Latent heat of vortex lattice melting in two-dimensional superconductors under high magnetic fields

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The latent heat of vortex lattice melting transition in a two-dimensional superconductor at high perpendicular magnetic field is calculated within the framework of the Ginzburg-Landau functional integral approach. The result is found to be smaller than that obtained from various numerical simulations, which tend to overestimate the latent heat due to finite-size effect.

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Phase fluctuations of the superconducting order parameter play a crucial role in controlling the stability of the vortex lattice and its possible melting processes. In two-dimensional (2D) systems the energy scale of these fluctuations is much smaller than the superconducting (SC) condensation energy, implying melting temperature T_m well below the mean field T_c.[1] However, the nature of the vortex lattice melting transition in 2D superconductors is, at present, not yet fully understood. A weak first-order melting transition was predicted in the framework of the Ginzburg-Landau (GL) theory by several Monte Carlo simulations[2–6] and by using high-order perturbation expansion.[7,8] It has been shown recently[1] that shear motions of Bragg chains along the principal crystallographic axes of the vortex lattice cost a very small fraction of the SC condensation energy and are responsible for the low-temperature vortex lattice melting.

In our previous work[1,9] we were mainly interested in determining the melting temperature and the jump of the shear modulus at the melting point. These could be reasonably achieved without resort to explicitly calculating the entropy associated with fluctuating vortices, which is a very subtle matter. Here we make the additional, nontrivial technical effort, and calculate the vortex state entropy in order to evaluate the latent heat of the melting transition. This requires careful examination of the statistical ensembles appropriate for such a calculation, especially since within the GL functional integral approach used the connection between the continuous set of SC fluctuations accessible at high temperatures, and the highly restricted, discrete set of fluctuations controlling the vortex lattice at low temperatures, is very poorly understood.

Within the framework of the GL functional integral approach the vortex state at finite temperature can be described by the partition function

$$Z=\int \prod_{\mathbf{x}} D\psi(\mathbf{x})D\psi^*(\mathbf{x})e^{-\beta_T\mathcal{H}\{\psi(\mathbf{x}),\psi^*(\mathbf{x})\}}, \qquad (1)$$

where the effective "Hamiltonian" $\mathcal{H}\{\psi(\mathbf{x}),\psi^*(\mathbf{x})\}$ is a functional of the condensate wave function ("order parameter") $\psi(\mathbf{x})$. In the phenomenological GL model of a 2D superconductor under a strong magnetic field, perpendicular to the 2D layer, $\mathcal{H}\{\psi(\mathbf{x}),\psi^*(\mathbf{x})\}$ has a simple, local form

$$\mathcal{H}=F_{GL}=\int d^2\mathbf{x}\left(-\alpha|\psi(\mathbf{x})|^2+\frac{1}{2}\beta|\psi(\mathbf{x})|^4\right), \qquad (2)$$

where $\psi(\mathbf{x})$ is restricted to the lowest Landau level (LLL) subspace: $\psi(\mathbf{x})=\Sigma_q c_q\phi_q(x,y)$, with $\phi_q(x,y)=e^{iqx-(y+q/2)^2}$. Here, unless otherwise explicitly stated, all lengths are measured in units of the magnetic length $a_H=\sqrt{c\hbar/eH}$. The plane-wave factor of the Landau orbital (LO) wave function $\phi_q(x,y)$ is selected to propagate along some arbitrary axis x, whereas the Gaussian factor attenuates in the perpendicular direction over the smallest length scale in the problem, a_H. The number of terms in the sum should be equal to number of vortices in the system, N. The range of the spatial integration in Eq. (2) is the total 2D volume V of the superconductor, that is, $V=\pi N$.

It is well known that minimization of the GL energy functional leads to a state in which vortices form a periodic triangular lattice—the Abrikosov lattice. It can be described as a linear superposition of discrete set of the LLL wave functions with

$$q\to q_n=\frac{2\pi}{a_x}n;\quad c_q\to c_n=c_0e^{i\pi n^2/2}, \qquad (3)$$

where $n=-\sqrt{N}/2+1,\ldots,\sqrt{N}/2$. In this representation there are only $\sqrt{N}$ LO's, so that every LO, labeled by n, embodies $\sqrt{N}$ frozen internal degrees of freedom, corresponding to $\sqrt{N}$ guiding centers having the same projection q_n on the y axis. The parameter a_x determines the interguiding center distance in the x direction.

The positions of vortices distributed near such a LO are determined by the interference among LO's located in a tube of radius $\sim a_H$ around it. For a selected x axis along a crystallographic direction with a distance $a_x a_H$ between vortices the number of LO's contributing significantly to this interference is proportional to a_x. It is clear that vortex chains along the principal crystallographic axes are formed by the minimal number (i.e., two) of widely separated LO's (see Fig. 1).

The ground (ordered) vortex state is strongly anisotropic with respect to shear deformations: the shear stiffness is strongly suppressed in directions of the principal axes. The reason for the anisotropy can be clearly understood from the LO picture of the vortex state. It arises from the short-range (i.e., of the order magnetic length) character of the LO inter-

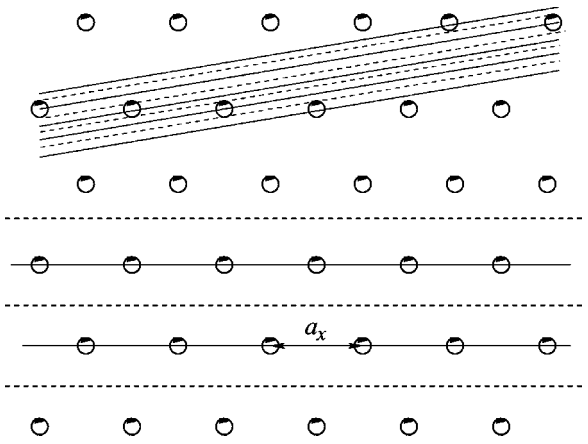

FIG. 1. Vortices (circles) and two Bragg families of Landau orbitals (dashed lines) in the Abrikosov lattice.

action. The strength of the interaction is proportional to the overlap integral between orbitals, which attenuates exponentially with distance between LO's. Thus, the shear deformation in an arbitrary direction involves several closely packed LO's along this axis. The corresponding shear energy has a scale of the condensation energy per unit vortex, $\varepsilon_0 = \pi\alpha^2/2\beta\beta_A$, when the overlap integral is of the order of unity. In contrast, for shear stress along the principal axes, only three LO's separated by a relatively large distance $\sim\pi/a_x$ are involved in the distortion. The energy of such a deformation is of the order $\lambda^2\varepsilon_0$, where $\lambda=\exp(-s)$, with $s=\pi^2/a_x^2$, being a small parameter, $\lambda\ll 1$. For a shear stress along the short diagonal of the unit cell, corresponding to $a_x^2=2\pi/\sqrt{3}$, $\lambda\approx 0.066$, whereas along the long diagonal, with $a_{x'}^2=2\sqrt{3}\pi$, $\lambda\approx 0.16$.

Thus, the partition function, Eq. (1), at low temperatures can be very well approximated by exploiting the former chain representation, and to a lesser extent the latter one. The corresponding GL free energy is given by

$$F_{GL}=\pi N f(c_n,c_n^*); \quad f(c_n,c_n^*) = \frac{1}{\sqrt{N}}\sum_n \left\{ -\overline{\alpha}|c_n|^2+\frac{\overline{\beta}}{2} \times \sum_{n_1,n_2} e^{-s^2(n_1^2+n_2^2)} c_{n+n_1+n_2}^* c_n^* c_{n+n_1} c_{n+n_2} \right\}, \quad (4)$$

where $\overline{\alpha}=a_x\alpha/\sqrt{2\pi}$ and $\overline{\beta}=a_x\beta/\sqrt{4\pi}$. Recalling that any LO embodies $\sqrt{N}$ frozen internal degrees of freedom, the partition function can be written as $Z=\varsigma^{\sqrt{N}}$, where the functional integral

$$\varsigma=\varsigma_0\int\prod_n dc_n dc_n^* \exp[-\beta_T\pi\sqrt{N}f(c_n,c_n^*)] \quad (5)$$

is carried out over all possible values of $c_n=|c_n|e^{i\varphi_n}$, in which the fluctuating phases φ_n correspond to all possible sliding chains configuration along the selected principal crystallographic axis.[1] The prefactor ς_0 is an unknown parameter, which takes into account the statistical weight of the frozen internal degrees of freedom. It depends on the choice of the family of chains, that is, on the parameter a_x.

The thermodynamic properties of the fluctuating system can be derived from the free energy function $f(T,a_x) = -\ln\varsigma/\beta_T\pi\sqrt{N}$ (computed per unit area), which may be separated into an internal energy $u(T,a_x)= -\partial\ln\varsigma/\pi\sqrt{N}\partial\beta_T$ and a contribution associated with the entropy $S(T,a_x)$ arising from thermal motion of sliding vortex chains:

$$f(T,a_x)=u(T,a_x)-TS(T,a_x). \quad (6)$$

In the nearest-neighbor approximation of interaction between chains $u(T,a_x)$ has been calculated in Ref. 1 for Bragg chain families parallel to a principal axis. Here, to increase the accuracy of calculations, we use the next-nearest-neighbor approximation, which incorporates terms in the energy expansion up to λ^5. The result can be written as

$$\pi u(T,a_x)=-\varepsilon_0\frac{\beta_A}{\beta_{fl}(T,a_x)}, \quad (7)$$

$$\beta_{fl}(T,a_x)\simeq\sqrt{\frac{s}{\pi}}[1+4\lambda-4\lambda^2\eta(\tau)+4\lambda^4+8\lambda^5\eta(\tau)^2],$$

where $\eta(\tau)=I_1(\tau)/I_0(\tau)$, $\tau\equiv 4\lambda^2/(1+4\lambda)\beta_T\varepsilon_0\equiv T_{cm}/T$, and $I_k(\tau)$ is modified Bessel function.

The function $\eta(\tau)$, which is proportional to the shear modulus of the vortex lattice along the selected axis,[1] undergoes a rather sharp drop at $\tau\sim 1$, i.e., at the temperature $T\sim T_{cm}$ which strongly depends on the interchain distance π/a_x. The strong suppression of the shear modulus at $T\sim T_{cm}$ is a rough indication for the melting of the vortex lattice. The parameter a_x (or more conveniently $s=\pi^2/a_x^2$) may be regarded as an order parameter for the corresponding solid-liquid transition.[10] Strictly speaking, the partition function, Eq. (5), should include summation over all possible (discrete) values of a_x, corresponding to the various families of Bragg chains in the vortex lattice. However, due to the factor $\sqrt{N}$ in the exponent, and the finite energy difference between states with different values of a_x, the partition function in the thermodynamic limit $N\to\infty$ is dominated by a single term in this sum corresponding to the minimum of $f(c_n,c_n^*)$.

The prevailing Bragg family of sliding vortex chains depends on temperature. Below some finite temperature $T_m\sim T_{cm}$ the partition function is dominated by fluctuations of chains along the large diagonal of the unit cell (x' axis), for which the mean deviation of vortices from their ground-state positions is very small. Above T_m the dominant Bragg family consists of vortex chains along the short diagonal of the unit cell (x axis). Due to larger interchain distance between the x chains, their shear fluctuations are much stronger than those of the x' chains,[1] so that the vortex state above T_m is essentially disordered. It should be stressed, however, that on both sides of this "melting" transition the average vortex positions constitute a periodic lattice. The rotational symmetry of this lattice above T_m is significantly reduced with respect to its symmetry below T_m, which is very close to the ideal

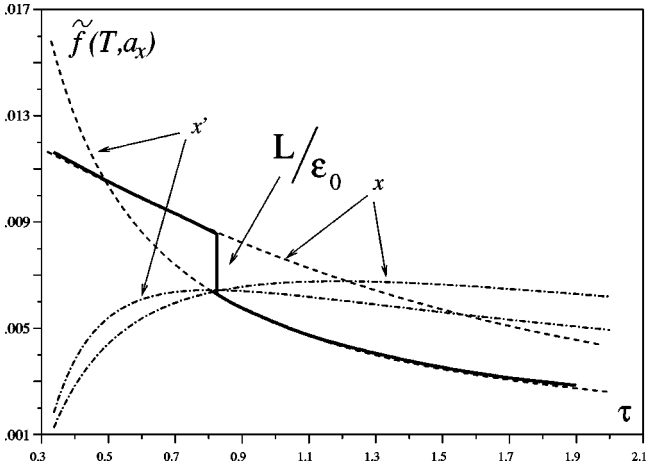

FIG. 2. Dependence of the free energy (dashed-dotted lines) and internal energy (dashed lines) on the inverse temperature $\tau = T_{cm}/T$ for the two principal chain systems x and x' in the canonical ensemble. The solid line depicts the internal energy at equilibrium with a discontinuous jump at the crossing point, $T=T_m$, of the x and x' free energies.

hexagonal symmetry of the Abrikosov lattice. In contrast to this positional ordering, SC order above T_m exists only along the chain direction, reflecting a strong orientation anisotropy of the liquid state just above the melting transition. The destruction of the nematic structure and gradual transition to rotationally invariant liquid with increasing temperature have been discussed in Ref. 10.

The calculation of the entropy $S(T,a_x)$ is a very subtle problem since the density of states factor ς_0 in Eq. (5), which determines the zero-temperature entropy $S(T=0,a_x)\equiv S_0$, is not known to us, as it includes contribution associated with the collapse of the continuum of vortex degrees of freedom into the discrete system of chains. However, for computation of the entropy contribution to the melting transition we need to know only the difference between the entropies corresponding to the x and x' chain systems, $S(T,a_{x'}) - S(T,a_x)$, which does not depend on S_0. This will be done in both the canonical ensemble (CE) and the microcanonical ensemble (MCE).

In the CE the entropy can be obtained indirectly from the free energy, which is evaluated by integrating the internal energy over temperature. For the sake of convenience we consider the thermal increase of the free energy calculated per single vortex, $\tilde{f}(T,a_x)\equiv\pi[f(T,a_x)-f(0,a_x)]/\varepsilon_0$, as a function of τ. Denoting $\tilde{u}(T,a_x)\equiv\pi[u(T,a_x)-u(0,a_x)]/\varepsilon_0$ and using the relations

$$\tilde{f}(\tau,\tau_x)=\frac{1}{\tau}\int_{\tau_x}^{\tau}\tilde{u}(\tau',a_x)d\tau'+\frac{\pi\tau_x}{\tau},$$

$$\tilde{f}(\tau,\tau_{x'})=\frac{1}{\tau}\int_{\tau_{x'}}^{\tau}\tilde{u}(\kappa\tau',a_{x'})d\tau'+\frac{\pi\tau_{x'}}{\tau}, \qquad (8)$$

where the last terms on the right-hand side arise from integration of the ground-state energy, and $\kappa = T_{cm}(a_{x'})/T_{cm}(a_x)\approx 21.8$, the free energies of the chain systems can be determined up to constants of integration τ_x and $\tau_{x'}$, which should satisfy the limiting condition $S(T,a_x)-S(T,a_{x'})\to 0$, as $T\to 0$, or

$$\lim_{\tau\to\infty}\tau[\tilde{f}(\tau,\tau_x)-\tilde{u}(\tau,a_x)-\tilde{f}(\tau,\tau_{x'})+\tilde{u}(\tau,a_{x'})]\to 0. \quad (9)$$

Due to the classical nature of the vortex fluctuations under study here, the entropy obtained from Eq. (8) diverges logarithmically with $T\to 0$. However, using the expansion (7) of the internal energy, up to second order in λ, which is given by $\tilde{u}(\tau,a_x)=(T_{cm}/\varepsilon_0)[1-I_0(\tau)/I_1(\tau)]$, in the integrals, Eq. (8), one finds that the divergent term in the entropy $S(T,a_x)\sim\frac{1}{2}\ln\tau$ does not depend on τ_x. Under these circumstances condition (9) is satisfied when $\tau_x=\tau_{x'}=\tau_0\approx 0.3$. Taking into account, however, higher-order corrections in λ, it is possible to cancel the divergent terms only for $\tau_x \neq \tau_{x'}$, namely, with $\tau_x\approx 0.3$ and $\tau_{x'}\approx 0.31$ in the present approximation.

The temperature dependence of the thermodynamic functions calculated per single vortex, $\tilde{f}(T,a_x)$ (dash-dot lines) and $\tilde{u}(T,a_x)$ (dashed lines), is shown in Fig. 2 for vortex chains along the principal axes x and x'. The crossing point of the free energies, where $\tilde{f}(T,a_x)=\tilde{f}(T,a_{x'})$, determines a discontinuous (first order) transition from a strongly correlated array of vortex chains, characterized by the order parameter a_x, into a weakly correlated array of vortex chains with an order parameter $a_{x'}$.[11]

Note that the crossing of the GL energies, where $\tilde{u}(T,a_x)=\tilde{u}(T,a_{x'})$, takes place at a temperature (corresponding to $\tau\approx 0.5$) slightly above the melting point $T_m \approx 1.2T_{cm}$, ensuring that the sign of the jump in the internal energy is consistent with the endothermic nature of the melting. Thus, our calculation yields a latent heat $L/\varepsilon_0 = \tilde{u}(T_m,a_x)-\tilde{u}(T_m,a_{x'})\approx 2.2\times 10^{-3}$ (or $L\simeq 0.1T_m$) per single vortex.

In the MCE the entropy of vortex configurations, $S(T,a_x)$, is determined by the number of states with a given energy $u(T,a_x)$. It can be derived from the expression

$$e^{\pi\sqrt{N}S(T,a_x)}=e^{\pi\sqrt{N}S_0}\frac{\int\prod_n dc_n dc_n^*\,\delta(f(c_n,c_n^*)-u(T,a_x))}{\int\prod_n dc_n dc_n^*\,\delta(f(c_n,c_n^*)-u(0,a_x))}, \qquad (10)$$

where the entropy at $T\to 0$ is assumed to be independent of the chain representation.

Expanding the energy functional $f(c_n,c_n^*)$, written in the nearest-neighbor approximation, in the small-amplitude fluctuations about their mean-field values, $c_0^2=\alpha/\beta\beta_A$, one may rewrite the integral in the numerator of Eq. (10) as

$$\int\prod_n dc_n dc_n^*\,\delta\left(\sum_n\left[\left(\frac{c_n^2-c_0^2}{c_0^2}\right)^2-\frac{T_{cm}}{\varepsilon_0}[\cos\overline{\chi_n}-\eta]\right]\right),$$

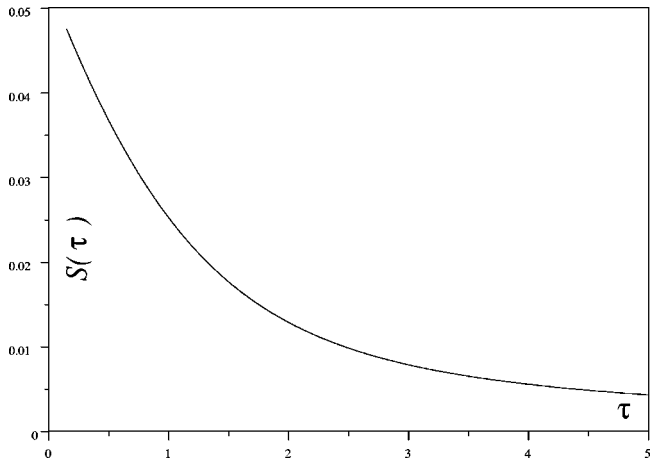

FIG. 3. Dependence of the entropy calculated in the microcanonical on $\tau = T_{cm}/T$.

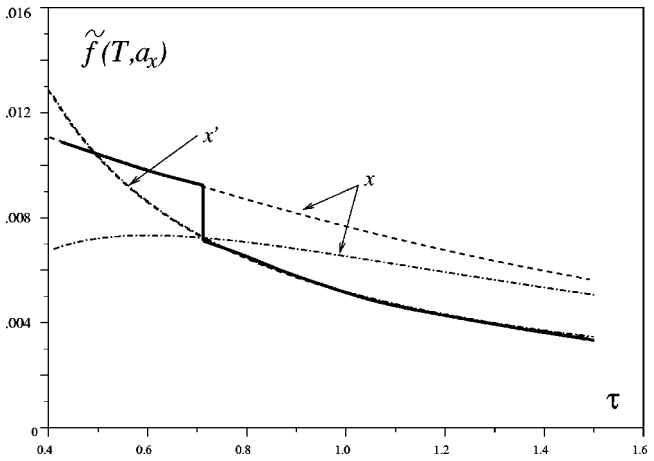

FIG. 4. The same as in Fig. 2 but for the microcanonical ensemble.

where $\bar{\chi}_n = \bar{\varphi}_{n+1} + \bar{\varphi}_{n-1} - 2\bar{\varphi}_n$, $\bar{\varphi}_n = \varphi_n - \varphi_{0n}$, and $\varphi_{0n} = \pi/2n^2$ is the mean-field value of the corresponding phase. It should be stressed that the calculation of the entropy is restricted to the nearest-neighbor approximation (i.e., to terms up to second order in λ) since the entropy contribution to free energy is multiplied by $T \sim T_m \sim \lambda^2 \varepsilon_0$. Introducing the new variables of integration $y_n = 2\sigma_n(x_n - \sigma_n)$, with $x_n = \varepsilon_0^{1/2}[(c_n^2 - c_0^2)/c_0^2]$, and $\sigma_n^2 = T_{cm}[\cos\bar{\chi}_n - \eta(\tau)]$, the multiple integral can be rewritten as $\int \Pi_n d\varphi_n dx_n \delta(\Sigma_n(x_n^2 - \sigma_n^2)) \simeq \int \Pi_n (d\varphi_n/2\sigma_n) dy_n \delta(\Sigma_n y_n)$, where second-order terms in the small-amplitude fluctuations are neglected. Noting that the multiple integration over y_n yields a temperature-independent constant (while recalling that the denominator in Eq. (10) is also a constant), and changing phase variables of integration to $\bar{\chi}_n$, we find that

$$S(T,a_x) - S_0 = \frac{1}{\pi\sqrt{N}} \sum_n \ln\left[\frac{\sqrt{2}}{\pi}\int_0^{\bar{\chi}_0} \frac{d\bar{\chi}_n}{\sqrt{\cos\bar{\chi}_n - \eta(\tau)}}\right], \tag{11}$$

where $\cos\bar{\chi}_0 \equiv \eta(\tau)$. Here the normalization in Eq. (10) was selected to satisfy the condition $S(T \to 0, a_x) \to S_0$.

The plot of the entropy $S(T) - S_0$ as a function of the dimensionless inverse temperature $\tau = T_{cm}(a_x)/T$ is shown in Fig. 3. It is seen that while the entropy sharply increases in the crossover region, $\tau \sim 1$, its contribution to the free energy is $0.03 T_{cm}(a_x)$ at $\tau = 1$, which should be compared with relatively large increase of the internal energy there, $u(T,a_x) - u(0,a_x) = T_{cm}(a_x)(1 - \eta(1))/\pi \approx 0.18 T_{cm}$.

The resulting dependence of the GL energy and free energy is demonstrated in Fig. 4. Within the accuracy of our calculations, the crossing point of the free-energy curves for the x and x' chain systems, found at $\tau_m = 0.71$, close to that obtained in the CE (see Fig. 2). The latent heat found in the MCE is estimated as $L/\varepsilon_0 \approx 2 \times 10^{-3}$, which agrees well with the latent heat obtained in the CE. Note that the form of the curves for the MCE and CE is different because of the different zero-temperature entropies S_0 used. While it is selected to be zero in the MCE, it diverges logarithmically to ∞ in our CE calculation.

The present calculation of the free energy has been carried out including terms $\sim \lambda^5$ (next-nearest-neighbor approximation with respect to the phase-dependent interaction between vortex chains). Such accuracy is required because of the relatively large value of the expansion parameter for the chain system along the x' principal axis, $\lambda(a_{x'}) = 0.4$. Invoking the next-nearest-neighbor approximation shifts the crossing point of the GL energies from $t = -16.5$ (Ref. 1) to $t = -12.8$, where t is defined by $t = -2\sqrt{\beta_A \varepsilon_0/T}$. Due to the entropy contribution, the free-energy crossing point occurs at $t_m = -15.4$ for MCE and $t_m = -16.6$ for CE. These values are within the range of melting temperatures obtained in the various numerical simulations, i.e., $t_m = -(14-17)$.[2–6] The latent heat obtained in our chain model, i.e., $\sim 2 \times 10^{-3} \varepsilon_0$, is smaller than that found in Refs. 2 and 3, which is $\sim 6 \times 10^{-3} \varepsilon_0$. The discrepancy seems to arise from finite-size effect of the vortex system employed in the numerical simulations. The results of Ref. 3 clearly show that the numerically computed melting temperature decreases with the sample size N. It is therefore plausible that the latent heat also reduces with the increasing sample size, suggesting that the internal energy jump calculated at $N = 256$ may be considered as an upper bound for the latent heat of a macroscopic sample. It is therefore interesting to note that our result, $L \simeq 0.1 T_m$, is in a considerably better agreement with that calculated within the frustrated XY model, $L \simeq 0.15 T_m$, in which a significantly larger sample was employed in the simulation.[12]

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[1] V. Zhuravlev and T. Maniv, Phys. Rev. B **60**, 4277 (1999).
[2] Z. Tesanovic and I.F. Herbut, Phys. Rev. B **50**, 10389 (1994); Z. Tesanovic and L. Xing, Phys. Rev. Lett. **67**, 2729 (1991).
[3] Y. Kato and N. Nagaosa, Phys. Rev. B **48**, 7383 (1993).
[4] Jun Hu and A.H. MacDonald, Phys. Rev. Lett. **71**, 432 (1993).
[5] R. Sasik and D. Stroud, Phys. Rev. B **49**, 16074 (1994).
[6] R. Sasik, D. Stroud, and Z. Tesanovic, Phys. Rev. B **51**, 3042 (1995)
[7] S. Hikami, A. Fujita, and A.I. Larkin, Phys. Rev. B **44**, 10 400 (1991).
[8] D. Li and B. Rosenstein, Phys. Rev. B **65**, 220504(R) (2002).
[9] T. Maniv, V. Zhuravlev, I.D. Vagner, and P. Wyder, Rev. Mod. Phys. **73**, 867 (2001).
[10] V. Zhuravlev and T. Maniv, Phys. Rev. B **66**, 014529 (2002).
[11] V. Zhuravlev and T. Maniv, in *Recent Trends in Theory of Physical Phenomena in High Magnetic Fields*, edited by I.D. Vagner, P. Wyder, and T. Maniv (Kluwer Academic Publishers, Dordrecht, 2003).
[12] X. Hu, S. Miyasita, and M. Tachiki, Physica C **282–287**, 2057 (1997).