Possible Tricritical Point in Phase Diagrams of Interlayer Josephson-Vortex Systems in High-T_c Superconductors

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A critical value in the product of the anisotropy parameter and the magnetic field is observed in interlayer Josephson-vortex systems by extensive Monte Carlo simulations. Below (above) this critical value the thermodynamic phase transition between the normal and the superconducting states upon temperature sweeping is first (second) order. It is discussed that the origin of this tricritical point is the highly anisotropic layered structure of high-T_c superconductors.

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In the superconducting state, an external magnetic field applied parallel to the Cu-O plane of a high-T_c superconductor induces the so-called Josephson vortices. The center of a Josephson vortex enters into a block layer, the layer between two neighboring superconducting Cu-O layers, in order to save the condensation energy of superconductivity [1]. The thermodynamic phase transition and the lattice structure of interlayer Josephson vortices have been attracting considerable interest since the discovery of high-T_c superconductivity. Using a London theory, the structure of Josephson-vortex lattice was derived as the compressed hexagons of triangular lattice pointing along the c axis by Ivlev, Kopnin, and Pokrovsky [2]. The interlayer shear modulus was shown to be exponentially small, and the shear deformation of a rhombic lattice might arise through a second-order phase transition. However, at higher temperatures fluctuations are more important, and the London theory is generally inaccurate for discussions about phase transitions. Considerable effort has been made in order to clarify the thermodynamic phase transition in Josephson-vortex systems both experimentally [3–7] and theoretically [8–13] thereafter. Nevertheless, the understanding for the problem is still not satisfactory yet. Results obtained by different techniques even seem to be contrary to each other. The difficulty in approaching this problem is twofold. On the experimental side, a small deviation of the direction of the magnetic field from the Cu-O plane can lead to a strong influence from the c-axis component of the magnetic field on thermodynamic properties of the systems, since all the high-T_c superconductors are very anisotropic. On the theoretical side, one has to treat simultaneously anisotropic intervortex forces, the commensuration of the vortex alignment with the underlying layered structure, and thermal fluctuations.

In the present Letter, we report new results of extensive Monte Carlo (MC) simulations on the thermodynamic phase transition and the lattice structure of interlayer Josephson vortices. Our results suggest the existence of a tricritical point corresponding to a critical value of product of the anisotropy parameter and the magnetic field, such that below (above) this critical value the thermodynamic phase transition between the normal and the superconducting states is first (second) order upon temperature sweeping. A theoretical argument is also provided supporting this variation in the nature of the phase transition.

The model Hamiltonian used for the present simulations is the so-called 3D anisotropic, frustrated XY model defined on the simple cubic lattice [14–16]:

$$H = -J \sum_{\langle i,j\rangle \| x,y\,\mathrm{axis}} \cos(\varphi_i - \varphi_j) - \frac{J}{\gamma^2} \sum_{\langle i,j\rangle \| c\,\mathrm{axis}} \cos\!\left(\varphi_i - \varphi_j - \frac{2\pi}{\phi_0}\int_i^j A_c\, dr_c\right). \tag{1}$$

Here the y axis is along the external magnetic field, and $\mathbf{y} \perp \mathbf{c} \perp \mathbf{x}$. The unit length of the simple cubic lattice is the distance d between the neighboring Cu-O layers in a cuprate. Therefore, the discreteness in the c axis comes from the underlying layered structure of cuprates, while that in the Cu-O planes is introduced merely for computer simulations. The coupling constant is given by $J = \phi_0^2 d/16\pi^3\lambda_{ab}^2$. The anisotropy parameter is defined by $\gamma = \lambda_c/\lambda_{ab}$, and determines the ratio between the couplings in the Cu-O plane and along the c axis. In the present model, fluctuations in amplitudes of superconducting order parameters and in the magnetic induction are neglected.

Details of simulation technique are summarized as follows: The density of flux lines induced by the external magnetic field is $f = Bd^2/\phi_0 = 1/32$. A Landau gauge is adopted so that $A_c = -xB$. The system size is $L_x \times L_y \times L_c = 384d \times 200d \times 20d$, which is compatible with the filling factor $f = 1/32$. There are 240 Josephson flux lines in the ground state. Periodic boundary conditions are applied on phase variables in all directions. A typical simulation process is started from a random configuration of the phase variables at a high temperature, such as $T = 1.5J/k_B$. 30 000 and 90 000 MC sweeps are used for equilibration and statistics, respectively, at each temperature. The last configuration

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at a temperature is used as the initial configuration at a slightly lower temperature, where the temperature difference is $\Delta T = 0.1 J/k_B$. Around the transition temperature, more than 1×10^6 MC sweeps are adopted at each temperature, and meanwhile the cooling rate is reduced to $\Delta T = 0.005 J/k_B$. Vortices are identified by counting phase differences around plaquettes.

In order to compare our simulation results with existing experimental observations, we choose to study first a system of anisotropy parameter $\gamma = 8$, which is near to that of $YBa_2Cu_3O_{7-\delta}$. The magnetic field corresponding to $f = 1/32$ in our simulations is much stronger than those in experiments, and we come back to this point later. The temperature dependence of the helicity modulus (a quantity proportional to the superfluid density) along the magnetic field and the specific heat is depicted in Fig. 1. There is a clearly observable δ-function like peak in the specific heat at $T_m \simeq 0.96 J/k_B$, where the helicity modulus along the direction of magnetic field increase sharply from zero [17]. Shown in the same figure is the temperature dependence of the intensities of Bragg peaks in diffraction patterns at $\mathbf{q}_{xc}^{(1)} = (\pm\pi/8d, 0)$ and $\mathbf{q}_{xc}^{(2)} = (\pm\pi/16d, \pm\pi/d)$. Therefore, a thermodynamic first-order phase transition occurs at T_m, where the gauge symmetry and translation symmetry are broken simultaneously, corresponding to the realization of superconductivity and Josephson-vortex lattice, respectively.

The lattice structure of Josephson vortices at low temperatures is shown in Fig. 2. The unit cell is rhombic with short axis along the c direction and of a length of $2d$, and the long axis along the x direction and of a length of $32d$. Josephson vortices are distributed in every block layer for the present parameters $\gamma = 8$ and $f = 1/32$. This structure is the same as that predicted by Ivlev, Kopnin, and Pokrovsky [2].

The lattice structure in Fig. 2 is obviously the ground state for $\gamma \geq 8$ when the filling factor is fixed at $f = 1/32$. Therefore we can use it for investigations of thermodynamic properties for large anisotropy parameters by a heating process. The specific heats thus obtained are shown in Fig. 3 for anisotropy parameters $\gamma = 8$, 9, and 10 ($\Delta T = 0.001 J/k_B$ and over 7×10^6 MC sweeps for $\gamma = 10$ around the transition point). The δ-function peak in the curves for $\gamma = 8$ and 9, is suppressed for $\gamma = 10$ [13]. In Fig. 4 we display the temperature and anisotropy parameter dependence of the gauge invariant phase difference between nearest neighboring Cu-O layers $\langle \cos\phi_{n,n+1} \rangle$. There is a jump in $\langle \cos\phi_{n,n+1} \rangle$ for $\gamma = 8$ and 9, which is smeared out for $\gamma = 10$. As the jump in $\langle \cos\phi_{n,n+1} \rangle$ is nothing but the jump in the Josephson energy in units of J/γ^2, there exists a latent heat at the transition temperature for $\gamma = 8$ and 9, but not for $\gamma = 10$, consistent with the data for the specific heat. The value of the latent heat itself is too tiny, about γ^2 times smaller than that in $\langle \cos\phi_{n,n+1} \rangle$, to be detected directly. On the other hand, from a standard finite-size scaling theory for a first-order phase transition, the height of the δ-function like peak in the specific heat is proportional to the system size [16]. Therefore, by using a large system such as the one in our simulations, the δ-function like peak in the specific heat becomes observable as in Figs. 1 and 3 for the first-order phase transitions.

As the anisotropy parameter increases, the melting temperature decreases because the lattice becomes softer. This is observable in Fig. 4 where a detailed scale is used around the transition points. On the other hand, the melting temperature is bounded from below by the Kosterlitz-Thouless transition point of a 2D unfrustrated XY model, $T_{\mathrm{KT}} \simeq 0.89 J/k_B$. For large anisotropy parameters

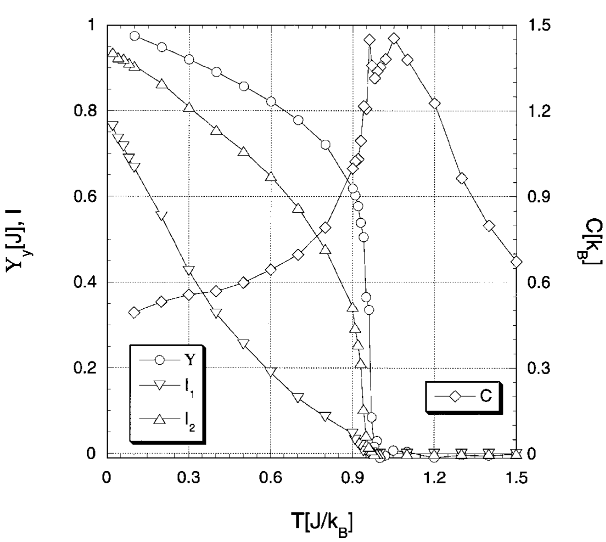

FIG. 1. Temperature dependence of the helicity modulus along the magnetic field, Υ_y, the specific heat, C, and the intensities I_1 and I_2 for the Bragg peaks at $\mathbf{q}_{xc}^{(1)} = (\pm\pi/8d, 0)$ and $\mathbf{q}_{xc}^{(2)} = (\pm\pi/16d, \pm\pi/d)$, respectively, for $\gamma = 8$ and $f = 1/32$.

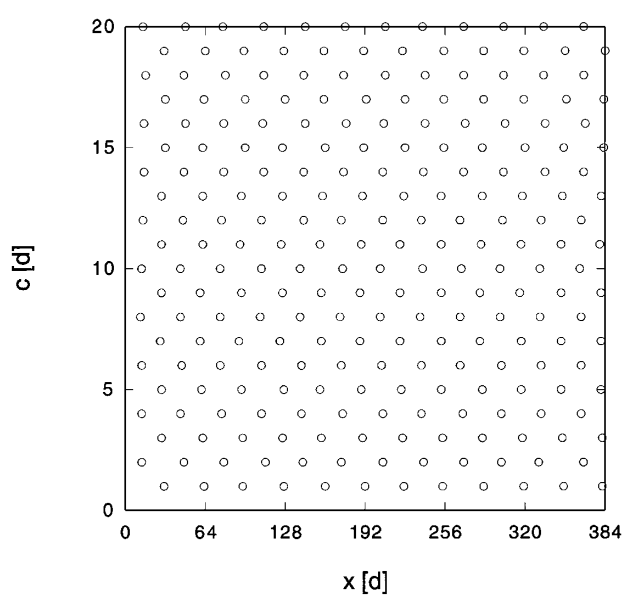

FIG. 2. Josephson vortex lattice for $\gamma = 8$ and $f = 1/32$ obtained by MC simulations of a cooling process from a random state at high temperatures.

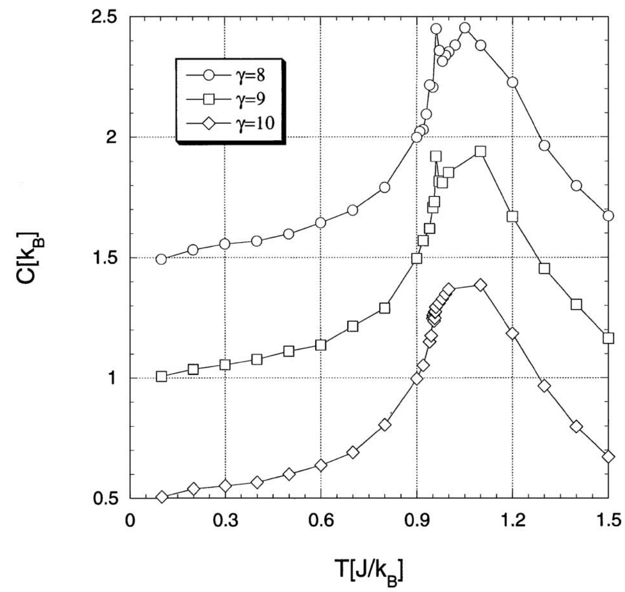

FIG. 3. Temperature dependence of the specific heat for $\gamma = 8$, 9, and 10 and $f = 1/32$. Data for $\gamma = 8$ and 9 are shifted by constants.

discussed here, the decrease of transition temperature is already very small.

We have performed simulations for anisotropy parameters $\gamma = 7, 6, \ldots,$ down to the isotropic case of $\gamma = 1$ [18] fixing the filling factor at $f = 1/32$, and observed first-order phase transitions in all the cases. Therefore, the present simulation results indicate that there is a critical anisotropy parameter in between $\gamma = 9$ and $\gamma = 10$ for $f = 1/32$, below (above) which the phase transition is first (second) order.

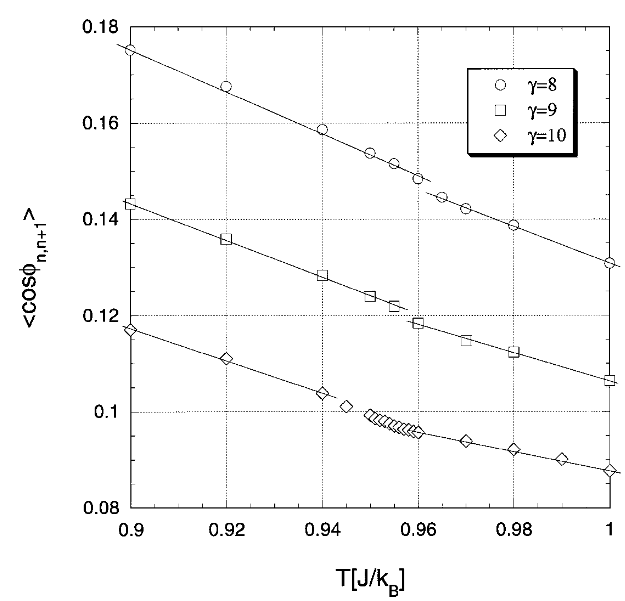

FIG. 4. Temperature dependence of the gauge invariant phase difference between nearest neighboring Cu-O layers for $\gamma = 8$, 9, and 10 and $f = 1/32$. The statistical errors estimated by the standard block averaging are smaller than the size of marks by an order. The lines are for guiding the eye.

Now we look for the reason for the suppression of the first-order phase transition when the anisotropy parameter is increased. Suppose a complete commensuration is achieved between the alignment of the Josephson vortices shown in Fig. 2 and the underlying layered structure of high-T_c cuprates. In other words, the Cu-O layers do not influence the lattice structure of Josephson vortices, but merely fix its position in the c direction. In such a case, the Josephson-vortex lattice should be rescaled into equilateral triangular lattice using the anisotropy parameter γ, and we have the relation

$$(2d)^2 = d^2 + (d/2f\gamma)^2$$

as in Fig. 5, which results in

$$f\gamma = \frac{1}{2\sqrt{3}}. \tag{2}$$

Now we increase the anisotropy parameter from that determined by the above relation when the filling factor f is fixed. Since the repulsive force between Josephson vortices in the c direction is reduced, the Josephson-vortex lattice would be compressed in this direction. However, this reconstruction of Josephson-vortex lattice is forbidden by the underlying layered structure of the high-T_c superconductor. Therefore, the above relation provides a criterion for onset of the intrinsic pinning effect of the layered structure on the formation of Josephson-vortex lattice. For anisotropy parameters larger than that evaluated by the above relation, the lattice structure of Josephson vortices is determined by both the intervortex repulsions and the pinning force of the underlying layered structure. The thermodynamic phase transition associated with the formation of the Josephson-vortex lattice can be different in the two regions divided by the above relation.

Numerically, the critical anisotropy parameter for the filling factor $f = 1/32$ is evaluated as $\gamma = 16/\sqrt{3} \simeq 9.24$ by the relation (2). This estimate coincides well with our simulation results, in which first-order phase transitions are observed for $\gamma \leq 9$ but not for $\gamma \geq 10$. We have also performed simulations for the filling factor $f = 1/25$, and found the variation of phase transition from first to second order around $\gamma = 8$. This observation is consistent with the relation (2), since for $f = 1/25$ one has the critical anisotropy parameter $\gamma \simeq 7.22$. For $f = 1/36$, we have observed a first-order phase transition even for $\gamma = 10$, consistent with the critical value $\gamma \simeq 10.39$. Therefore, our simulation results indicate

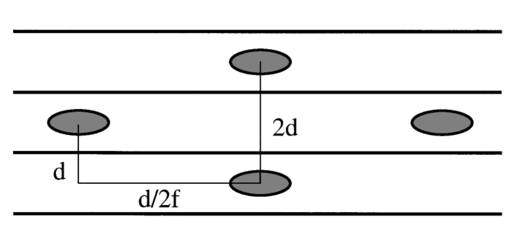

FIG. 5. Real-space unit cell of the Josephson-vortex lattice in a layered, highly anisotropic superconductor under a strong magnetic field.

clearly that the critical anisotropy parameter increases with decreasing filling factor, or magnetic field. Quantitatively, the simple relation (2) seems to give a reasonable estimate on the critical anisotropy parameter.

The same variation in nature of the phase transition should be observed when the anisotropy parameter is fixed while the filling factor, or the strength of the magnetic field, is tuned. The relation (2) can be rewritten as

$$B = \frac{\phi_0}{2\sqrt{3}\,\gamma d^2}\,. \tag{3}$$

For $YBa_2Cu_3O_{7-\delta}$ with $\gamma \simeq 8$ and $d = 12$ Å, the critical magnetic field is estimated as $B \simeq 50$ T. Therefore the phase transition in the Josephson-vortex systems in $YBa_2Cu_3O_{7-\delta}$ is first order for magnetic fields available experimentally now, according to our present study. For $Bi_2Sr_2CaCu_2O_{8+y}$ with $\gamma \simeq 150$ and $d = 15$ Å, the critical magnetic field is evaluated as $B \simeq 1.7$ T, which can be checked experimentally. We notice the similarity between our critical magnetic induction (3) and the first transition field derived by Bulaevskii and Clem [19].

The phase transition observed in the present study occurs in between the transition temperatures of the 2D XY model for a single superconducting layer T_{KT} and of the 3D XY model for infinite superconducting layers coupled by the same anisotropy parameter (e.g., $T \simeq 1.1J/k_B$ for $\gamma = 10$). While the thermodynamic phase transition is second order without frustrations for both 2D and 3D, it is first order for small anisotropy parameters and second order for large anisotropy parameters when an external magnetic field is applied parallel to the layer.

In highly anisotropic systems, many pairs of Josephson vortices and antivortices are excited thermally since the energy cost $\sim J/\gamma^2$ is small. In these systems, Josephson flux lines induced by the magnetic field collide with each other in the same block layers frequently even at low temperatures, and jump into neighboring block layers via thermally excited pancake vortices when temperature is elevated (but still below the transition point). There is no sharp decrease in the number of collisions and entanglements at the transition point, in contrast with the first-order Abrikosov lattice melting when the magnetic field is along the c axis [16,20].

A possible second-order shear deformation, or decoupling, of Josephson vortex lattice has been discussed theoretically by Efetov [21], Ivlev, Kopnin, and Pokrovsky [2], Blatter, Ivlev, and Rhyner [8], and Horovitz [11]. For anisotropy parameters larger than the critical value in (2), weakening in the c-axis correlations and the shear modulus by thermal fluctuations should be predominant in the melting of 3D Josephson vortex lattice. According to Balents and Nelson [12], a smectic phase (see also [8]) can freeze either into a crystal free of interstitials (normal solid) via a first-order transition, or into a crystal of interstitials (supersolid [22]) via a second-order transition. The phenomena observed in the present study are consistent with these theoretical studies. It should be mentioned that there are also theoretical works against the decoupling scenario mentioned above [9,10]. While there seems to be some consensus for the low magnetic field limit where there are no flux-line collisions in the same block layers [9], the high magnetic field limit, the main target of the present study, has not been settled theoretically with satisfaction. Therefore, further studies for the present problem are highly anticipated.

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