Energy landscape and shear modulus of interlayer Josephson vortex systems

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The ground state of interlayer Josephson vortex systems is investigated on the basis of a simplified Lawrence-Doniach model in which spatial dependence of the gauge field and the amplitude of superconducting order parameter is not taken into account. Energy landscape is drawn with respect to the in-plane field, the period of insulating layers including Josephson vortices, and the shift from the aligned vortex lattice. The energy landscape has a multi-valley structure and ground-state configurations correspond to bifurcation points of the valleys. In the high-field region, the shear modulus becomes independent of field and its anisotropy dependence is given by $\xi_0 \propto \gamma^{-4}$.

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Introduction. Although interlayer Josephson vortex systems in cuprate high-$T_c$ superconductors have been intensively studied, their phase diagrams have not been established yet even in the ground state. For high in-plane fields, Josephson vortices penetrate into every insulating layer, and the ground state is given by an elongated triangular lattice aligned along the superconducting layers. As the field decreases, such an aligned vortex lattice becomes unstable owing to the shear instability \[1\], and the shearing angle of vortex lattices increases continuously \[2\]. As the field further decreases, the rotated vortex lattices have been considered to be the ground state \[3\]-\[5\]. The studies mentioned above (except for Ref. \[2\]) were based on the London model, and effects of the layered structure were included only as geometrical constraint.

This layered structure can be directly taken into account by using the Lawrence-Doniach model. Bulaevskii and Clem \[6\] first introduced this model in order to investigate interlayer Josephson vortex systems for high fields. Ichioda \[7\] calculated the energies of the aligned vortex lattices including vacant insulating layers. Stability of some rotated-vortex-lattice configurations was first pointed out by Hu and Tachiki \[8\] in the frustrated XY model, and Ikeda \[9\] reported similar results in the Lawrence-Doniach model within the lowest-Landau-level approximation. Quite recently, Koshelev \[10\] systemically evaluated the ground-state phase diagram (including the sheared and rotated vortex lattices) based on a simplified Lawrence-Doniach model, in which spatial dependence of the gauge field and the amplitude of superconducting order parameter is neglected.

The ground state of this simplified model is completely given by the in-plane field $h$, the period $N$ between insulating layers including Josephson vortices, and the shift $\Delta$ of the vortex lattice from the aligned one. In Ref. \[10\], $\Delta$ is fixed at fractional numbers which correspond to the rigid rotated vortex lattices. In the present study, we draw the full energy landscape for the first time, and find that the energy landscape has a multi-valley structure, and that the ground state for low fields shows systematic deviation from the rigid rotated vortex lattices. We also find that field dependence of the shear modulus is quite different from previous estimation based on the London theory \[1\] in the high-field region.

Formulation. When spatial dependence of the gauge field and the amplitude of superconducting order parameter is neglected, the Lawrence-Doniach free energy functional is expressed by the phase component $\phi_n$ as

$$ F\{\phi_n(r)\} = \frac{\phi_0^2}{16\pi^2\lambda_{ab}} \int d^3r \left\{ \frac{1}{2} \left( \nabla \phi_n \right)^2 + \frac{1}{(\gamma d)^2} \left[ 1 - \cos \left( \phi_{n+1} - \phi_n - \frac{2\pi}{\phi_0} dB_x y \right) \right] \right\}, \quad (1) $$

where $\phi_0$ is the flux quantum, $\lambda_{ab}$ is the penetration depth in the $ab$ plane, $\gamma$ is the anisotropy parameter, and $d$ is the interlayer distance. The distance $a$ between Josephson vortices in the same layer and the period $N$ (see Fig. \[4\]a) are related with the in-plane field along the $x$ axis $B_x$ as $a = adN B_x$. Since the ground state should be uniform along the field direction, the free energy functional per unit volume is expressed as

$$ f\{\phi_n(y)\} = \frac{\phi_0 B_x}{16\pi^2\gamma\lambda_{ab}} u\{\phi_n(y)\}, \quad (2) $$

$$ u\{\phi_n(y)\} = \frac{1}{\pi} \sum_{n=1}^N \int_0^\bar{a} d\bar{y} \left\{ \frac{1}{2} \left( \frac{d\phi_n}{d\bar{y}} \right)^2 + 1 - \cos \left( \phi_{n+1} - \phi_n - \gamma d \bar{y} \right) \right\}, \quad (3) $$

where the following normalized quantities are introduced:

$$ \bar{y} = y / \gamma d, \quad \bar{a} = a / \gamma d, \quad h = 2\pi / \phi_0 \gamma d^2 B_x. \quad (4) $$

By minimizing the free energy functional \[4\] with respect to $\phi_n$, we have

$$ \frac{d^2\phi_n}{d\bar{y}^2} \sin(\phi_{n+1} - \phi_n - h\bar{y}) - \sin(\phi_n - \phi_{n-1} - h\bar{y}) = 0. \quad (5) $$

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Hereafter the energy function will be a ground state. As will be revealed below, it is not the case. However, it is not trivial that any rigid rotated vortex lattice can respond to the ground state with $\Delta = 0$. As the field decreases to $h \approx 1.33$, a sheared vortex lattice with finite $\Delta$ becomes the ground state. The shearing angle increases continuously as the field decreases, and such continuous field dependence cannot be represented by the rotated-lattice index. Although the ground state changes to the $(1,0,2)$ aligned lattice at $h \approx 0.99$, the sheared vortex lattice state is still the lowest energy state in the $N = 1$ subspace, and it becomes the ground state again at $h \approx 0.80$. The field dependence of $\Delta$ is quite small around $h \approx 0.7$, which corresponds to the simplest rigid rotated vortex lattice labeled with $(2,1,1)$ and characterized by $\Delta_{\text{rigid}} = 1/7$. Since each ground-state configuration is separated in the energy landscape, these configurations can be labeled by the rotated-lattice indices $(n, m, N)$, even though the parameter $\Delta$ may deviate from the fractional values $\Delta_{\text{rigid}}$ corresponding to the rigid rotated vortex lattices. Typical ground-state configurations are shown in Fig. 3 where all the rotated-lattice configurations of the rotated lattices are connected with the corresponding rotated-lattice indices $(n, m, N)$.

Results. The energy landscape of eq. $3$ is shown in Fig. 2(a), where $-g$ is taken instead of $g$ because the valley structure is hard to visualize. The ridges in this figure correspond to the valleys in the actual energy landscape. Energy functions for various $N$'s are drawn in the same figure, and different colors correspond to different $N$'s. The ground state denoted by dark solid lines often jumps between two different values of $\Delta$ as drawn in dashed lines. The pale solid lines represent the lowest-energy state (but not the ground state) for each $N$. As will be revealed below, it is not the case. Hereafter the energy function $g \equiv u + \frac{1}{2} \log h - 1.432$ is used instead of $u$, following Ref. 2.

FIG. 1: Definition of (a) the unit cell of a vortex lattice and (b) the labeling of a rigid rotated vortex lattice (here $(n, m, N) = (2, 1, 1)$). Scaled coordinate $\bar{y} \equiv y/(\gamma d)$ is used.

FIG. 2: (a) Energy function $-g$ versus the shift from the aligned vortex lattice $\Delta$ and the normalized in-plane field $h$. Each color stands for the energy function for each $N$ [color online]. The dark [blue] solid lines denote the ground state, and the pale [green] solid lines stand for the lowest-energy state (not the ground state) for each $N$. The rotated-lattice index $(n, m, N)$ for each ground state configuration is displayed. (b) Top view of the above figure [gif figure appended].

FIG. 3: Ground-state configurations for various in-plane fields $h$ with the corresponding rotated-lattice indices $(n, m, N)$.
FIG. 5: Deviation of $\Delta$ from that of the rigid rotated vortex lattice ($\Delta_{\text{rigid}}$) versus normalized field $h$ in the $N=1$ subspace, and it takes minimum at $h = h_{\text{min}}$ (dashed lines). The fields corresponding to the rigid rotated vortex lattices ($h_{\text{rigid}}$) are marked by arrows. In the inset, the deviation of $\Delta$ ($|\Delta_{\text{rigid}} - \Delta|$) at $h = h_{\text{min}}$ is plotted versus that of $h$ ($h_{\text{rigid}} - h_{\text{min}}$) together with the rotated-lattice indices.

each other by lines of local energy minima, and such ground-state configurations correspond to the bifurcation points of local minima. Similar bifurcating structure is expected for $N \geq 2$ at much low fields.

From precise analyses of $\Delta$, we find that the rigid rotated vortex lattices expected from the London theory can never be the ground state. The deviation of $\Delta$ from the values corresponding to the rigid rotated lattices $\Delta_{\text{rigid}}$ is plotted versus $h$ in Fig. 5. The inequality $\Delta_{\text{rigid}} - \Delta > 0$ holds for $n \geq m/2$, and vice versa. The field corresponding to the rigid rotated vortex lattice $h_{\text{rigid}}$ is marked by arrows in the same figure, and $|\Delta_{\text{rigid}} - \Delta|$ takes minima at $h = h_{\text{min}}$ (dashed lines). The deviation decreases as $h$ decreases, and seems to vanish in the $h \to 0$ limit. In the inset, the deviation of $\Delta$ at $h = h_{\text{min}}$ is plotted versus that of the field, $h_{\text{rigid}} - h_{\text{min}}$.

Finally, we observe the shear modulus $c_{66}$ defined by

$$c_{66} = \frac{d^2 N^2}{a^2} \frac{\partial^2 f}{\partial \Delta^2} = \frac{\phi_0^2}{(8\pi \lambda_{ab})^2} \frac{\tilde{c}_{66}}{2 \pi \gamma d^2}, \quad \tilde{c}_{66} = N^4 h^3 \frac{\partial^2 u}{\partial \Delta^2},$$

where $\phi_0 = adNB_x$ and eq. (6) are substituted and parameter dependence on $h$, $N$ and $\Delta$ is only included in the scaled shear modulus $\tilde{c}_{66}$. Field dependence of $\tilde{c}_{66}$ is displayed in Fig. 6 and this quantity converges to a constant value $C \approx 39.4$ in the $h \to \infty$ limit. Namely, the shear modulus becomes field independent for high fields,

$$c_{66} \approx \frac{\phi_0^2}{(8\pi \lambda_{ab})^2} \frac{C}{2 \pi \gamma d^2} = \frac{C \phi_0}{2 \pi \gamma d^2}.$$  

This behavior is in sharp contrast to the exponentially vanishing $c_{66}$ of the London model [2], and is also different from that of the elastic theory, $c_{66} = [\phi_0 B_x (8\pi \lambda_{ab})^2]^{-3} [11]$. Introducing a “saturated field” $\tilde{B}$ defined below, eq. (7) can be expressed similarly to the elastic theory as

$$c_{66} \approx \tilde{\phi}_0 \tilde{B}_x \frac{\gamma^{-3}}{(8\pi \lambda_{ab})^2} = \frac{C \phi_0}{2 \pi \gamma d^2}.$$  

and $\tilde{\phi} \equiv \phi_0 / (d \tilde{B}^2) = (2 \pi / C) \gamma d \approx 1.57 \gamma d$ corresponds to the effective core size of a Josephson vortex. As the field decreases, $\tilde{c}_{66}$ vanishes at the shear instability field of the aligned vortex lattice [11], increases again together with the increase of the shearing angle, and jumps when the rotated-lattice index changes.

Discussion. In the London model, only the rigid vortex lattices can be the ground state by definition. Therefore, the sheared vortex lattices are specific to the models including the layered structure explicitly such as the present model. We find that the rotated vortex lattices with $\Delta_{\text{rigid}}$ cannot be the ground state even at the fields corresponding to the rigid rotated lattices, which is another nontrivial effects of the layered structure.

It would be interesting to investigate how the above description is altered by various kinds of fluctuations. Hu et al. [12] studied the phase diagram of interlayer
Josephson vortex systems in the vicinity of the melting temperature using the density functional theory. They found the vortex smectic state around the \((n,m,N) = (1,0,2)\) state, while no sheared vortex lattice states were observed between the \((1,1,1)\) and \((1,0,2)\) states. This finding may suggest that the sheared vortex lattice state is affected very much by thermal fluctuations. Study on temperature dependence of the deviation from the rigid rotated lattices would be an interesting future problem.

The screening effect is also studied in the present framework, and we find that the rotated vortex lattices are almost unchanged, while the sheared vortex lattices or the \(N \geq 2\) aligned vortex lattices are affected very much. These facts suggest that the rotated vortex lattice structure is robust against the screening effect. Details of this study will be reported elsewhere [13].

**Summary.** Ground state of interlayer Josephson vortex systems is investigated on the basis of the simplified Lawrence-Doniach model, in which spatial dependence of the gauge field and the amplitude of superconducting order parameter is neglected. The free energy functional is minimized in the unit cell with one Josephson vortex. We draw the energy landscape with respect to the in-plane field, the period of insulating layers including Josephson vortices, and the shift from the aligned lattice.

As the in-plane field decreases, the aligned vortex lattice along superconducting layers changes to the sheared vortex lattice and then to the rotated vortex lattices, in which the shift from the aligned lattice is approximately given by that of the corresponding rigid rotated lattices. Systematic deviation from the rigid configurations is clarified for the first time. Ground-state configurations of the rotated lattices are connected with each other by local minima in the energy landscape to form a multi-valley structure, and such ground-state configurations correspond to the bifurcation points of the valleys.

In the high-field region, the shear modulus becomes independent of field and its anisotropy dependence is given by \(c_{66} \propto \gamma^{-4}\), quite different from the London theory in which \(c_{66}\) decays exponentially with field. This quantity vanishes at the onset of the sheared vortex lattice, and jumps when the rotated-lattice index changes.

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[1] B. I. Ivlev et al., J. Low Temp. Phys. 80, 187 (1990).
[2] A. E. Koshelev, cond-mat/0602341.
[3] L. J. Campbell et al., Phys. Rev. B 38, 2439 (1988).
[4] L. S. Levitov, Phys. Rev. Lett. 66, 224 (1991).
[5] M. F. Laguna et al., Phys. Rev. B 62, 6692 (2000).
[6] L. Bulaevskii and J. R. Clem, Phys. Rev. B 44, 10234 (1991).
[7] M. Ichioka, Phys. Rev. B 51, 9423 (1995).
[8] X. Hu and M. Tachiki, Phys. Rev. Lett. 80, 4044 (1998).
[9] R. Ikeda, J. Phys. Soc. Jpn. 71, 587 (2002).
[10] A. E. Koshelev, Private Communication.
[11] V. G. Kogan and L. J. Campbell, Phys. Rev. Lett. 62, 1552 (1989).
[12] X. Hu et al., Phys. Rev. B 72, 174503 (2005).
[13] Y. Nonomura and X. Hu, in preparation.
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