δ-Function Peak in the Specific Heat of High-T_c Superconductors: Monte Carlo Simulation

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(Received 24 March 1997)

A δ-function peak in the specific heat is observed at the melting point T_m of the flux lattice in high-T_c superconductors. It is $18.5k_B$ and $17.5k_B$ in the liquid and the solid phases per flux per layer, respectively, and increases to $23k_B$ in $\Delta T = 0.009T_m$ around T_m. At T_m the system changes from the triangular flux lattice to a decoupled 2D liquid of vortices. The latent heat is $0.07k_BT_m$ per flux per layer. [S0031-9007(97)04306-8]

PACS numbers: 74.20.De, 74.25.Bt, 74.25.Dw, 74.60.Ge

Thermal fluctuations play important roles in determining properties of high-T_c superconductors, because of high operation temperature and large anisotropy [1–4]. The second-order phase transition from the Abrikosov flux lattice to the normal state in conventional superconductors [5] is thus switched into a first-order melting transition. From the thermodynamic point of view, a first-order phase transition should be accompanied by a 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 the case of the mixed state in high-T_c superconductors. The existence of the latent heat at the melting transition is verified by a calorimetric measurement in $YBa_2Cu_3O_{7-\delta}$ [6]. The discontinuous jump in the magnetization induction is observed in $Bi_2Sr_2CaCu_2O_8$ [7]. Observations on transport properties also provided consistent evidences of the first-order phase transition [8]. Computer simulations have been performed to investigate the melting transition as well about the latent heat [9,10] and the jump of the magnetic induction [11]. In the present Letter, we provide detailed results of Monte Carlo (MC) simulation observation on the δ-function peak in the specific heat and the temperature dependence of the internal energy. It is revealed from the present simulation that the sharp spike in the specific heat occurs in a very narrow temperature region and can be well simulated only in systems with large dimension along the c axis, over long simulation time. Very recently, the observations on the δ-function peak in the specific heat by thermal experiments [12,13] and by MC simulation [14] have briefly been reported.

The starting point of the present study is the Ginzburg-Landau Lawrence-Doniach free-energy functional for layered superconductors [15,16]. We concentrate on the phase degrees of freedom in the superconductivity order parameter in the ensemble of constant magnetic induction $\boldsymbol{B}$. The system is discretized in ab planes in order to implement simulation. The model Hamiltonian is therefore that of a three-dimensional frustrated XY model [9,17],

$$H = -J\left\{\sum_{\langle i,j\rangle\in ab\text{-plane}} \cos\left(\varphi_i - \varphi_j - \frac{2\pi d^2}{\phi_0}\int_i^j \frac{\mathbf{A}^{(2)}}{d}\frac{d\mathbf{l}}{d}\right) + \frac{1}{\gamma^2}\sum_{\langle i,j\rangle\in c\text{-axis}} \cos\left(\varphi_i - \varphi_j - \frac{2\pi d^2}{\phi_0}\int_i^j \frac{A_z}{d}\frac{dz}{d}\right)\right\}.$$

The coupling J is related to the flux quantum, the interplane distance, and the penetration length in the ab planes by $J = \phi_0^2 d/16\pi^3\lambda^2$. γ is the anisotropy constant. The gauge invariance of the magnetic field is kept in the explicit fashion in the present approach. The system is then subject to a MC simulation process which minimizes the free energy. Vortices and thus flux lines are identified by counting the gauge invariant phase differences around relevant cells.

In the present Letter, $\boldsymbol{B}$ is along the c axis. We have performed MC simulations of Metropolis algorithm for systems of a filling factor $d^2B/\phi_0 = 1/25$. The main body of the results is for a system of $\gamma^2 = 10$ and $L_z = 40$ ab planes with $L_{xy} \times L_{xy} = 50 \times 50$ square meshes in each plane. Periodic boundary conditions are put in all the directions. In a relation concerning the parameter dependence and the size dependence of the simulated results, some other systems are discussed. The number of MC steps are typically 100×10^3 after 50×10^3 for equilibration. Around the transition temperature, we have simulated up to 4×10^6 MC sweeps.

Instead of assuming any ordered structure [17], we start from a random configuration at a sufficiently high temperature, and investigate the behavior of the system upon cooling. At temperatures higher than $T_v = 1.1J/k_B$, many vortices and antivortices are excited. Without any correlation both in the structure function $S(\boldsymbol{q}_{ab}, z = 0)$, which describes the correlations among vortices within the same ab planes, and in the helicity modulus Y_c [17], which evaluates the coherence of the system along the c axis, the system behaves as a fully random gas of pancake vortices. On cooling down across T_v, the number of pancake vortices decreases significantly. Isotropic rings appear in the structure function $S(\boldsymbol{q}_{ab}, z = 0)$; meanwhile

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the helicity modulus Y_c remains vanishing, indicating that the system is decoupled into a two-dimensional (2D) liquid of pancake vortices. The phase change between the gas and the liquid is a crossover associated with a broad cusp in the specific heat.

As the system is cooled down further, the 2D vortex liquid is ordered at $T_m = 0.568J/k_B$ into a lattice of flux lines along the c axis and of hexagonal symmetry in the ab planes via a first-order thermodynamic phase transition. In Fig. 1, we present the temperature dependence of the specific heat, the central result of this Letter, evaluated from thermal fluctuations of the internal energy via the fluctuation-dissipation theorem,

$$C = (\langle H^2\rangle - \langle H\rangle^2)/k_B T^2.$$

The specific heat per flux line per layer increases sharply from $18.5k_B$ of the vortex liquid just above T_m to $23k_B$ right on T_m, within a temperature variation $\Delta T = 0.0015J/k_B$, and then drops to $17.5k_B$ of the flux lattice within $\Delta T = 0.0035J/k_B$. Taking place within $\Delta T = (0.009 \pm 0.002)T_m$, the spike of the specific heat is roughly $5k_B$ above those off, but very close to the transition region. We therefore conclude that a δ-function-like peak is observed in the specific heat at the transition point.

Consistently with appearance of the δ-function peak in the specific heat, the temperature dependence of the internal energy shows a kink-like anomaly around the melting point, as in Fig. 2. The data are obtained by averaging on 4×10^6 MC sweeps at each temperature after 150×10^3 steps for equilibration. From Fig. 2, the latent heat is estimated as $Q = 0.07k_BT_m$ per flux line per layer. The error bars in Fig. 2 are the variance of the internal energy evaluated on bins of 500×10^3 MC sweeps. Off the transition region the error bars are smaller than the marks of the data points. Within the transition region the error bars are larger, corresponding to the fact that the system fluctuates between two phases with different energies. These error bars decrease systematically as longer bins are adopted for statistics. By investigating time sequences of the fluctuation in the internal energy in the melting region, it is confirmed that the system vibrates with a period of about 150×10^3 MC steps between two states of different internal energies. During the total 4×10^6 MC sweeps enough numbers of vibrations occur. Therefore, the data shown in Figs. 1 and 2 are for the equilibrium state even in the transition region, rather than for metastable states as in a simulation using much shorter MC sweeps. The histograms for energy distribution [18] in the transition region are fitted well by two Gaussian functions, and the two values of the internal energy yielding the peaks of the two histograms are separated by $0.042J$. This value of the latent heat is consistent with the estimate from the data in Fig. 2.

Let us show the consistency of our data in Figs. 1 and 2. It is known that (see, for example, Ref. [19]) the δ-function peak in the specific heat associated with a first-order transition is smeared by the finite size of the simulated system to a spike with the maximum value

$$C^{\max} = \frac{Q^2}{4k_BT_m^2} L_{xy}^2 L_z f + \frac{C_+ + C_-}{2},$$

where $C_\pm = \lim_{T\to T_m\pm} C$, and the width of the peak

$$\Delta T = \frac{2k_BT_m^2}{QL_{xy}^2 L_z f}.$$

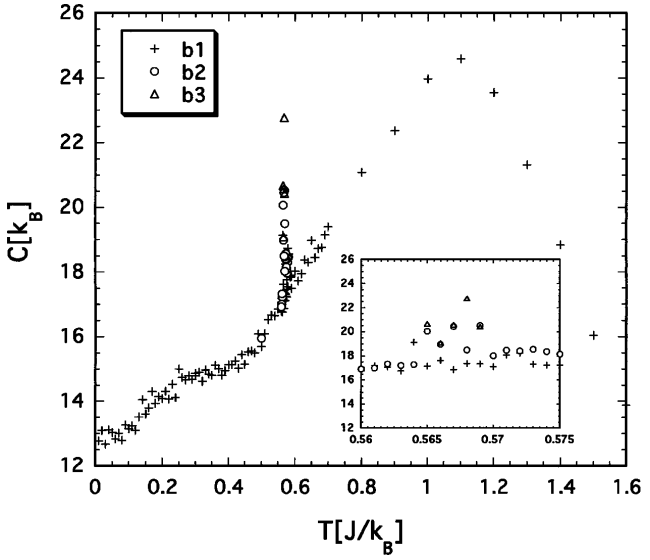

FIG. 1. Temperature dependence of the specific heat per flux line per layer evaluated in three simulation bins: b1 from 50×10^3 to 150×10^3, b2 for the next 2×10^6, and b3 for the successive next 2×10^6 MC sweeps at each temperature. The inset is for a narrow temperature region around the melting point.

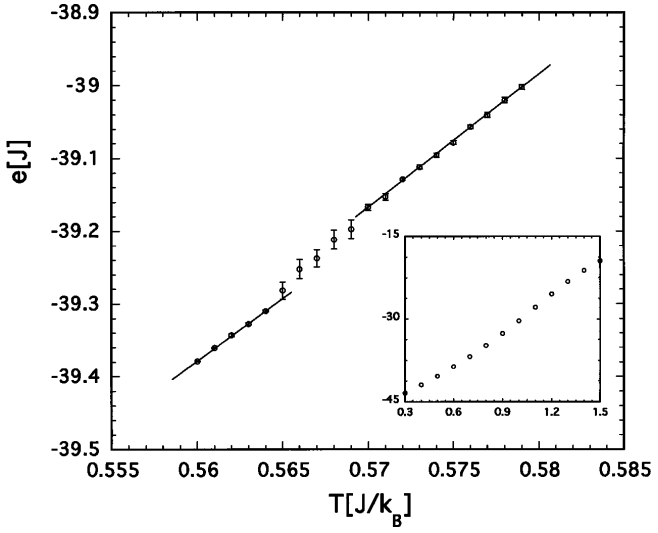

FIG. 2. Temperature dependence of the internal energy per flux line per layer evaluated by averaging over 4×10^6 MC sweeps after 150×10^3 MC sweeps for equilibration. Error bars are estimated from the standard variance of the internal energy over bins of 500×10^3 MC sweeps. The solid lines are guides for the eye. The inset is for a wide temperature region.

Our results for the specific heat and the internal energy satisfy these two relations very well. Namely, substituting our estimates for $Q, T_m, C_{\pm}$, and the system size and the filling factor used for the simulation into the above two relations, we obtain $C^{\max} = 22.9k_B$, and $\Delta T = 0.007T_m$. This maximal value of the specific heat is almost the same as we have observed by simulation and shown in Fig. 1. The width of the peak agrees with the transition region estimated from Figs. 1 and 2. As an additional evidence for the accuracy of the present simulation, we estimate the specific heat from the temperature dependence of the internal energy by $C = de/dT$. It is $25k_B$ in, and $17.5k_B$ off the transition region, consistent with those evaluated from the thermal fluctuation of the internal energy.

The difficulty in simulating the δ-function peak of the specific heat at the flux-lattice melting is twofold. First, as is seen in the inset of Fig. 1, almost no anomalous behavior in the specific heat can be detected during the overall cooling process in which 150×10^3 MC sweeps are used at each temperature. In the transition region the intrinsic fluctuations appear only after a long simulation time. As discussed above, our simulation time, more than 4×10^6 MC sweeps at each temperature, is sufficient to overcome this difficulty and to obtain the statistically correct results. The second hurdle for observing the δ-function peak in the specific heat at the melting point by computer simulation is the system size. As a matter of fact, we could not find any anomaly in the specific heat in a system of 20 *ab* planes with the same parameters discussed above, even though maximally 8×10^6 MC sweeps are monitored at several temperatures in the melting region. A small number of *ab* planes with a periodic boundary condition along the *c* axis for simulation enhances the ordering in this direction, and therefore has the effect of suppressing fluctuations. The boundary between this fluctuation-suppressed region and the well-fluctuating region looks to exist between 20 and 40 *ab* planes for the present value of anisotropy.

Corresponding to the big fluctuations of the internal energy within the temperature region of transition, we have observed the vibration of the structure function $S(\boldsymbol{q}_{ab}, z = 0)$ between rotational invariance and hexagonal symmetry. It is then clear that the higher/lower internal energy state is associated with the liquid/solid state. As in Fig. 3, the helicity modulus Y_c along the *c* axis is set up very sharply at T_m. This jump of Y_c is consistent with the fact that the phase transition is of first order. We have also investigated the number of nearest-neighboring vortices, sixfold and fourfold local orientational order parameters by Voronoi analysis. There are finite jumps in all these quantities at T_m. Simulations on heating processes have also been conducted. All the results indicate consistently that the system experiences a reversible, thermodynamic first-order phase transition between a triangular lattice of flux lines and a phase of decoupled 2D liquid of pancake vortices.

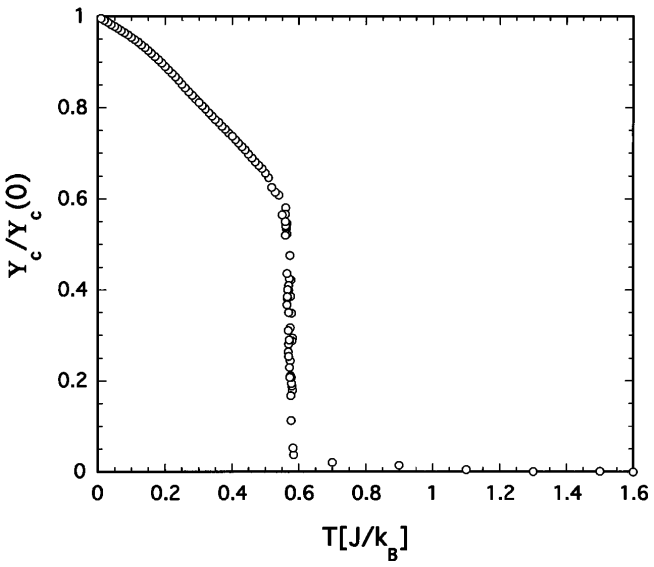

FIG. 3. Temperature dependence of the helicity modulus along the *c* axis.

The total number of pancake vortices and antivortices is counted as the temperature is swept. As in Fig. 4, it increases significantly at $T_v = 1.1J/k_B$, responsible for the broad cusp in the specific heat. More importantly, the total number of vortices and antivortices deviates from that in the ground state, even at $T = 0.4J/k_B$ fairly below T_m. The excited vortex-antivortex pairs are associated with the flux lines in the forms of overhang and knot. For higher temperatures, but still below T_m, isolated loops of vortices and antivortices are also excited beside the flux lines. At T_m, there are on average 0.6 thermally excited vortex-antivortex pairs per *ab* plane, increasing

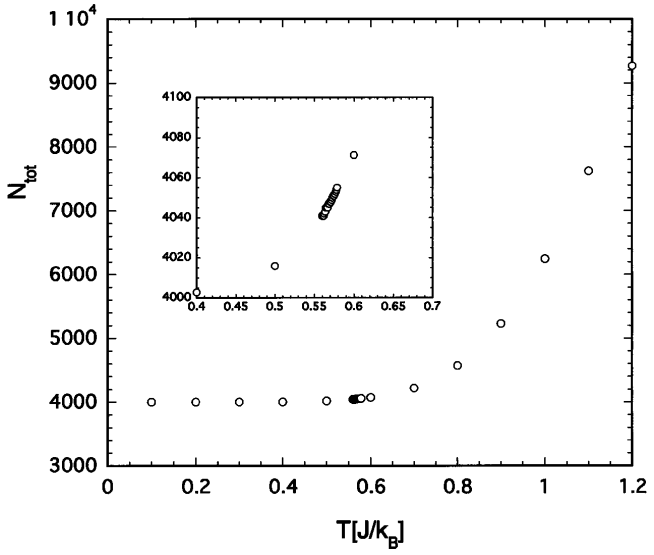

FIG. 4. Temperature dependence of total number of pancake vortices and antivortices. The inset is for a narrow temperature region around the melting point.

with a rate of 10 pair k_B/J per *ab* plane as seen in the inset of Fig. 4. The excitation of vortex-antivortex pairs in the various forms is characteristic of the present vortex system [20]. The perturbation of these excited flux loops on the system should be a key factor triggering the melting of the flux-line lattice, which was not taken into account in the boson analogy approach [2], and in the flux-line representation derived from the Ginzburg-Landau Lawrence-Doniach functional [10].

The temperature region of phase transition by the present simulation is about $\Delta T = 0.009T_m$, very close to the experimental observations [12,13]. It is, however, smaller than that in Ref. [9] by a factor of 4. With the differences in anisotropy, type of mesh grid, and system size between the two systems in mind, we notice that the results in Ref. [9] are obtained by a much quicker sweeping of temperature, 4×10^3 MC steps at each temperature.

We then turn to the discussion about the finite-size effect on the simulated results. In a system of the same parameters discussed above except for 20 *ab* planes, the latent heat is $0.01k_BT_m$ per flux line per layer. On the other hand, the latent heat for the system of 40 *ab* planes with 100 by 100 square meshes in each plane is almost the same as that of 40 *ab* planes of 50 by 50 meshes. Therefore, the latent heat associated with the phase degrees of freedom of the superconductivity order parameter is estimated as $0.07k_BT_m$ per flux line per layer. This value is still smaller than the experimental observation in the $Bi_2Sr_2CaCu_2O_8$ sample in Ref. [7], and the simulated result of $0.3k_BT_m$ in Ref. [9], but twice those in Refs. [10] and [11].

In order to see the effect of the anisotropy on the first-order melting transition in the vortex system, we have studied systems of various anisotropy constants with the filling factor fixed. For the system of $\gamma^2 = 100$ and 20 *ab* planes with 50 by 50 meshes in each plane, the melting transition is observed at $T_m = 0.176J/k_B$ associated with a latent heat $Q = 0.15k_BT_m$ [14]. A δ-function peak in the specific heat is observed, of $32.5k_B$ per flux line per layer at the melting point and $15k_B$ off the transition region. The jump in the helicity modulus Y_c at T_m is the same as that in Fig. 3 for $\gamma^2 = 10$, namely, $0.6Y_c(0)$, which suggests some universality. On the other hand, neither latent heat nor divergence of the specific heat can be observed for $\gamma^2 = 2$ by using simulation times similar to that in the present Letter and in systems up to 60 *ab* planes with 100 by 100 meshes in each plane. The strong interlayer coupling suppresses fluctuations along the *c* axis, and makes the first-order transition very weak if any. A systematic investigation about the effect of the anisotropy and of the number of *ab* planes on the first-order melting transition would be an interesting future problem.

The present simulations are performed on the Numerical Materials Simulator (SX-4) of National Research Institute for Metals (NRIM), Japan.

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