Flux-line entanglement as the mechanism of melting transition in high-temperature superconductors in a magnetic field

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Abstract

The mechanism of the flux-line-lattice (FLL) melting in anisotropic high-$T_c$ superconductors in $\mathbf{B} \parallel \hat{c}$ is clarified by Monte Carlo simulations of the 3D frustrated XY model. The percentage of entangled flux lines abruptly changes at the melting temperature $T_m$, while no sharp change can be found in the number and size distribution of vortex loops around $T_m$. Therefore, the origin of this melting transition is the entanglement of flux lines. Scaling behaviors of physical quantities are consistent with the above mechanism of the FLL melting. The Lindemann number is also evaluated without any phenomenological arguments.

74.60.Ge, 74.25.Dw, 74.20.De, 74.25.Bt
Nature of the mixed phase in type-II superconductors has been studied for many years, and much attention has been paid to this field since the discovery of high-$T_c$ superconductors (HTSC) because of short correlation lengths and large anisotropy. In HTSC in a magnetic field along the $c$ axis, the flux-line lattice (FLL) melts at much lower temperatures or in much weaker fields [1] than those predicted by the Abrikosov mean-field theory, where the superconducting phase transition is of second order regardless of details of models. The FLL melting in HTSC was first theoretically analyzed by Nelson and Seung [2] on the basis of the mapping to a two-dimensional Boson model, and they pointed out that the Lindemann criterion might be valid in this FLL melting because of large fluctuations in HTSC owing to large anisotropy and high transition temperatures. Similar theoretical analysis was also made by Houghton et al. [3] independently. Earlier experiments of “the FLL melting in HTSC” as reviewed in Ref. 1 were found to be explained better by the vortex-glass transition [4] rather than by the FLL melting transition. In clean systems, the “true” FLL melting was confirmed afterwards by experiments [3-10] and computer simulations [11-18], and the first-order FLL melting transition in a magnetic field has now been established in extremely type-II superconductors such as HTSC.

On the other hand, the mechanism of the FLL melting has not yet been well understood. Nelson argued [2,19] that the entanglement of flux lines is related to this transition, but this picture has only been confirmed numerically [17] within the two-dimensional Boson model. Thermal excitations of vortex loops [20,21] are not included in this picture and some authors claimed [21,22] that the FLL melting is characterized by the breakdown of flux-line description by the proliferation of large vortex loops, but the latter picture began to be modified recently [23]. In order to clarify the mechanism of the FLL melting numerically, the first-order phase transition should be identified by measuring thermodynamic quantities, and the behavior of flux lines induced by an external magnetic field and thermally excited vortex loops should be observed microscopically in the vicinity of the melting temperature.

In this article, the three-dimensional anisotropic, frustrated XY model is analyzed with the Monte Carlo method from the above point of view. Our main results are as follows: First,
the mechanism of the first-order FLL melting transition is exclusively the entanglement of flux lines. The percentage of entangled flux lines sharply changes at the melting temperature \( T_m \), while the number and the size distribution of loop excitations has a smooth temperature dependence around \( T_m \). Second, scaling properties around the melting temperature are clarified. As a consequence of the entanglement mechanism of the FLL melting, \( T_m \) is scaled by the inverse of the system size along the \( c \) axis. Third, the Lindemann number takes nearly a constant value \( c_L \approx 0.30 \) regardless of the anisotropy constant, and thus the use of the Lindemann criterion is justified for the determination of the melting line in a phase diagram.

As the model of the anisotropic, extremely type-II HTSC in a magnetic field along the \( c \) axis, we consider the three-dimensional anisotropic, frustrated XY model \([24,15]\) described by the following Hamiltonian,

\[
\mathcal{H} = -J \sum_{i,j \in ab \text{ plane}} \cos (\varphi_i - \varphi_j - A_{ij}) - \frac{J}{\Gamma^2} \sum_{i,j \parallel c \text{ axis}} \cos (\varphi_i - \varphi_j) ,
\]

\[
A_{ij} = \frac{2\pi}{\phi_0} \int_i^j \mathbf{A}^{(2)} \cdot d\mathbf{r}^{(2)} .
\]  

Here \( \varphi_i \) denotes the phase of the superconducting order parameter, \( \phi_0 \) stands for the flux quantum, and the anisotropy is represented by the parameter \( 1/\Gamma^2 \). Note that this model neglects fluctuations of the gauge field and the amplitude of the superconducting order parameter. The periodic boundary condition (PBC) is applied on the phase variable \( \varphi_i \) in all the directions in order to refrain from finite-size effects from free boundaries. We mainly investigate the case with the averaged number of fluxes per plaquette \( f = 1/25, \Gamma = 2 \) and 5. In these parameters, effects of the introduction of a square lattice in the \( ab \) plane is negligible [13]. Each phase variable takes a value \(-\pi < \varphi_i \leq \pi\), and the summation of the phase difference around a plaquette is given by

\[
\sum_{i,j \in \square} (\varphi_i - \varphi_j - A_{ij}) = 2\pi (n - f) , \quad n = 1, 0, -1 .
\]
When the integer $n$ takes 1 or $-1$, the plaquette is defined to have a vortex or an antivortex, respectively. The nearest-neighbor vortices are connected with one another to form vortex lines, which do not have end points inside the system. When a vortex line returns to itself inside the system, it is called as a vortex loop, and such a loop does not exist in the ground state. When a vortex line runs from one boundary to another along the direction of the external field, it is called as a flux line. The flux lines are straight in the ground state, and they begin to fluctuate at finite temperatures. A flux line is defined as entangled if it does not terminate at the same transverse position in the top and bottom boundaries in the PBC. The flux lines which wind with each other and return to the initial transverse positions inside the system are not included in this definition. Such excitations are negligible in the vicinity of the melting temperature, because they have higher energies.

The helicity modulus along the $c$ axis [15,25] is observed for the determination of the melting temperature. This quantity is proportional to the superfluid density, and therefore nonvanishing only in the superconducting phase. The numbers of vortex loops $N_{\text{loop}}$ and entangled flux lines $N_{\text{ent}}$ are counted. The distribution of sizes is also measured for Josephson loops, which are dominant below and slightly above the melting temperature. The transverse distance $w$ of a flux line between the top and bottom $ab$ planes is measured, and its averaged value over all the flux lines is denoted by $L_{\text{diff}}$. The fluctuation of a flux line is measured by the deviation $u$ from the projection of its mass center in each $ab$ plane, and averaged over all the flux lines and the $ab$ planes. The Lindemann number $c_L$ is defined by

$$c_L \equiv \lim_{T \to T_m-0} \langle u^2 \rangle^{1/2}/a_0,$$

where $a_0$ stands for the lattice constant of the triangular FLL, $a_0 = (2/\sqrt{3})^{1/2}/f^{1/2}$.

Monte Carlo simulations are performed on the basis of the Metropolis algorithm. Most results reported in this article are for systems with $L_x = L_y = 50$ and $L_c = 80$. Then, the number of total flux lines is $N_{\text{flux}} = 100$ in the present simulations with $f = 1/25$. In order to check the size dependence, we also simulate systems with $(L_x, L_c) = (50, 20), (50, 40), (50, 54), (50, 160), (25, 80)$ and $(100, 20)$. In addition, in order to check the flux-density
dependence, the \((L_x, L_c) = (50, 80)\) and \((100, 80)\) systems are calculated for \(f = 1/50\) and \(1/100\), respectively. Simulations are started from temperatures more than ten times higher than \(T_m\) and the system is gradually cooled down. Typical Monte Carlo steps (MCS) are \(1.0 \times 10^5\) and \(1.5 \times 10^5\) for equilibration (E-MCS) and measurement (M-MCS) at each temperature, respectively. Since the correlation time becomes longer in the vicinity of the melting point, E-MCS and M-MCS are taken as \(3.5 \times 10^5\) and \(8.0 \times 10^5\), respectively, and the cooling rate is reduced to \(\Delta T = 1.0 \times 10^{-3} J/k_B\). Moreover, for the precise determination of \(T_m\) and \(c_L\), supercooling behavior is reduced very carefully by using up to \(1.0 \times 10^7\) MCS at each temperature. The helicity modulus is measured at each MCS, and the numbers of vortex loops and entangled flux lines are measured once per 100 MCS.

The temperature dependence of the helicity modulus along the \(c\) axis, \(\Upsilon_c\), is displayed in Fig. 1 for \(\Gamma = 2\) and \(5\) with \(f = 1/25\). This quantity sharply drops from a finite value to zero at the melting temperature, \(T_m = 0.810 J/k_B\) for \(\Gamma = 2\) and \(T_m = 0.3445 J/k_B\) for \(\Gamma = 5\), which indicates the thermodynamic first-order phase transition \[13\]. The temperature dependence of the ratio of entangled flux lines to total flux lines, \(N_{\text{ent}}/N_{\text{flux}}\), is also displayed in Fig. 1. It shows a sharp jump at \(T_m\) for each of the anisotropy. Similar behavior is also observed for \(\Gamma = 5\) with \(f = 1/50\) and \(1/100\). The number of vortex loops per flux line per \(ab\) plane, \(N_{\text{loop}}/(N_{\text{flux}} L_c)\), is shown in Fig. 2 for \(\Gamma = 2\) and \(5\) with \(f = 1/25\). The temperature dependence of this quantity is not as drastic as that of the ratio of entangled flux lines. The size distribution of Josephson loops is also measured for \(\Gamma = 5\) with \(f = 1/25\), \(1/50\) and \(1/100\), and no drastic change is observed in this distribution around \(T_m\). The numbers of vortex loops are not of the same order for the different anisotropy constants at the melting temperatures. That is, the number of vortex loops at \(T_m\) for \(\Gamma = 5\) corresponds to that of \(T \approx 0.6 J/k_B\) for \(\Gamma = 2\), and this temperature is much lower than the melting point for \(\Gamma = 2\), \(T_m \approx 0.810 J/k_B\). These facts clearly indicate that the origin of the FLL melting is the entanglement of flux lines, at least up to \(f = 1/100\).

Then, we show the results for the finite-size-scaling behavior. The averaged end-to-end transverse distance of flux lines, \(L_{\text{diff}}\), is normalized by the lattice constant of FLL, \(a_0\), and
plotted versus temperature for $L_c = 40, 80$ and $160$ in Fig. 3. The size dependence of this quantity can be described by the random-walk-type scaling,

$$L_{\text{diff}}(L_c) \sim \text{const.} \times L_c^{1/2},$$

for a certain temperature range above $T_m$, as displayed in the inset of Fig. 3. Therefore, it is clear that the vortices form flux lines even above $T_m$. The inset of Fig. 3 shows that the data for $L_c = 160$ and $80$ deviate from the scaling (5) at $T \approx 0.4 J/k_B$ and $0.5 J/k_B$, respectively. These two temperatures correspond to the same transverse distance $L_{\text{diff}} \approx 2.7a_0$, as can be read from the two curves for $L_c = 160$ and $80$ in the main body of Fig. 3. This fact suggests that the random-walk behavior is restricted within a transverse diffusion distance approximately $2.7a_0$ independently of temperature even in bulk systems. Beyond this length scale, reconnection between flux lines occurs frequently, and the random-walk property is suppressed. Since the transverse distance between the bottom and top $ab$ planes in each entangled flux line cannot be smaller than $a_0$, the total number of entangled flux lines abruptly decreases at $T_m$ when temperature is gradually reduced. As a consequence of the scaling given in Eq. (5), the temperature characterized by $L_{\text{diff}} \approx a_0$, namely $T_m$, depends on $L_c$, as will be discussed below.

Simulations for systems with $(L_x, L_c) = (100, 20)$ and $(25, 80)$ are also performed, and the results coincide with those with $(L_x, L_c) = (50, 20)$ and $(50, 80)$, respectively. This is quite natural because the melting transition is characterized by the entanglement of flux lines along the $c$ axis, and the leading term of size dependence is only related to $L_c$. Finite-size effects in the $ab$ plane are indirect on thermodynamic quantities. As displayed in Fig. 4, our data exhibit the following finite-size scaling,

$$\delta T_m(L_c) \equiv T_m(L_c) - T_m(L_c = \infty) \sim \text{const.} \times L_c^{-1},$$

with $T_m(L_c = \infty) = 0.3354 \pm 0.0007$ for $\Gamma = 5$. This size dependence means that the FLL melting has a one-dimensional character, because the scaling form of the transition point in first-order phase transitions [26] is generally given by $\delta T(L) \sim \text{const.} \times L^{-D}$ with the spatial dimension $D$. This one-dimensional character is consistent with the entanglement picture.
Finally, we turn to see the temperature dependence of the fluctuation of flux lines and evaluate the Lindemann number. The quantity \( \langle u^2 \rangle^{1/2}/a_0 \) shows a sharp jump at \( T_m \) for \( \Gamma = 2 \) and 5 with \( f = 1/25 \) (Fig. 5). From the definition of the Lindemann number in Eq. (4), we have \( c_L \approx 0.30 \) for both the anisotropy constants. This result suggests that the Lindemann number does not depend on details of models, as assumed in previous studies \[3,27\]. The Lindemann number was evaluated as \( c_L \approx 0.18 \) by part of the present authors \[15\] by fitting the simulated melting line with a formula derived by Blatter et al. \[27\] based on the London theory. We believe that the present direct evaluation of \( c_L \) is more reliable.

In conclusion, the three-dimensional anisotropic, frustrated XY model has been analyzed with Monte Carlo simulations. The melting temperature \( T_m \) has been estimated as the point at which the helicity modulus along the \( c \) axis vanishes. The percentage of entangled flux lines shows a sharp jump at \( T_m \), while the number and size distribution of vortex loops do not show such drastic change at \( T_m \). This fact clearly indicates that the origin of the FLL melting in a magnetic field along the \( c \) axis is the entanglement of flux lines. The consistency of this picture with the size dependence of various quantities has been confirmed. Especially, the melting temperature is scaled by the system size along the \( c \) axis as \( T_m(L_c) - T_m(L_c = \infty) \propto L_c^{-1} \). The averaged deviation of flux lines from their mass centers also shows a sharp jump at \( T_m \) as a consequence of the entanglement of flux lines. The Lindemann number takes a constant value \( c_L \approx 0.30 \) regardless of the anisotropy. This numerical result justifies the use of the Lindemann criterion for characterizing the FLL melting in HTSC.

Numerical calculations were performed on the Numerical Materials Simulator (NEC SX-4) at National Research Institute for Metals, Japan.
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FIGURES

FIG. 1. Helicity modulus along the $c$ axis (squares) and the ratio of entangled flux lines to total flux lines (circles) versus temperature for $\Gamma = 2$ and 5 with $f = 1/25$.

FIG. 2. Normalized number of vortex loops (diamonds) versus temperature for $\Gamma = 2$ and 5 with $f = 1/25$. The ratio of entangled flux lines (circles) is also plotted for comparison.

FIG. 3. Normalized end-to-end transverse distance versus temperature for $L_c = 40$ (triangles), 80 (squares) and 160 (circles) for $\Gamma = 5$ with $f = 1/25$. Scaling plot of the same data according to Eq. (3) is shown in the inset with the same symbols.

FIG. 4. $L_c$ dependence of the melting temperature for $\Gamma = 5$ with $f = 1/25$. $T_m(L_c = \infty)$ is estimated by the least-squares fitting of the data with $L_c = 40$, 54, 80 and 160.

FIG. 5. Fluctuation of flux lines (triangles) versus temperature for $\Gamma = 2$ and 5 with $f = 1/25$. The helicity modulus along the $c$ axis (squares) is also plotted for comparison.
Fig. 1: Y. Nonomura, X. Hu, and M. Tachiki

\[ \frac{N_{\text{ent}}}{N_{\text{flux}}} \]

\[ \Upsilon \]

\[ \Gamma = 5 \]

\[ \Gamma = 2 \]
Fig. 2: Y. Nonomura, X. Hu, and M. Tachiki

\[ \frac{N}{N_{\text{flux}}} \]

\[ T \ [J/k_B] \]

\[ \Gamma = 5 \]

\[ \Gamma = 2 \]
Fig. 3: Y. Nonomura, X. Hu, and M. Tachiki
Fig. 4: Y. Nonomura, X. Hu, and M. Tachiki

\[ T_m(L_c) \ [J/k_B] = \frac{40}{5480} \]

\[ L_c = 40 \]
Fig. 5: Y. Nonomura, X. Hu, and M. Tachiki

\[ \frac{1}{2}a_0 \]

\[ \Gamma = 5 \]

\[ \Gamma = 2 \]

\[ \langle u^2 \rangle \]

\[ T \text{ [J}/k_B \text{]} \]

\[ \chi \text{ [J}/\Gamma^2 \text{]} \]