Lifetime of vortices in two-dimensional easy-plane ferromagnets

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We use a combination of classical Monte Carlo and spin dynamics simulations for the two-dimensional (2D) classical easy-plane ferromagnet to estimate the lifetime of free vortices near the Kosterlitz-Thouless transition temperature. 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. We compare the lifetime results with simulations and ideal-gas phenomenology for the dynamic structure function, $S^{\alpha\alpha}(\mathbf{q},\omega)$. Motion of the vortices is observed only on a short-range scale and the magnitude of the lifetime is mainly determined by processes of creation and annihilation of vortex-antivortex pairs rather than by vortex motion.

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 $n \geqslant 2$. 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 (MC) simulations. The question of vortex dynamics is also of much interest in understanding the physical properties of the mixed state of type-II superconductors and has been studied recently too.[8–10]

In this paper we study the vortex dynamics in 2D easy-plane ferromagnets, in which case an ideal-gas theory[11] 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. This 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 paper is to investigate the time and space fluctuations of vortices in 2D easy-plane ferromagnets to determine 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. Understanding vortex motion is of considerable interest not only in XY magnets but also in all the other systems mentioned above.

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

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

where the sum is over nearest-neighbor lattice sites, $J>0$ determines ferromagnetic coupling and $0\leqslant\lambda<1$ 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[12,14] 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.*[11] obtained the asymptotic behavior for the in-plane correlation function $S^{xx}(\mathbf{r},t) = \langle S^x(\mathbf{r},t)S^x(\mathbf{0},0)\rangle$:

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

The characteristic time implied by this equation is $t_{\mathrm{char}}=2\xi/\sqrt{\pi}\bar{u}$, which is approximately the time for a vortex to move one correlation length. Thus, the theory is reasonable provided the free-vortex lifetime is at least that long. For an order of magnitude result the characteristic time is approximately $t_{\mathrm{char}}\approx 5.9$ from the estimates[11] $\xi\approx 4.4$ 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[11] $S^{xx}(\mathbf{q},\omega) = S^2\gamma^3\xi^2/2\pi\{\omega^2+\gamma^2[1+(\xi q)^2]\}^2$, where $\gamma=1/t_{\rm char}$, with a wave-vector-dependent characteristic frequency width $\Gamma_{\rm char}(q)=\bar{u}/2\xi\{\pi(\sqrt{2}-1)[1+(\xi q)^2]\}^{1/2}$. 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 lifetime, $1/\tau_{\rm free}$. Thus, $1/\tau_{\rm free}$ will represent a cutoff frequency below which the ideal-vortex gas theory for $S^{xx}(\mathbf{q},\omega)$ cannot be a valid description.

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. But 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,[11] it is important to compare the free-vortex lifetime in this case with the case $\lambda=0$, where the spin-wave peak is strongly softened and the central peak can be attributed to the motion of vortices.

Simulations. We study classical spins on a square $L\times L$ lattice, for L between 16 and 100, with periodic boundary conditions. The simulation is a combination of Monte Carlo and spin-dynamics methods[12] applied to Hamiltonian (1). We use the Metropolis Monte Carlo method[15] to produce initial spin configurations (IC) at a given temperature $T>T_{\rm KT}$, but close to $T_{\rm KT}$. Then, each IC is evolved in time solving numerically the Landau-Lifshitz spin equations of motion.[16] The time evolution simulation implements a fourth-order Runge-Kutta scheme. We accumulate 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 eight surrounding unit cells. This is one of the simplest definitions to determine the free vortices, particularly for $\lambda<\lambda_c$, in a given distribution of the spins of the system at a given instance of time. More complicated classification schemes will slightly change the total number of free vortices but will also change the time scale over which this number fluctuates. Therefore, we expect that the vortex lifetime, as defined below, will remain approximately unchanged if a more elaborate definition of the free vortices is adopted. For the out-of-plane vortices $(\lambda>\lambda_c)$, the vortex radius is determined by[12]

$$r_v=\frac{1}{2}\left(\frac{\lambda}{1-\lambda}\right)^{1/2}, \tag{3}$$

which for $\lambda=0.9$, a case studied here, $r_v=1.5$, comparable to the length scale beyond which we classify vortices as free on the square lattice (no nearest neighbors closer than $\sqrt{2}$). When $\lambda\to 1$, r_v diverges and for $\lambda=1$ there is no characteristic length scale in the model; this is the isotropic Heisenberg model in two dimensions with well-known exact solution.[13]

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

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

$$\tau_i=\frac{N_i\Delta t_i}{|\Delta N_i|}. \tag{4}$$

The factor N_i is needed because any of the N_i vortices present could have annihilated in this event. The denominator introduces a weighting factor that correctly accounts for the number of vortices annihilated. This formula is applicable if $\min(\Delta t_i)\geqslant dt$, where dt is the integration time step. This condition assures that the observed fluctuations 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.) A free-vortex lifetime is calculated for each IC as an average over all τ_i's and the final value $\tau_{\rm free}$ is an average over the lifetimes from all initial configurations. 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 use is $dt=7\times 10^{-5}$ for a 64×64 system at temperature $T=1.3$.

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

$$C(t)=\frac{\langle[N(t)-\bar{N}][N(0)-\bar{N}]\rangle}{\langle(\delta N)^2\rangle}, \tag{5}$$

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

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 $\tau_{\rm rxn}$,

$$C(t)=\exp(-t/\tau_{\rm rxn}). \tag{6}$$

We use 40 IC and a time step $dt=0.01$ for all temperatures during the simulation of $C(t)$. Each IC is integrated in time up to $t_{\rm tot}=350$ with $C(t)$ calculated for t in the interval $dt\leqslant t\leqslant 50$. Each $C(t)$ point is from approximately 300 measurements since the successive measurements for a given IC are taken with a shift of 1.0 time unit in order to minimize correlation in the data. Finally, an average over the initial configurations is performed.

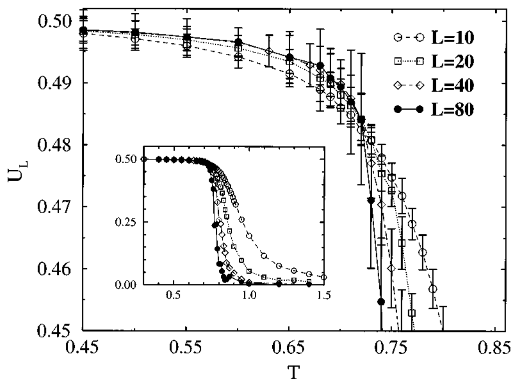

FIG. 1. MC data for the fourth-order cumulant of Eq. (7), vs temperature for various sizes L. The inset shows the data over a larger temperature range.

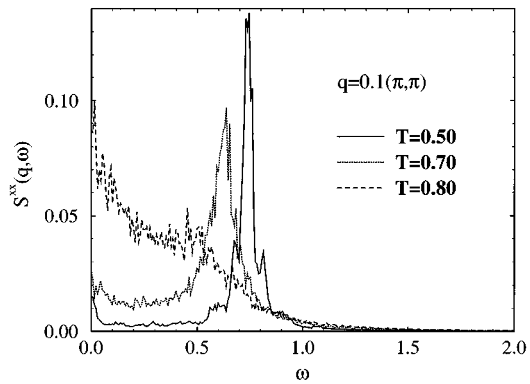

FIG. 3. In-plane dynamic correlation function $S^{zz}(\mathbf{q},\omega)$ for a 100×100 system with $\lambda=0$, at small wave vector $\mathbf{q}=0.1(\pi,\pi)$, averaged over 40 IC.

Results. As a preliminary step we made a Monte Carlo finite-size scaling[17] study to determine accurately the KT temperature for $\lambda=0.0$. Using $L=$ 10, 20, 40, and 80, and averaging over 160 000 states at each temperature, we calculated the reduced fourth-order cumulant,

$$U_L=1-\frac{\langle M^4\rangle}{3\langle M^2\rangle^2}, \tag{7}$$

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 $T_{\rm KT}\approx 0.72\pm 0.005$. This is consistent with the prediction of Menezes *et al.*[18] [$T_{\rm KT}(\lambda=0)\approx 0.73\times T_{\rm KT}$ (planar rotator)], combined with the MC calculations of Gupta *et al.*[19] [$T_{\rm KT}$ (planar rotator) ≈ 0.90], although the theory of Menezes *et al.* does not give the correct $T_{\rm KT}$ for either model. On this basis, to have enough vortices for lifetime measurements, we consider the temperature range $0.75\leqslant T\leqslant 1.3$ with a step $\Delta T=0.05$.

We obtain the free-vortex lifetime for two values of the anisotropy parameter $\lambda=0.0$ and $\lambda=0.9$, as shown in Fig. 2 for system sizes $L=32,\ 64,\ 80,\ 100$. 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 $t_{\rm char}\approx 5.9$. This implies a cutoff frequency $1/\tau_{\rm free}$ several times greater than the characteristic frequency $1/\tau_{\rm char}$ in the theory of Mertens *et al.*[11] 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 central peak is strong for higher temperatures, and for frequencies well below our measured values of $1/\tau_{\rm free}$. This shows that the ideal vortex gas description for frequencies below $1/\tau_{\rm free}$ is inappropriate.

For $\lambda=0$, the first two data points of the 32×32 system size are higher than the corresponding points of the larger sizes (see the inset of Fig. 2). When the system size is decreased as T approaches $T_{\rm KT}$ from above, there will be zero or very few free vortices present, which is the case for $L=32$ and $T=0.75$. In such a case, the statistics of data from Eq. (4) is not reliable, unless much larger systems are simulated. For $\lambda=0.9$ and $L=32$ there are many more free vortices because $T_{\rm KT}^{\lambda=0.9}<T_{\rm KT}^{\lambda=0.0}$.[18]

In Fig. 4 we show the free-vortex number-number correlation function for temperatures 0.75, 0.8, and 0.9, for $\lambda=0.0$ and system size 64×64. As expected, it decays faster

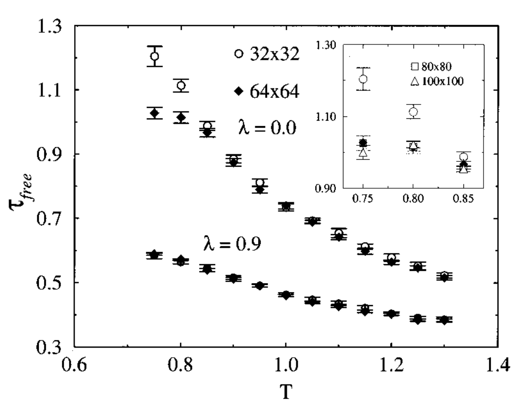

FIG. 2. Free-vortex lifetime as obtained from number fluctuations for $\lambda=0$ and 0.9, system sizes 32×32 and 64×64. The inset shows the first three data points for $\lambda=0$ including also the results for system sizes 80×80 and 100×100.

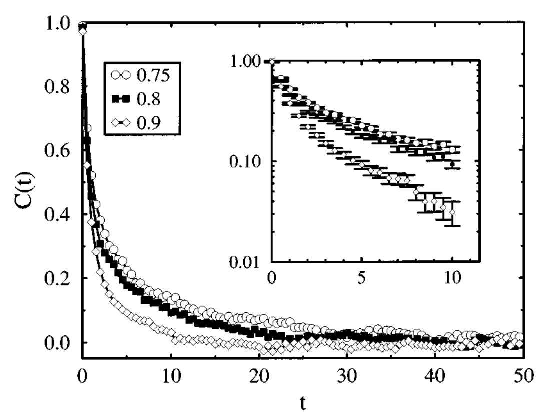

FIG. 4. Free-vortex number-number correlation function for temperatures $T=0.75$, 0.8, and 0.9. The system size is 64×64 and $\lambda=0.0$; the error bars are of the size of the data points. The inset shows the initial decay of the correlation function on a semilog scale.

and decorrelates at earlier times for larger temperature. The correlation function cannot be described by the 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. The relaxation time $\tau_{\rm rxn}$, determined from the small-t decay of $C(t)$, has the same behavior with T as $\tau_{\rm free}$, remaining greater than $\tau_{\rm free}$ for $T_{\rm KT}<T\leqslant 1.0$ and approaching $\tau_{\rm free}$ when T approaches 1.0. 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 but at large times $C(t)$ decorrelates slightly slower than for the case $\lambda=0.0$.

Discussion and Conclusions. Two classes of processes determine the *free*-vortex lifetime-pair creation or annihilation and motion of vortices. 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 free vortices making up a bound pair. The opposite process occurs when bound vortices move apart which leads to creation of one or more free vortices.

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, and this results in the short free-vortex lifetime we observe. This effect is very similar to that reported by Song[10] in experiments on vortex dynamics in $YBa_2Cu_3O_{7-\delta}$, where long-range diffusive vortex motion is also absent, while short-range motion is observed.

In conclusion, we carried out the first study to estimate the lifetime of free vortices in the three-component classical *XY* model with easy-plane anisotropy, at two values of the anisotropy parameter λ. The lifetime $\tau_{\rm free}$ increases when approaching $T_{\rm KT}$ from above and reaches $\tau_{\rm free}\approx 1.03$ for $\lambda=0.0$, system size 64×64, and $T=0.75$. The study of the free-vortex number-number correlation function gives a relaxation time from its initial decay $\tau_{\rm rxn}>\tau_{\rm free}$ for $T_{\rm KT}<T\leqslant 1.0$. The maximum deviation of $\tau_{\rm rxn}$ from $\tau_{\rm free}$ does not exceed 60%. But the slow decay of the correlation function at large times shows that its behavior cannot be described by the linear-response theory. The values of both $\tau_{\rm rxn}$ and $\tau_{\rm free}$ for $\lambda=0.9$ are smaller than those for $\lambda=0.0$. Since the existing theory[11] 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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