A δ-function-like peak in the specific heat of two-dimensional vortex lattice: Monte carlo study*

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Abstract: A repulsive vortex-vortex interaction model was used to numerically study the melting transition of the two-dimensional vortex system with Monte Carlo method. Then a δ-function-like peak in the specific heat was observed and the internal energy showed a sharp drop at the melting temperature, which indicated that there exists a first-order melting transition at finite temperatures. The Lindemann criterion was also investigated and valid, but different from previous simulation results.

Key words: vortex lattice, Monte Carlo method, melting transition, Lindemann criterion

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INTRODUCTION

In the conventional superconductors, thermal-fluctuation effects are very small because of the large coherence length. Mean-field theory, therefore, can give a good description of these systems. In contrast, because of the short coherence lengths and large anisotropy, thermal fluctuation plays an important role in determining the thermodynamic properties of the cupric high-T_c superconductors (Blatter et al. 1994; Luo et al., 2001). Brezin et al. (1985) were the first who discussed the contribution of thermal fluctuation beyond the mean-field theory. From the thermodynamic point of view, a first-order phase transition should be accompanied by latent heat and a δ-function-like peak in the specific heat, as well as a jump in the magnetic induction, provided the transition is relevant to a magnetic ordering as in the case of the mixed state in high-T_c superconductors. The first concrete experimental evidence for the first-order melting transition in the vortex states of high-T_c superconductors was provided by Zeldov et al(1995), who observed a discrete jump in the magnetic induction by using microscopic Hall sensors in the $Bi_2Sr_2CaCu_2O_8$ sample. Then the existence of the latent heat and a δ- function peak in the specific heat were observed by Schilling et al. (1996) in a single crystal of $YBa_2Cu_3O_{7-\delta}$ using calorimetric measurement. More recently, based on the three-dimensional uniformly frustrated, anisotropic XY model, Hu et al. (1997) in their Monte Carlo simulations observed a δ-function peak in the specific heat at the melting point T_m of the flux lattice in high-T_c superconductors.

However, magnetic-transport measurement on thin $YBa_2Cu_3O_{7-\delta}$ films seemed to indicate that the melting temperature decreases to $T_m = 0$. Theoretically Moor(1992)argued that due to the absence of long-range phase coherence, the melting transition does not exist at a finite temperature. Whereas it is believed that the vortex pinning is strong in thin films, which could explain the absence of a finite- temperature melting transition (Yates et al., 1995). Monte Carlo studies (Tesanovic et al., 1991; Ryn et al., 1992) on various approximations to the full Landau-Ginzburg partition function have been claimed to be consistent with the existence of a finite-temperature melting transition.

In this work, based on a generally used model of repulsive vortex-vortex interacting po-

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tential, we reexamine the melting of the 2D vortex lattice with the Monte Carlo method.

THEORY

The vortices are treated as massless classical particles, with repulsive interaction potential (Fisher et al., 1980):

$$V(\boldsymbol{R}) = V_0 \{H_0(\boldsymbol{R}/\Lambda) - Y_0(\boldsymbol{R}/\Lambda)\} \quad (1)$$

Where H_0^2 is a Struve function and Y_0 is a Neumann function, $V_o = \Phi_0^2/2\mu_0\Lambda$ with Φ_0^2 being the flux quantum, μ_0 the permeability constant, and the effective two-dimensional penetration depth $\Lambda = 2\lambda_B^2/d$, with λ_B the bulk penetration depth and d the film thickness. In our simulations, λ_B and d were chosen as the typical values of high-T_c compounds: $\lambda_B = 1000$Å and $d = 1$Å. The equilibration in the Abrikosov lattice a_0 was taken to be presenting an internal field of 1 T. The potential function is plotted in Fig. 1. Our model potential is different from that of Yates et al. (1995), where a logarithmic form was chosen.

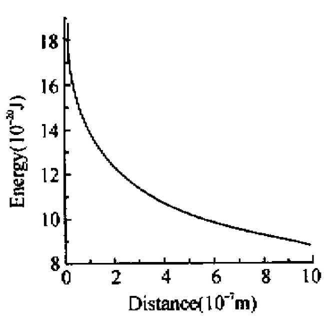

Fig. 1 The vortex-vortex interaction potential as a function of vortex separation

RESULTS AND DISCUSSIONS

The potential is cut off to a fixed value at a finite range in order to avoid artificial ordering effects induced by the periodic boundary. The Monte Carlo simulation technique used here employs the standard Metropolis algorithm. We start with the ideal triangular lattice subject to the periodic boundary conditions. The results reported in this work are for a system of 108 vortices. The typical step size is adjusted during the run in order to ensure that approximately halt of the moves are accepted.

The specific heat is evaluated from the thermal fluctuations of the internal energy via the fluctuation-dissipation theorem:

$$C = (\langle \boldsymbol{E}^2 \rangle - \langle \boldsymbol{E} \rangle^2)/\kappa_B \boldsymbol{T}^2 \quad (2)$$

During a run, 10^4 Monte Carlo sweeps are taken for equilibration and twice that for the energy measurement.

Fig. 2 shows the temperature dependence of the specific heat. The specific heat per vortex increases sharply from $T = 17.9$ K and drops when the temperature is increased to higher than $T = 18.1$ K. We therefore conclude that the δ-function-like peak observed in the specific heat at the transition point indicates existence of a melting transition at a finite temperature.

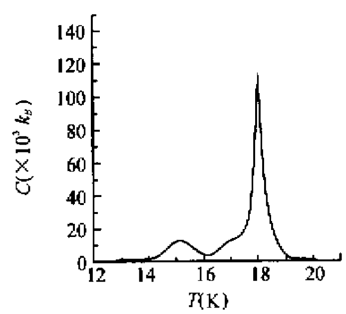

Fig. 2 Temperature dependence of the specific heat per vortex

Along with the appearance of the δ- function-like peak in the specific heat, the temperature dependence of the internal energy shows a sharp drop at the melting point. The results are shown in Fig. 3. Study of Fig. 2 and Fig. 3 led us to conclude that a first-order melting transition occurs at finite temperature.

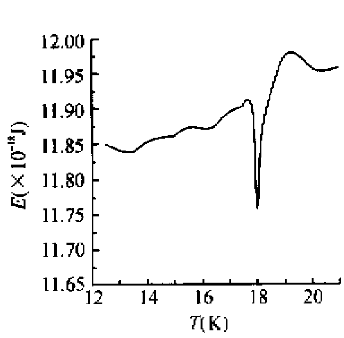

Fig. 3 Temperature dependence of the internal energy per vortex

Finally, we calculate the root mean square displacement of the thermal fluctuations $<u^2>_{th}^{1/2}$. The temperature dependence of $<u^2>_{th}^{1/2}$ is presented in Fig. 4. showing significant thermal motion at the melting temperature. This accords with the Lindemann criterion (Blatter et al., 1994); but differs from the finding of Yates et al. (1995).

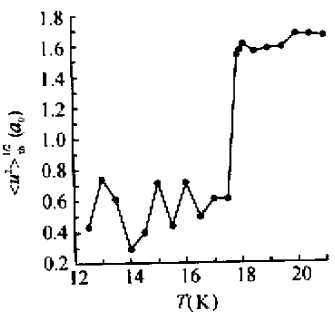

Fig. 4 Temperature dependence of the root mean square displacement of the thermal fluctuations $<u^2>_{th}^{1/2}$

In conclusion, using a model of repulsive vortex-vortex interacting potential, we have performed Monte Carlo simulation for the 2D vortex lattice. A δ- function-like peak is observed in the specific heat and the internal energy shows a jump drop at the melting temperature, which indicates that there exists a first-order melting transition at finite temperatures. The Lindemann criterion has also been investigated to be valid.

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