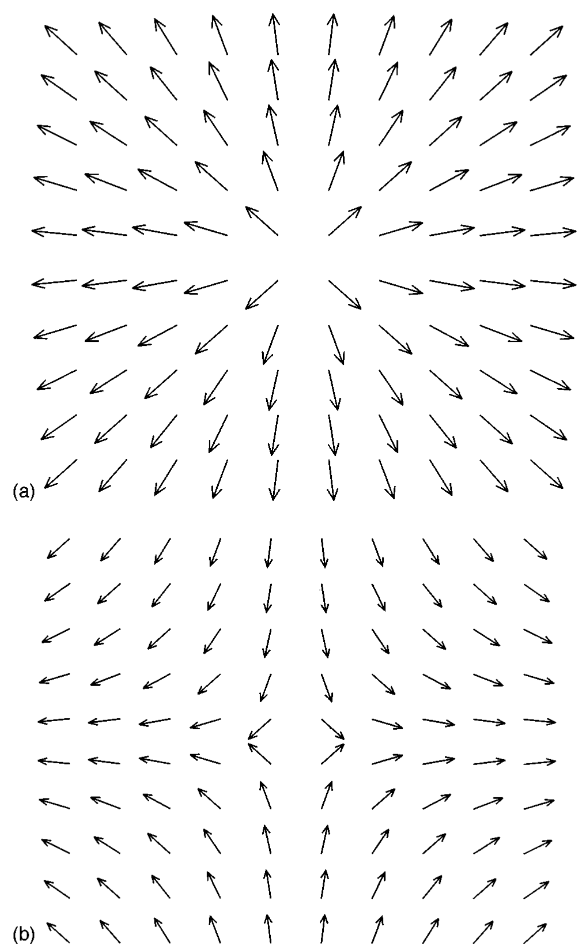

FIG. 1. Schematic view of a vortex (a) and antivortex (b) for spins of equal length.

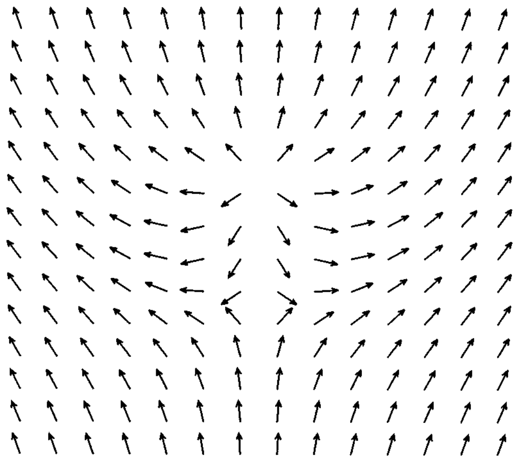

FIG. 2. Schematic view of a vortex-antivortex pair for spins of equal length.

in-plane correlation function $[S^{xx}(q,\omega)]$. More recently Menezes *et al.*,[21] using a harmonic approximation, reported a logarithmic central peak. Pereira and Costa,[22] using a vortex pair gas approach, found a Lorentzian central peak. In the high-temperature region $(T>T_{\mathrm{KT}})$, Huber[23] discussed how a vortex gas approximation could contribute to a central peak in the Fourier transform of the spin-correlation functions in the hydrodynamic regime. Mertens *et al.*[24] calculated the dynamical correlation functions above T_{KT} using a diluted ideal gas approach which was successful in treating one-dimensional soliton dynamics in magnetic spin chains.[25] The main ingredient in such an approach is the assumption that a vortex can wander through the lattice obeying a Maxwellian velocity distribution. A vortex passing between the positions $r=0$ and $r=r_0$ flips the spins within that interval, diminishing the correlations. They found a Lorentzian central peak for the in-plane dynamical structure factor $[S^{xx}(q,\omega)]$ and a Gaussian peak for the out-of-plane $[S^{zz}(q,\omega)]$ one which should be present for all values of the anisotropy λ. They also performed some spin-dynamics calculations. However, the statistics were not sufficient to give any quantitative result. Costa *et al.*,[26] in an exploratory work, discussed the

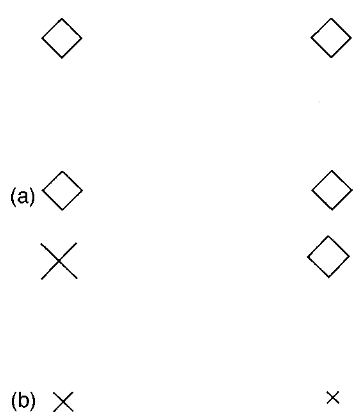

FIG. 3. Schematic view of vortices showing possible configurations for the out-of-plane spin component around a plaquette in the XY model. (a) Ordered and (b) random arrangement. The symbol size is proportional to the modulus of the S^z component. Diamonds $(\times)$ are for S^z positive (negative).

origin of the central peak in the 2D-XY model using Monte Carlo and spin dynamics. In their work they calculated the vortex density-density correlation function

$$C(R,t)\equiv\frac{\langle\Delta\rho(0,0)\Delta\rho(R,t)\rangle}{\langle[\Delta\rho(0,0)]^2\rangle}, \tag{1}$$

where $\Delta\rho(R,t)=\langle\rho(R,t)\rangle-\rho(R,t)$ and $\rho(R,t)$ is the vortex density at position R at time t. They found that $C(R,t)$ is nonzero only for $R=0$ and $C(0,t)$ has an exponential behavior

$$C(0,t)\sim\exp\left(-\frac{t^{\theta}}{\tau}\right), \tag{2}$$

with $\theta=0.4$ and $\tau\sim\exp(-\alpha\overline{T})$, where $\overline{T}$ is defined by $\overline{T}=T_{\mathrm{KT}}/(T-T_{\mathrm{KT}})$. Those results suggest that vortices cannot move through the lattice for more than a few lattice spacings. What they observed is that motion in general is followed by a creation-annihilation process. The behavior of the vortex creation-annihilation rate τ suggests that below T_{KT} vortices and antivortices become a static condensate of pairs. In an independent work, Dimitrov and Wysin[27] using an approach similar to that of Costa *et al.*[26] confirmed the creation-annihilation picture.

More recently Evertz and Landau,[16] in a very extensive work, calculated the in-plane and out-of-plane correlation functions $S^{xx}(\vec{q},\omega)$ and $S^{zz}(\vec{q},\omega)$, respectively. For $T<T_{\mathrm{KT}}$ they observed spin-wave peaks in both in-plane and out-of-plane correlation functions. In addition they observed a central peak in the in-plane function even for temperatures well below T_{KT}. For $T>T_{\mathrm{KT}}$ they found a strong central peak in $S^{xx}(\vec{q},\omega)$ and only damped spin waves in $S^{zz}(\vec{q},\omega)$. This result is in clear disagreement with the vortex gas picture where a central peak should be observed in $S^{zz}(\vec{q},\omega)$ for any value of the anisotropy in the high-temperature phase. Costa and Costa[28] reported results of Monte Carlo and spin dynamics (MCSD) for the anisotropic Heisenberg model for several values of the anisotropy λ. They found that there is a critical value of the anisotropy λ_c characterized by the appearance of a central peak in $S^{zz}(\vec{q},\omega)$ for $\lambda>\lambda_c$ and $T>T_{\mathrm{KT}}$. Below λ_c only spin-wave peaks are seen. From the experimental point of view Wiesler *et al.*[5] reported measurements in the $CoCl_2$ intercalated compound which is a good realization of the 2D-XY model. They found an indication of a Kosterlitz-Thouless transition and tested the ideal diluted gas picture. Their results for the in-plane central peak intensity were not conclusive, but they measured a central peak width which was not consistent with the theoretical predictions of Mertens *et al.*[24] More recently Song[29] made NMR measurements on a type-II superconductor $(YBa_2Cu_3O_{7-\delta})$ around the vortex lattice melting temperature. The NMR experiment can directly measure the local spin field distributions, therefore giving a direct measurement of the vortex fluctuations. His results were consistent with local vortex motion only. The purpose of the present work is to report some MCSD simulations for the vortex density fluctuation, pair vortex-antivortex distance distribution, lifetime of pairs and the time needed for a vortex to move one lattice spacing. We also calculate the out-of-plane spin component and the energy density at the vortex core. We hope that our results can lead to a better understanding of the vortex contribution to the 2D-XY model dynamical behavior.

II. MODEL

The 2D-XY model is described by the Hamiltonian

$$\mathcal{H} = -J\sum_{\langle i,j\rangle} (S_i^x S_j^x + S_i^y S_j^y), \tag{3}$$

where $\vec{S}_i$ is a classical three-component spin variable defined on the site i of a square lattice, $|\vec{S}_i|=1$ and $J>0$ is a coupling constant. (This model should not be confused with the planar rotator in which the spin variable has only two degrees of freedom which has no true dynamics.) A vortex gives a logarithmic contribution to the Hamiltonian as obtained by Kosterlitz and Thouless[13] for the planar rotator. In the XY model case a correction to the vortex energy due to the extra degree of freedom should be expected. At $T=0$ the minimum energy configuration is obtained as a ferromagnetic arrangement of the spins $(J>0)$. As long as the temperature increases vortices are created in the system. For very low T the most stable vortex has no out-of-plane component.[28,30] However, the development of an out-of-plane component as temperature increases should not be surprising. Of course a development of such a component should be reflected in the vortex energy, as well as in its dynamical behavior. We observe that for small out-of-plane fluctuations compared with the in-plane one the appropriate canonical variables are polar angles, ϕ, associated with the in-plane components of the spins and the conjugate momenta S^z. From Hamilton's equation we can write $\dot{\phi}\approx 4JS^z$.[18,31] This relation shows that in order to move a vortex has to develop a S^z component. One can always define a stochastic model which has kinetics and which can be studied by Monte Carlo, but this would be a very different situation. Inelastic neutron-scattering experiments on XY-like systems[5,32] show deterministic propagating modes thus indicating the Hamiltonian dynamics is more physical.

III. SIMULATION

In order to better understand the vortex dynamics we performed a very careful Monte Carlo spin dynamics (MCSD) simulation of the 2D-XY model. We calculated the vortex density as a function of time and temperature, the vortex pair density as a function of the distance between vortex and antivortex, the time needed for a pair to annihilate and the time needed for a vortex (antivortex) to move one lattice spacing. Following the discussion in the preceding paragraph we calculate the vortex contribution to the energy and the out-of-plane spin fluctuations inside the vortex core. Here we have a difficulty to define the vortex core. Any definition will be *ad hoc*. In order to give a reasonable definition we follow Ref. 33. For $\lambda>\lambda_c$, the out-of-plane vortex spin asymptotic behavior is known from a continum approach

$$S^z(r)\sim (r_v/r)^{1/2} e^{-r/r_v},$$

where

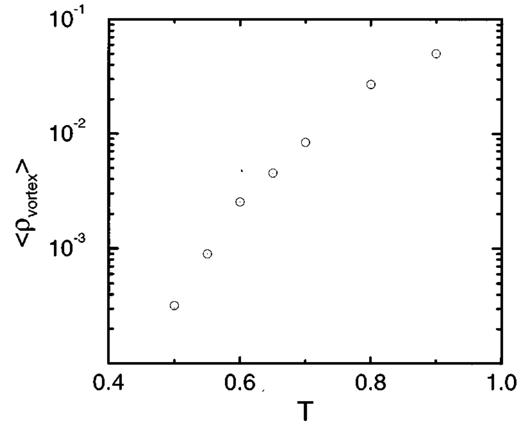

FIG. 4. Vortex density as a function of temperature.

$$r_v = \frac{1}{2}[\lambda/(1-\lambda)]^{1/2}$$

is the vortex core radius and r is the distance from the vortex center. At critical λ ($\lambda_c \simeq 0.7035$) (Ref. 34) $r_v\simeq 1$. Since we are interested in the limit $\lambda=0$ it is reasonable to define the vortex core as the plaquette which contains the vortex. The vortex position is obtained by calculating the sum of the difference between adjacent polar angles around a plaquette. If the sum is 2π (-2π) we have a vortex (antivortex). Our simulations were carried out on a 100×100 lattice with periodic boundary conditions at temperatures from $T=0.3$ up to 0.9 (T is measured in units of J/k_B).

The dynamic of the spins for the 2D-XYmodel is described by

$$\frac{d}{dt}\vec{S}_i = \vec{S}_i \times \vec{V}_i, \tag{4}$$

where

$$\vec{V}_i = J\sum_{nn} (S^x \hat{e}_x + S^y \hat{e}_y). \tag{5}$$

Here the sum is over nearest-neighbors sites of i and $\hat{e}_x$ and $\hat{e}_y$ stand for the unit vectors in the x,y directions, respec-

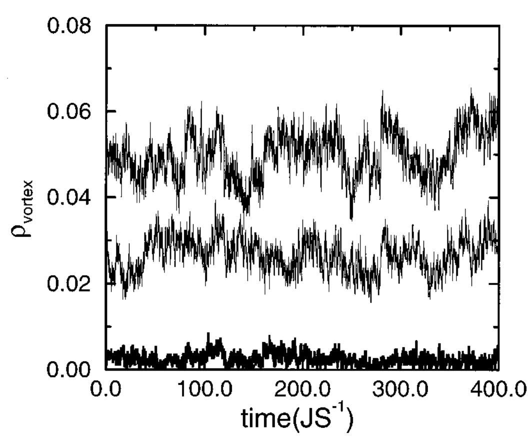

FIG. 5. Vortex density as a function of time for three different temperatures. From bottom to top are seen curves for $T=0.6$, 0.8, and 0.9.

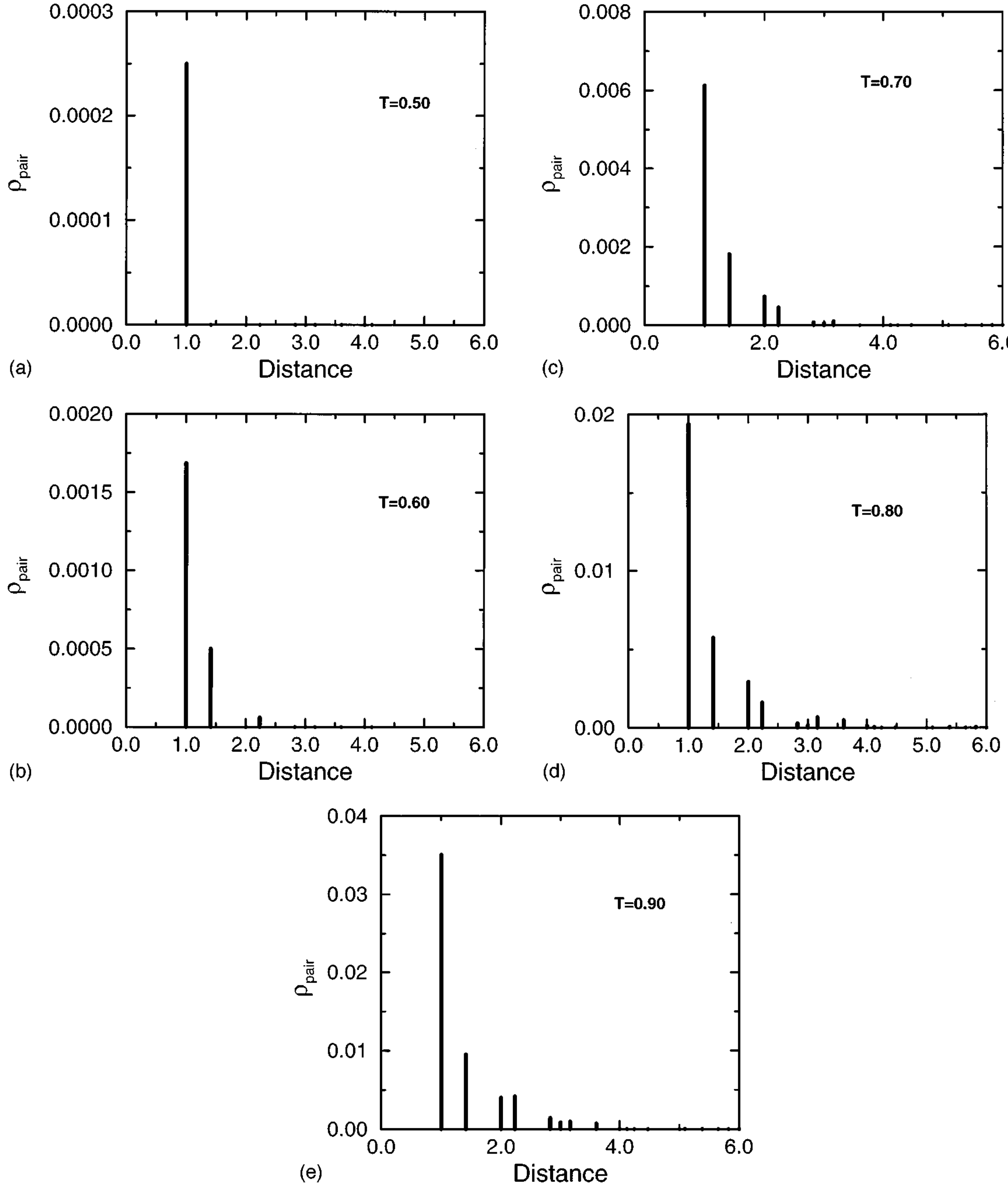

FIG. 6. Number of the vortex-antivortex pairs as a function of the distance between them. Temperatures are indicated as inserts.

tively. Equation (4) is correct in the limit of large $|\vec{S}|$.[35] This equation is derived from Eq. (3) and preserves the total energy. We reinforce that the plane rotator model does not possess Hamiltonian equations of motion; there is only relaxational dynamics. To obtain the dynamical behavior we first equilibrate the system at a desired temperature, then we integrate numerically the Hamiltonian equations of motion. Equilibrium configurations were generated by using a hybrid Monte Carlo method,[16,36] which combines the Metropolis algorithm with Wolff updates. (After each Wolff update six Metropolis sweeps were performed.) This procedure is essential, since the critical slowing down becomes severe as the Kosterlitz-Thouless temperature is approached. (The dynamical critical exponent $z=1.00$ for all $T<T_{\mathrm{KT}}$.[16]) Two hundred initial configurations were generated from independent runs in which the first 10 000 hybrid sweeps were discarded for equilibration. Starting with each thermalized configuration we integrated the equations of motion generated by the Hamiltonian (3) by using a vectorized fourth-order Adams-Moulton method[37] with time steps of $\delta t=0.04J^{-1}$ which ensures a deviation in energy of less than 0.1% after 2000 time steps. The results we present here were obtained every ten time steps and then averaging over all different initial configurations.

Results

In Fig. 4 we plot the average vortex density as a function of temperature. The density increases almost exponentially and shows no indication of T_{KT}. In Fig. 5 we show the vortex density as a function of time for temperatures $T=0.6$, 0.8, and 0.9. It clearly has large fluctuations even at

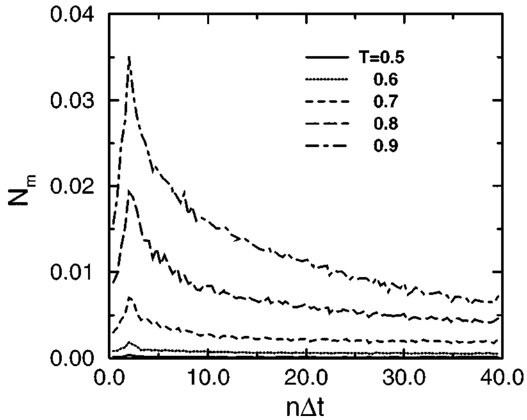

FIG. 7. Histogram showing the time spent for a vortex (antivortex) to move for one lattice spacing. The bin size is $\Delta t = 0.4J^{-1}$.

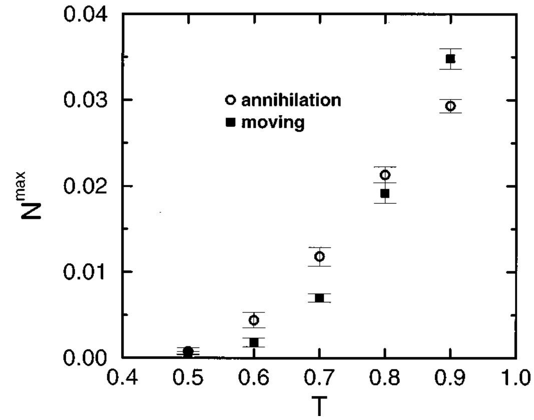

FIG. 9. Maximum of the curves for moving and annihilated vortex, obtained from Figs. 7 and 8, as a function of temperature.

temperatures well below T_{KT}. Our next step was to calculate the position of every vortex and antivortex in the system. We measured the distances from each vortex to the antivortex selecting the smaller one for each, storing the result in a table. The same procedure is applied for each antivortex. By comparing both tables we define a pair as the couple which are at the smaller distance. Our results are shown in Figs. 6(a)–6(e), where we plot the pair density as a function of distance. From those figures it is clear that the pair size has no discontinuous behavior upon passing through T_{KT}, but it grows continuously with temperature. At $T = 0.50$ only pairs at a distance of one lattice spacing are seen, between $T = 0.50$ and $T = 0.60$ the separation starts to grow and at $T = 0.80$ well separated pairs can be seen. At $T = 0.90$ the vortex density is almost saturated and the distribution looks the same as at the previous temperature, except by a scale factor. Our next step was to calculate the time for a vortex (antivortex) to move a distance of one lattice constant. For that, we followed each vortex and antivortex for a long time. At the beginning we created a table with the vortex and antivortex position and for each a corresponding time table. Once a vortex (antivortex) moves we refreshed the time table as well as the position table; then by inspecting both tables we decided if the motion was larger than one lattice spacing. If not, we stored the time spent for this motion to take place. We never observed any motion for more than one lattice spacing in our simulation. Next we calculated the time needed for a pair vortex-antivortex to annihilate. The procedure is basically the same one we used above. The results are presented in Figs. 7 and 8 as histograms using a bin size of $\Delta t = 0.4J^{-1}$. In both cases we found a very well-defined peak around $t = 2J^{-1}$ for all temperatures. An important change occurs when passing through T_{KT}. Below $T = 0.70$ the number of annihilated vortices (N_{c-a}) is larger than that of moving vortices (N_m). At $T = 0.80$ they are almost the same, and at $T = 0.90$ $N_{c-a} < N_m$. Figure 9 shows the maxima $N_{c-a}^{\max}$ and $N_m^{\max}$. The position of the peak does not change with temperature; however, it is clear that longer-lived processes become important. For some configurations we visually followed the annihilation process of an isolated vortex, understood here as a vortex whose distance from its partner is the largest possible for that particular temperature. The vortex does not move to meet an antivortex; instead, a new pair is created in its vicinity and the first vortex can annihilate with the new antivortex. There are some reports in the literature about the movement of vortices in the XY model[38,39] which deserve some comment. In those works the approach used to see the vortex motion was to put a vortex-antivortex pair far apart in the lattice. A dissipative term was added to the equations of motion in order to maintain the

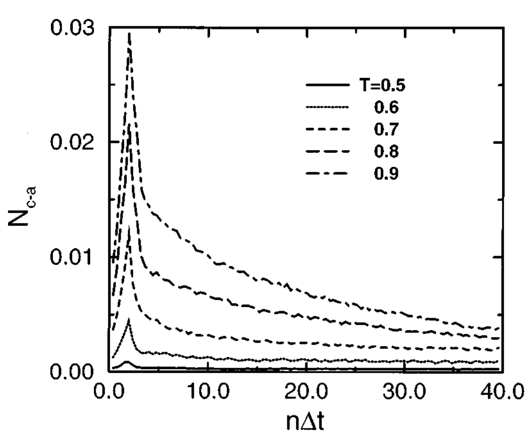

FIG. 8. Lifetime of a vortex-antivortex pair showed as a histogram. The bin size is the same as in Fig. 7.

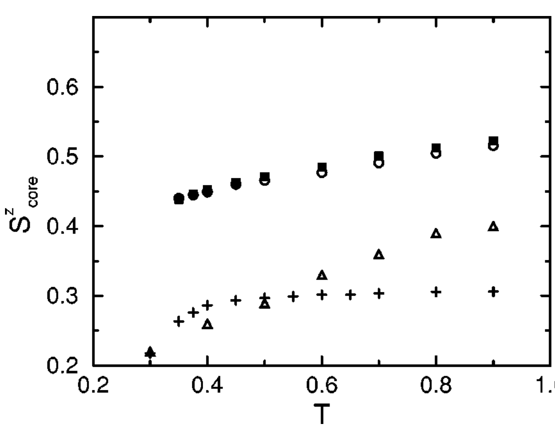

FIG. 10. Average of the modulus of the S^z component at the vortex core as a function of temperature. Squares and circles are for vortices which will disappears or move inside a time interval of $\delta t = 0.04J^{-1}$, the crosses are for all vortices and triangles are for the entire lattice.

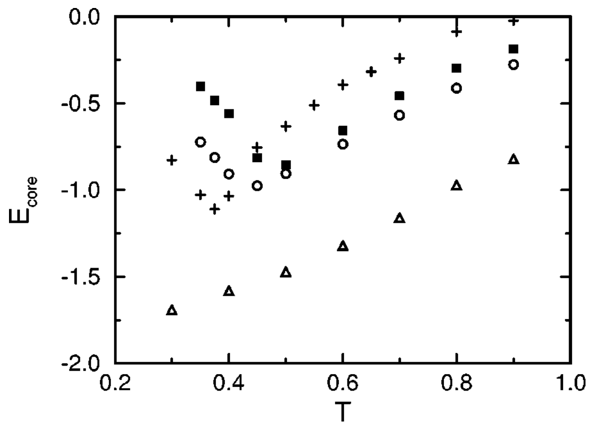

FIG. 11. Energy due to the vortex core as a function of temperature. Symbols are the same as in Fig. 10.

vortex shape and then they were integrated. Clearly such a system is not in thermodynamical equilibrium and the expected behavior could only be the movement of the vortex against the antivortex under the action of the logarithmic attractive potential such that they finally annihilate each other. From the above results it seems that the dynamical behavior of vortices in the XY model comes mainly from the creation-annihilation process and local vortex motion which occur at all temperatures. If vortices play any role in the observed central peak for the XY model it should be seen at all temperatures. In fact such a central peak was reported by Evertz and Landau.[16] Finally we calculated the energy density and the out-of-plane fluctuation at the vortex core. [We define the vortex core as the plaquette which contains the vortex (antivortex).] From our simulations we observed only random core vortices structures as shown in Fig. 3(b). So, for each vortex we calculated the module of the z components ($S^z_{\rm core}$) of the spins around the plaquette. We also obtained the contribution to the energy ($E_{\rm core}$) due to that plaquette using the bonds and spins on the plaquette and none of their other neighbors. They were calculated at each time step $\delta t = 0.04J^{-1}$ in three different situations. We averaged over vortices which will disappear or move at $t+\delta t$ and over all kinds of vortices. The curves for annihilated and moving vortices are similar, since to be annihilated the vortex has to move one lattice spacing. Results of this calculations are seen in Figs. 10 and 11 as squares, circles, and crosses, respectively. We also show S^z and the energy by considering the entire system (all spins), as triangles. We see that an out-of-plane component is developed coherently well below $T_{\rm KT}$. The lowest temperature we could reach was $T=0.30$, below which the time required to equilibrate the system is too large and the vortex density too small to give a reasonable statistics in a reasonable cpu expenditure. Thus, we do not know if $S^z_{\rm core}$ goes to zero at a finite temperature or if this regimen is reached only at $T=0$. On the high-temperature side, $S^z_{\rm core}$ seems to saturate quickly, almost reaching an asymptotic value of $S^z_{\rm core} \approx 1/3$. The out-of-plane component for spins in the case of annihilated and moving vortices is much larger than for all vortices. It clearly indicates that for both processes to take place, the S_z component is important, in agreement with our earlier discussion, and stable vortices have a smaller S^z component. In Fig. 11 we show the core energy behavior of a single vortex. All three curves present a minimum close to $T=0.40$. The origin of these minima seems to lie in the fact that at low, but finite T the spins have enough energy to break the perfect vortex-antivortex arrangement (see Fig. 2) and each vortex (antivortex) core gives a small net ferromagnetic contribution to the energy. At very low T, $E_{\rm core}$ should be zero since the planar vortex configuration has zero energy, i.e., adjacent spins around the plaquette are orthogonal. For $T > T_{\rm KT}$ the energy goes to zero again but now with a well developed out-of-plane component.

IV. DISCUSSION

We have performed a detailed study, from the microscopic point of view, of the vortex dynamics in the 2D-XY model by using a Monte Carlo and spin-dynamics approach. Our study covered both temperature region $T < T_{\rm KT}$ as well as $T > T_{\rm KT}$. The results show that the vortices (antivortices) in this system cannot move freely through the lattice as suggested in early studies and they have only local motion. We also found a quite huge creation-annihilation process which competes in importance with the local vortex motion. If the vortices are really the important excitation responsible for the central peak found in the in-plane dynamical correlation function, then these processes should play the role and a central peak should be seen in the whole range of temperature $T > 0$.

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