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LETTER TO THE EDITOR

Modulated and commensurate vortex structures in layered superconductors

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Abstract. The metastable states of a vortex lattice in a layered superconductor in the presence of a magnetic field parallel to the layers are shown to form structures that are modulated or commensurate to the layers. A number of commensurate structures with equivalent energies are found. The incommensurate structures can rotate abruptly when the magnetic field is varied. The structure factor and the London free energy of the incommensurate structures are calculated.

We consider vortex lattices in layered superconductors in magnetic fields parallel to the layers. Such structures have been shown to be metastable in a wide range of temperatures due to strong periodic pinning [1]. In previous work [1] the vortex structures were implicitly assumed to be commensurate with the layers. Moreover, only the most symmetric orientation of the vortex lattice with respect to the layers was considered. In this work we generalize the theory [1] include incommensurate lattices and non-symmetric orientations of commensurate lattices.

We assume the following experimental procedure. One should apply the external magnetic field parallel to the layers at a temperature higher than T_c. Then the temperature is decreased until at some $T^* < T_c$ the periodic pinning becomes very strong. The vortex structure that appears by this procedure is metastable, i.e. the vortices cannot change their coordinates perpendicular to the layers. We search for a minimum energy of the vortex system under these conditions.

If the external field is chosen in such a way that the vortex lattice becomes commensurate, this metastable state coincides with the stable state. Otherwise the vortices should be shifted in order to occupy positions defined by the layers. Displacements should be minimal to minimize the interaction energy of vortices.

In this case the London free energy assumes the form:

$$F = \frac{1}{8\pi}\int \mathrm{d}V\left[H^2 + \lambda_c^2\left(\frac{\partial H}{\partial x}\right)^2 + \lambda_{ab}^2\left(\frac{\partial H}{\partial z}\right)^2\right] \tag{1}$$

and after rescaling $x \to x\lambda_c$, $z \to z\lambda_{ab}$ we get:

$$F = \frac{1}{8\pi}\int \mathrm{d}V\left[H^2 + \left(\frac{\partial H}{\partial x}\right)^2 + \left(\frac{\partial H}{\partial z}\right)^2\right]. \tag{2}$$

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The energy is obviously invariant with respect to rotations in the x–z plane. So, without layers there exists a continuous set of symmetric hexagonal lattices with the same energy. In non-layered uniaxial superconductors an infinitesimal tilt of the external magnetic field lifts this degeneracy [2], and the most symmetrically oriented structure with triangle edges parallel to the x-axis, has minimal energy. We call such a configuration the symmetric configuration. However, layered superconductors have been shown to screen the component of the external field normal to the layers, until it reaches some critical value H_z [3]. So, it is reasonable to consider strictly parallel orientation of the magnetic induction B to the layers and therefore various positions of the vortex lattice.

A periodic lattice can be made commensurate to the layered structure with period s if there exist reciprocal lattice vectors with the modulus equal to $2\pi/s$. So, we can define $s_b = (0, 2\pi/s)$. For commensurability this vector must coincide with one of the reciprocal lattice vectors G, say G_1. Orientation of this vector in the reciprocal lattice gives the orientation of the lattice with respect to the layers. For a symmetric hexagonal lattice with $a = (2\phi_0/\sqrt{3}B)^{1/2}$ the vectors of reciprocal lattice are defined by two integers n_1 and n_2:

$$G = 2\pi(n_1/a(2n_2 - n_1)/a\sqrt{3}) \tag{3}$$

and the commensurability condition is

$$n_1^2 - n_1n_2 + n_2^2 = 3a^2/4s^2 = \alpha^2. \tag{4}$$

Here B is the space average of the local magnetic field H. Equation (4) defines particular values of the magnetic field

$$B_{n_1n_2} = (\phi_0/d^2)1/(n_1^2 - n_1n_2 + n_2^2)$$

corresponding to commensurate vortex lattices. One should expect the critical current to have maxima at these values of magnetic field, as was observed in the experiments by Martinoli and coworkers [4] with periodically corrugated aluminium films.

Equation (4) possesses an obvious reflection symmetry: if (n_1, n_2) is a solution then $(n_1, n_1 - n_2)$ is also a solution. These solutions correspond to the orientations of G_1 transformed into one another by a reflection transformation of the reciprocal lattice, and give configurations with the basis of triangle rotated by β and $-\beta$ with respect to the x-axis, where $\sin\beta = n_1 s/a$. Other symmetry transformations of the reciprocal lattice (and (4)) give rise to vectors G_1 that are turned to the angle $n\pi/6$ with respect to two aforementioned vectors. So, in general (when these two vectors do not coincide and there are no independent solutions) there exist two different non-symmetric positions of the lattice. We show the arrangements of the reciprocal lattice in figure 1(a). Sometimes the number of these positions is larger. The symmetric configuration appears when α is an integer $\alpha = m$. Special values of m, for which a non-symmetric configuration is possible in addition to the symmetric one, are defined by two integers p and q, so that $m = p^2 + q^2 - pq$, $n_1 = p(2q - p)$ and $n_2 = q(2p - q)$ and $q/2 < p < 2q$. The first non-trivial solution, corresponding to $p = 2, q = 3, m = 7$, is shown in figure 1(b); the next one corresponding to $p = 3, q = 4, m = 13$ is shown in figure 1(c). If, for example, (4) can be satisfied for $\alpha = m_1$ and $\alpha = m_2$, where m_1 and m_2 are integers then for $\alpha = m_1m_2$ it

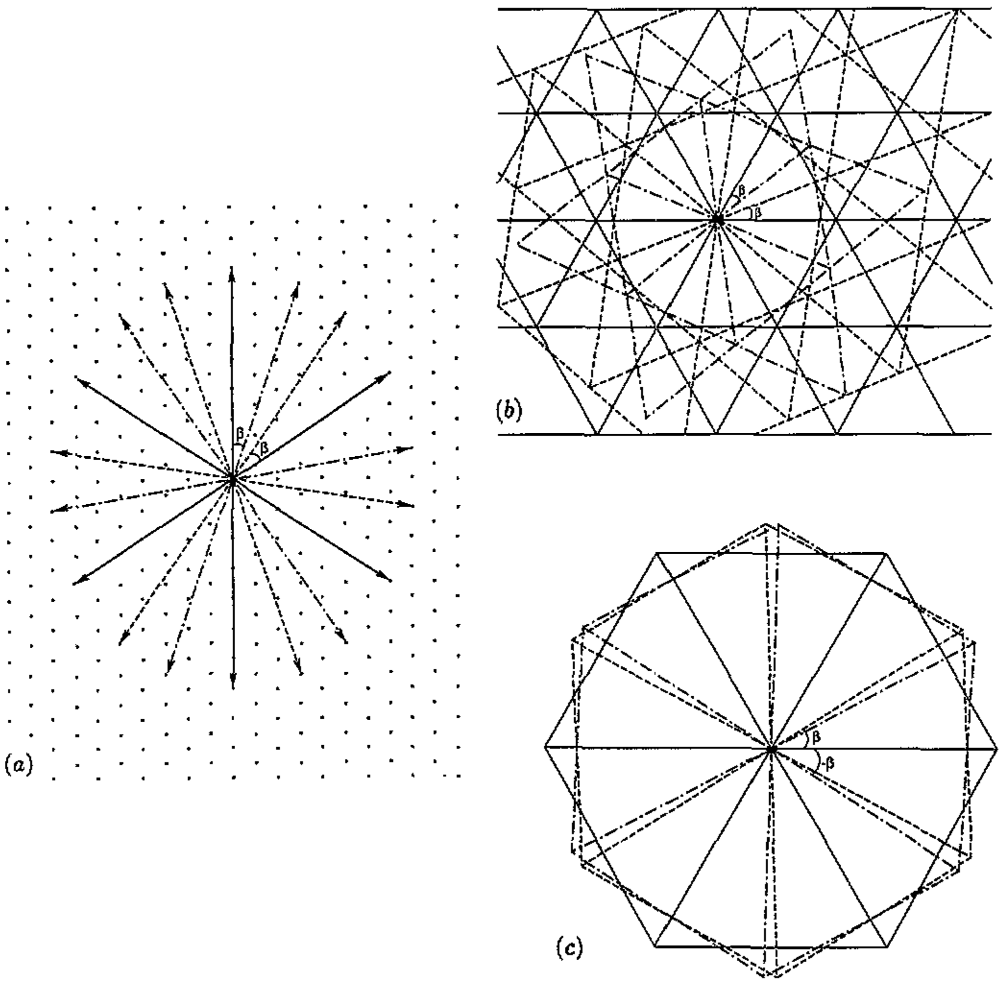

Figure 1. (*a*) The reciprocal lattice of a vortex structure (points) and different orientation of reciprocal lattice vectors of layers (arrows) for $\alpha = 7$. Three inequivalent orientations are shown by solid, dashed and point-dashed lines, respectively. (*b*) The elementary cells of three inequivalent structures for $\alpha = 7$. According to the notation of (4) they correspond to $n_1 = 7$, $n_2 = 0$; $n_1 = 8$, $n_2 = 5$ and $n_1 = 8$, $n_2 = 3$, respectively. (*c*) The same for $\alpha = 13$ and $n_1 = 13$, $n_2 = 0$; $n_1 = 15$, $n_2 = 7$ and $n_1 = 15$, $n_2 = 8$.

can also be satisfied, and for this value of α there are at least five different solutions including four non-symmetric ones.

For incommensurate phases we assume that their orientations will be defined by the reciprocal lattice vector closest by modulus to $|s_b| = 2\pi/s$. This vector is a discontinuous function of s at fixed B; therefore, a set of orientational phase transitions can be found. To find these transitions one should first increase the temperature at fixed magnetic field until $T > T^*$ and then decrease it again. Let us consider an incommensurate configuration close to some symmetric commensurate configuration. If the vortices are displaced to the nearest interlayer spaces, the z

component of the displacement is:

$$u_z(z) = \left[\tfrac{1}{2} - \{z/s + \tfrac{1}{2}\}\right] s \tag{5}$$

where braces denote the fractional part of a number. We believe that there are no displacements u parallel to the layers. At least, for $a \gg 1$ the expansion to second order in u of the pairwise vortex interaction shows that such displacements are unfavourable.

The magnetic field H can be found from the generalized London equation:

$$H - \frac{\partial^2 H}{\partial x^2} - \frac{\partial^2 H}{\partial z^2} = \phi_0 \sum_{m,n} \delta[\boldsymbol{r} - \boldsymbol{r}_{m,n} - \boldsymbol{u}(\boldsymbol{r}_{m,n})]. \tag{6}$$

Here $\boldsymbol{u}(\boldsymbol{r}_{m,n})$ is the displacement of the site $\boldsymbol{r}_{m,n}$ with z component given by (5) and zero x component. After the Fourier transformation we find:

$$H_q(1+q^2) = B \sum_G \int \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\boldsymbol{u}(\boldsymbol{r}) - \mathrm{i}\boldsymbol{r}(\boldsymbol{q}-\boldsymbol{G})}\, \mathrm{d}^2\boldsymbol{r}. \tag{7}$$

As a result we find:

$$H_q(1+q^2) = (2\pi)^2 B \sum_{G,n} \delta(\boldsymbol{q} - \boldsymbol{G} - n\boldsymbol{s}_b) \sin \frac{\boldsymbol{G}\boldsymbol{s}_a}{2} \Big/ \left(\frac{\boldsymbol{G}\boldsymbol{s}_a}{2}\right) \tag{8}$$

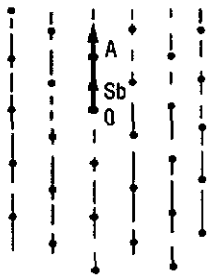

Figure 2. A set of parallel lines filled by reciprocal vectors of the vortex lattice when it is incommensurate to the layers.

where $\boldsymbol{s}_a = (0, s)$. Consider two cases. If $n\boldsymbol{s}_b$ does not belong to the reciprocal lattice for any integer n then the set of vectors $\boldsymbol{G} + n\boldsymbol{s}_b$ fills, densely, a set of parallel lines in the plane (see figure 2) and the representation of a vector in such a form is unique. The vortices form a double-periodic lattice. This is a typical modulated structure or a quasicrystal. The Fourier components of the field at $\boldsymbol{q} = \boldsymbol{G} + n\boldsymbol{s}_b$ are

$$H_q = \phi_0 N \sin(\boldsymbol{G}\boldsymbol{s}_a/2)/(\boldsymbol{G}\boldsymbol{s}_a/2) 1/(1+q^2) \tag{9}$$

where N is the total number of vortices. If $m\boldsymbol{s}_b$ belongs to the reciprocal lattice at some integer m then H_q is also non-zero for $\boldsymbol{q} = \boldsymbol{G} + n\boldsymbol{s}_b$ and

$$\begin{aligned} H_q = \phi_0 N &\left[\sin(\boldsymbol{G}\boldsymbol{s}_a/2)/m \sin(\boldsymbol{G}\boldsymbol{s}_a/2m)\right]\left[(\cos(\boldsymbol{G}\boldsymbol{s}_a/4m))^2\right. \\ &\left. - (-1)^m (\sin(\boldsymbol{G}\boldsymbol{s}_a/4m)^2\right] 1/(1+q^2). \end{aligned} \tag{10}$$

Note that in this case, α of the RHS of (4) is rational and m is its denominator. The vortex structure is commensurate and its period along the z axis is $m\alpha s$. As α converges to an irrational number, $m \to \infty$ and the period also tends to infinity. The structure becomes double-periodic and its Fourier components converge to the RHS of (9). At $m = 1$, the RHS of (10) gives the ordinary Fourier components. We can unify (9) and (10) by writing:

$$H_q = \phi_0 N f(Gs_a/2, \alpha) 1/(1+q^2). \tag{11}$$

Then the London free energy per unit volume becomes:

$$F = \frac{B^2}{8\pi} \sum_{G,n} \frac{f^2(Gs_a/2,\alpha)}{1+(G+ns_b)^2}. \tag{12}$$

The summation in (12) proceeds over all G which are inequivalent by modulus ms_b.

The scattering amplitude f_q of polarized neutrons in the Born approximation is proportional to H_q, namely $f_q = \mu_n(\boldsymbol{s}\boldsymbol{H}_q)$, where μ_n is the neutron magneton and $\boldsymbol{s}$ is the neutron polarization vector [5].

The function f is continuous at every irrational point and discontinuous at every rational point. We can show that the free energy is a continuous function of magnetic field. However, we have no definite predictions on the behaviour of the magnetization and the magnetic susceptibility. One should keep in mind that at each measurement, heating to a temperature $T > T^*$ and subsequent cooling is assumed. Otherwise the vortices move only along the x-axis and all thermodynamic variables are continuous with the exception of special singular points [1].

In conclusion, we emphasize that in experimental observations the modulated structure will exhibit a series of satellites in addition to main reflections of the triangular lattice, with orientational phase transitions and with singular behaviour of magnetization versus magnetic field. We also expect the appearance of complex commensurate structures in strong magnetic fields ($B \geqslant 5$ T), when the period of the regular lattice becomes less than interplane distance.

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