Lifetime of vortices in 2D easy-plane ferromagnets

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Abstract— We use a combination of classical Monte Carlo and spin dynamics simulations for the 2D classical easy-plane ferromagnet to estimate the lifetime of free vortices near the Kosterlitz-Thouless transition temperature. Using thermal equilibrium initial states from Monte Carlo, the spin equations of motion are integrated numerically and the number fluctuations of free vortices are used to calculate the lifetime. The inverse lifetime gives an estimate for a cutoff frequency below which an ideal gas description of vortex dynamics is inappropriate. For this reason we compare the lifetime results with simulations and ideal gas phenomenology for the dynamic structure function, $S^{\alpha\alpha}(\mathbf{q},\omega)$.

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It is well known [1] that in two-dimensional (2D) systems with continuous symmetry there is no long range order: $\langle \mathbf{S} \rangle = 0$ for all temperatures, where $\mathbf{S} = (S_1, S_2, \ldots, S_n)$ and $n \geq 2$. But for continuous Abelian symmetry, a finite-temperature topological phase transition exists [2] and occurs through unbinding of topological point defects. [3] These systems include superfluids [4], 2D crystalline solids [5], and XY magnets. [2]

While the static thermodynamic properties are well described by the Kosterlitz–Thouless theory [3], the dynamical properties are not so well understood. There are variety of quasi-2D magnetic materials, such as $BaCo_2(AsO_4)_2$, Rb_2CrCl_4, and others, [6] where the dynamical properties were tested at low frequencies and long wavelengths using inelastic neutron-scattering measurements. More recent experiments [7] show some deviations from existing theories and Monte Carlo simulations. Mertens *et al.* [8] built a theory which accounts qualitatively well for the behavior of the dynamical form factor above the transition temperature for both the in-plane and out-of-plane correlations. The theory assumes an ideal gas of unbound vortices above the Kosterlitz–Thouless transition temperature T_{KT} and it has as adjustable parameters the root-mean-square vortex velocity $\bar{u}$ and the mean vortex-vortex separation 2ξ, where ξ is the correlation length. The validity of this theory may depend on the lifetime of free vortices. Though the ideal gas theory supposes infinite lifetime, it will remain approximately correct for a dilute gas too, if the lifetime τ_{free} is greater than the characteristic time which describes their motion $\xi/\bar{u}$.

The purpose of this Letter is to investigate the free vortex lifetime, for which there is no theory, and to consider its implications for the ideal vortex gas theory. The finite lifetime we measure also suggests that creation and annihilation processes may make substantial contributions to dynamic correlations.

The Model.—We consider a system of classical spins on the sphere S^2 ($\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$, $|\mathbf{S}_i| = 1$), interacting on a 2D square lattice. The Hamiltonian is

$$H = -J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z), \qquad (1)$$

where the sum is over nearest-neighbor lattice sites, $J > 0$ determines ferromagnetic coupling and $0 \leq \lambda < 1$ introduces easy-plane anisotropy.

There are two types of static vortices which arise in this model—*out-of-plane* and *in-plane* ones, depending on the presence or absence respectively of nonzero out-of-plane spin components (S^z), with identical in-plane spin structure. A study of their static properties [9–11] shows that their stability depends on the anisotropy parameter λ. Below a specific value λ_c (≈ 0.70 for square lattice) only the *in-plane* vortex is stable while for $\lambda > \lambda_c$ only the *out-of-plane* one is stable. Because the out-of-plane structure may influence the vortex interactions and therefore their lifetime, we consider both $\lambda < \lambda_c$ and $\lambda > \lambda_c$.

Assuming an ideal gas of free vortices with infinite lifetime, Mertens *et al.* [8] obtained the asymptotic behavior for the in-plane correlation function $S^{xx}(\mathbf{r}, t) = \langle S^x(\mathbf{r}, t) S^x(\mathbf{0}, 0) \rangle$:

$$S^{xx}(\mathbf{r}, t) \simeq \frac{1}{2} S^2 \exp\left(- \left[\left(\frac{r}{\xi}\right)^2 + \left(\frac{\sqrt{\pi}\bar{u}}{2\xi} t\right)^2 \right]^{1/2} \right). \qquad (2)$$

The characteristic time implied by this equation is $t_{\text{char}} = 2\xi/\sqrt{\pi}\bar{u}$, which is approximately the time for a vortex to move one correlation length. Thus, the theory is reasonable provided the vortex lifetime is at least that long. For an order of magnitude result the characteristic time is approximately $t_{\text{char}} \approx 5.9$ from the estimates [8] $\xi \approx 4.4$ and $\bar{u} \approx 0.84$ at temperature $T = 0.9$ (length is in lattice constant units, T in J/k_B, and time in $\hbar/J$). We use this value to compare with the lifetime we obtain from our simulation at this particular temperature.

The space-time Fourier transformation of Eq. (2) leads to a squared Lorentzian central peak form [8] $S^{xx}(\mathbf{q}, \omega) = \frac{S^2}{2\pi} \frac{\gamma^3 \xi^2}{\left(\omega^2 + \gamma^2 \left(1 + (\xi q)^2\right)\right)^2}$, where $\gamma = 1/t_{\text{char}}$, with a wavevector-dependent characteristic frequency width $\Gamma_{\text{char}}(q) = \frac{\bar{u}}{2\xi} \left(\pi(\sqrt{2} - 1)(1 + (\xi q)^2)\right)^{1/2}$. However, a finite vortex lifetime will lead to fluctuations in the number of free vortices on a length scale of $1/q$ of the order of $(1/q\xi)$, with frequency higher than the inverse vortex lifetime, $1/\tau_{\rm free}$. Thus, $1/\tau_{\rm free}$ will represent a cut-off frequency below which the ideal vortex gas theory for $S^{xx}(\mathbf{q},\omega)$ cannot be a valid description.

As mentioned above, the two types of static vortices have the same xy behavior of their spin components but different S^z components. For $\lambda < \lambda_c$, there is no contribution to $S^{zz}(\mathbf{q},\omega)$ from static in-plane vortices and the vortex contribution can only be from *moving* vortices. On the other hand, for $\lambda > \lambda_c$, the main contribution can be from static (out-of-plane) vortex structures. In either case, the ideal gas theory predicts a central peak in Fourier space, but with a Gaussian shape for $S^{zz}(\mathbf{q},\omega)$ rather than the squared Lorentzian for the in-plane correlation function. Since for $\lambda_c < \lambda < 1$, the theory for $S^{zz}(\mathbf{r},t)$ may be built in first approximation by assuming that the out-of-plane structure of a moving vortex can be approximated by the static structure [8], it is important to compare the vortex lifetime in this case with the case $\lambda = 0$, where the spin-wave peak is strongly softened and the central peak can be clearly attributed to the motion of vortices.

Simulations.—We studied classical spins on a square $L \times L$ lattice, for $L = 16$, 32 and 64, with periodic boundary conditions. The simulation was a combination of Monte Carlo and spin-dynamics methods applied to Hamiltonian (1). We used the Metropolis Monte Carlo method to produce initial spin configurations (IC) at a given temperature $T > T_{KT}$, but close to T_{KT}. Then, each initial configuration was evolved in time using the equations of motion for the spins. We accumulated statistics of the fluctuating number of free vortices during the time evolution to determine the free vortex lifetime. A vortex in a given unit cell is considered free if there are no vortices or antivortices in any of the 8 surrounding unit cells.

In the Monte Carlo, we used the first 10^4 Monte Carlo steps (MCS) for equilibration, writing data after each 500 or 1000 MCS. Individual spins were updated by adding increments in arbitrary directions, and then renormalizing to unit lengths. We generated between 25 and 100 IC at each temperature, so that the relative error in $\tau_{\rm free}$ is 1 to 3 percent.

The time evolution simulation solves numerically the Landau—Lifshitz spin equations of motion, [12] using a fourth order Runge—Kutta scheme.

The free vortex lifetime was determined during the time evolution simulation. The number of free vortices was counted at each time step and the times of its decrements were recorded. If Δt_i is the time between the $(i-1)^{th}$ and i^{th} decrements, N_i is the number of free vortices (plus antivortices) in the system before the i^{th} decrement, and ΔN_i is the change of N_i, then from this event the estimate of the vortex lifetime from the time interval Δt_i is

$$\tau_i = \frac{N_i \Delta t_i}{|\Delta N_i|}. \tag{3}$$

The denominator introduces a weighting factor that reduces the importance of fluctuations involving a change in N_i of more than one. This formula gives correct results if $\min(\Delta t_i) \geq dt$, where dt is the integration time step. Also, this condition assures that most of the fluctuations and the processes which occur will change N_i by one or two. [$\Delta N_i = \pm 2$ for vortex pair creation/annihilation, $\Delta N_i = \pm 1$ when a vortex changes from bound to free or vice-versa.] The choice of the time step dt depends on T and L. Increasing either of these increases the average number of vortices, and diminishes the time scale over which their numbers fluctuate, and requires a decrease of dt. The smallest dt we used was $dt = 7 \times 10^{-5}$ for a 64×64 system at temperature $T = 1.3$. In order to check the reliability of the simulations with small time steps we compared the components of the spins(S_i^α, $\alpha = x, y, z$) with precision 10^{-6} at equal times for runs with $dt = 0.01$ and $dt = 7 \times 10^{-5}$ out to a final time $t_{\rm tot} = 50$, finding no differences.

We also considered the free-vortex number-number time correlation function, as another way to obtain the time scale of the vortex number fluctuations, and as a check of the lifetime measurement. The definition is

$$C(t) = \frac{\langle (N(t) - \overline{N})(N(0) - \overline{N}) \rangle}{\langle (\delta N)^2 \rangle}, \tag{4}$$

where $\delta N(t) = N(t) - \overline{N}$ is the instantaneous deviation in $N(t)$ from its time-independent average, $\overline{N} = \langle N \rangle$.

Under the phenomenological assumption of linear response, if the number of free vortices deviates slightly from the equilibrium number at a given temperature, then the rate at which the system relaxes back to equilibrium is proportional to the deviation from equilibrium. If it is valid, it leads to a relaxation time $\tau_{\rm rxn}$;

$$C(t) = \exp(-t/\tau_{\rm rxn}). \tag{5}$$

For the simulations of the correlation function we used 40 initial configurations and a time step $dt = 0.01$ for all temperatures. Each IC was integrated in time up to $t_{\rm tot} = 350$. Each $C(t)$ point is from approximately 300 measurements since we constrained the argument of $C(t)$ in the interval $dt \leq t \leq t_{\rm max} = 50$ ($t_{\rm tot} = 350$). The successive measurements for a given IC and time t in Eq. (4) were taken with a shift of 1.0 time unit in order to minimize the correlation of the data. The final data points were obtained using a weighted average [13] over the initial configurations.

Results.—As a preliminary step we made a Monte Carlo finite-size scaling [14] study to determine accurately the KT-temperature, for $\lambda = 0.0$, since the precise critical point for this model is not known. Using $L = 10$, 20, 40 and 80, and averaging over 160,000 states at each temperature, we calculated the reduced fourth-order cumulant,

$$U_L = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}, \quad (6)$$

where M is the total *in-plane* magnetic moment. This definition is appropriate for systems with XY symmetry, with U_L approaching 0.5 in the low-temperature phase and 0.0 in the high-temperature phase. The result is shown in Fig. 1; the curves for different L cross at $T_{KT} \approx 0.72 \pm 0.005$. This is consistent with the prediction of Menezes *et al.* [15] [$T_{KT}(\lambda = 0) \approx 0.73 \times T_{KT}$(planar rotator)], combined with the MC calculations of Gupta *et al.* [16] [T_{KT}(planar rotator) ≈ 0.90], although the Menezes *et al.* theory does not give the correct T_{KT} for either model. On this basis, to have enough vortices for lifetime measurements, we considered the temperature range $0.75 \leq T \leq 1.3$ with a step $\Delta T = 0.05$.

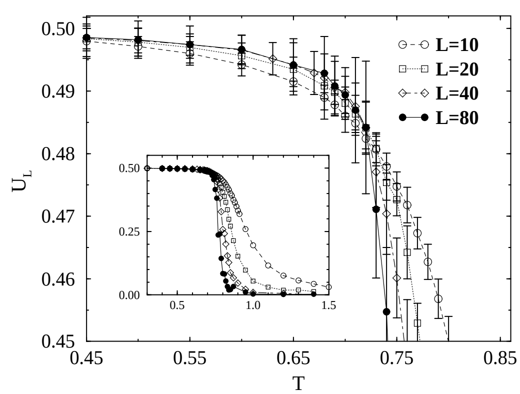

FIG. 1. MC data for the fourth order cumulant of Eq. (6), vs. temperature for various sizes L. The inset shows the data over a larger temperature range.

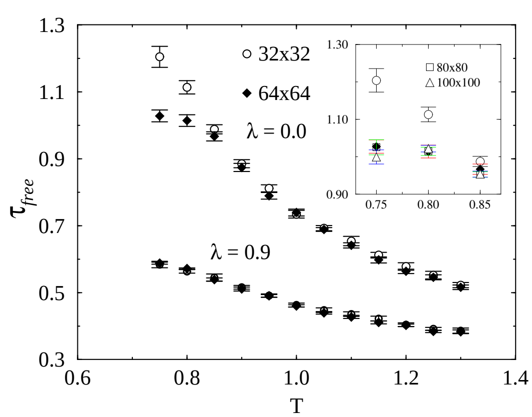

FIG. 2. Free vortex lifetime as obtained from number fluctuations for $\lambda = 0$ and 0.9, system sizes 32×32 and 64×64.

We obtained the free vortex lifetime for two values of the anisotropy parameter $\lambda = 0.0$ and $\lambda = 0.9$, as shown in Figure 2 for system sizes $L = 32, 64$. The lifetime decreases starting from $T = 0.75$ and it is close to saturation when approaching $T = 1.3$. The data points for $\lambda = 0.0$ are higher than those for $\lambda = 0.9$ for all T studied. For $T = 0.9$ and $\lambda = 0.0$, we have $\tau_{\rm free} \approx 0.87$, whereas $t_{\rm char} \approx 5.9$ (see Sec.). This implies a cutoff frequency $1/\tau_{\rm free}$ several times greater than the characteristic frequency $1/\tau_{\rm char}$ in the Mertens *et al.* [8] theory. For comparison, some typical results for $S^{xx}(\mathbf{q}, \omega)$ from an $L = 100$ system are shown in Fig. 3, for $\mathbf{q} = 0.1(\pi, \pi)$. The observed CP is strong for higher temperatures, and for frequencies well below our measured values of $1/\tau_{\rm free}$. This implies that the ideal vortex gas description for frequencies below $1/\tau_{\rm free}$ is inappropriate.

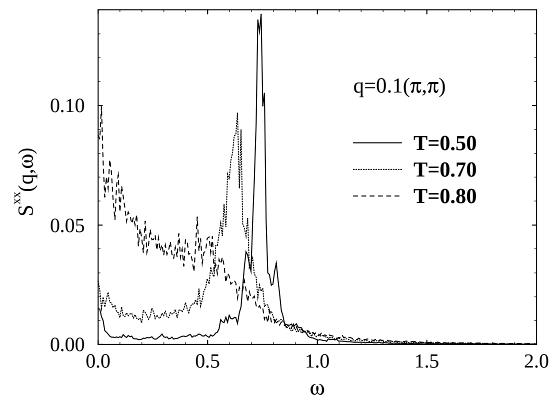

FIG. 3. In-plane dynamic correlation function $S^{zz}(\mathbf{q}, \omega)$ for a 100×100 system with $\lambda = 0$, at small wavevector $\mathbf{q} = 0.1(\pi, \pi)$, averaged over 40 IC.

The lifetime does not show dependence on the size of the system for $\lambda = 0.9$; the data points for 32×32 and 64×64 overlap within their error bars. On the contrary, there is a pronounced finite size effect when approaching the critical region from above for $\lambda = 0.0$. This indicates that the 32×32 system size is too small to be used to study the bulk properties, unless some finite size scaling is applied in a domain close enough to the critical temperature. The presence of this finite size effect and its absence for $\lambda = 0.9$ is because the correlation length for $\lambda = 0.0$ is greater than that for $\lambda = 0.9$ for the corresponding temperatures, since $T_{KT}^{\lambda=0.9} < T_{KT}^{\lambda=0.0}$ [15].

In Fig. 4 we show the free vortex number—number correlation function for temperatures 0.75, 0.8, and 0.9, for $\lambda = 0.0$. As expected, the correlation function decays faster and decorrelates at earlier times for larger temperature. The correlation function cannot be described by linear response theory, implying that $C(t)$ is not governed by a single time scale. This is also confirmed by the tails of these curves. For example, for $T = 0.75$, a linear fit to $\ln C(t)$ from the first 4–5 points gives $\tau_{\rm rxn} \approx 1.8$. However $C(t)$ decorrelates at large times $t > 40$, which contradicts the simple $C(t) = \exp(-t/\tau_{\rm rxn})$ behavior. On the other hand, relaxation times determined from the small-t linear fits are of the same order of magnitude and have the same behavior with temperature as $\tau_{\rm free}$ determined above. Similar results for $\lambda = 0.9$ show a faster decay of $C(t)$ than for $\lambda = 0.0$, completely in agreement with our measurements of $\tau_{\rm free}$ for both values of λ, however, at large times $C(t)$ decorrelates slightly slower than for the case $\lambda = 0.0$.

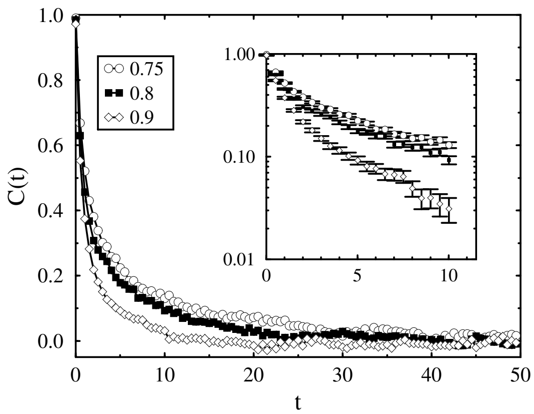

FIG. 4. Free vortex number—number correlation function for temperatures $T = 0.75$, 0.8, and 0.9 for $\lambda = 0.0$.

Discussion and Conclusions.—Different processes determine the *free* vortex lifetime. In general, they can be divided into two classes—pair creation or annihilation and motion of vortices.

Vortices are created or annihilated in pairs due to topological charge conservation. The pair creation process may change the number of *free* vortices in the system by one or more. For instance, a pair may be created in the neighboring cells of a free vortex, thus making all these vortices bound. A different possibility occurs in a group of four bound vortices(two positive and two negative is the most common case) where two of them annihilate and the rest of them become free.

Vortex motion influences the lifetime in a different way. One possibility is the motion of one or both of two vortices which make up a bound pair. When they move apart from each other they may become free and this leads to creation of one or two more free vortices. The opposite process occurs when a free vortex moves closer to another one, they bind and the number of free vortices decreases.

Simulations show that pair creation and annihilation processes occur more frequently than vortex motion over a distance of one lattice constant. A free vortex almost never travels more than one lattice constant before it becomes a bound one in the cases studied.

In conclusion, we carried out the first study to estimate the lifetime of free vortices in the classical XY model, at two values of the anisotropy parameter λ. The lifetime $\tau_{\rm free}$ increases when approaching T_{KT} from above and reaches $\tau_{\rm free} \approx 1.03$ for $\lambda = 0.0$, system size 64×64, and $T = 0.75$. The timescale $\tau_{\rm rxn}$ for decay of the free-vortex number-number correlations was found to be similar to the lifetime. The values of the lifetime and relaxation time for $\lambda = 0.9$ are smaller than those for $\lambda = 0.0$. Since the existing theory [8] assumes effectively infinite lifetime and its characteristic time scale is larger than $\tau_{\rm free}$, we conclude that the short lifetime should be incorporated in the theory, particularly the processes of vortex creation and annihilation which are the main reason for the short free-vortex lifetime.

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