Reconstruction of Vortex Lattices at Low Inductions

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The nonlocal elasticity and the normal modes of an unpinned flux-line lattice (FLL) in a uniaxially anisotropic superconductor are considered in the low induction regime $b=B/B_{c2}\ll 1$ at oblique angles θ between $\mathbf{B}$ and the $\hat{\mathbf{c}}$ axis. A novel feature of anisotropic superconductors is *strongly dispersive shear moduli* when $\theta>0$. Thus, the normal modes of the FLL may become soft away from the zone center, signaling a $\mathbf{k}\neq 0$ *structural* instability of the distorted hexagonal FLL. Vortex structures of a novel type are thus possible in anisotropic superconductors.

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Since the discovery, by Bitter pattern decoration experiments, of apparently thermally decorrelated flux lines in the high-T_c superconductors $YBa_2Cu_3O_7$ and $Bi_{2.2}Sr_2Ca_{0.8}Cu_2O_8$ even at quite low temperatures [1], a central and theoretically interesting issue has been whether or not a flux-line lattice (FLL) may melt [2]. Several groups have tackled this problem [2–4]. It is well established that the FLL in anisotropic extreme type-II superconductors is intrinsically soft due to the long range of vortex-vortex interactions [3–5].

More recent decoration experiments [6] at low T revealed fascinating, exotic vortex arrangements (vortex chains embedded in a vortex lattice) when the applied field was oriented at oblique angles with respect to the crystal $\hat{\mathbf{c}}$ axes. This observation was not expected from earlier work on anisotropic superconductors, which for very small B predicted vortex chains without a FLL in between [7]. This observation raises the interesting question of whether a "simple" FLL may be unstable due to the anisotropic character [8,9] of the long-range vortex-vortex interaction.

In this paper, we address the issue of the stability of a class of hexagonal FLLs so far believed to represent the (unpinned) vortex *ground state* in an anisotropic type-II superconductor. We will demonstrate the *instability* of these proposed ground states at sufficiently low inductions in very anisotropic superconductors at large angles $\theta=\angle(\mathbf{B},\hat{\mathbf{c}})$, provided that the nonlocal character of the anisotropic vortex-vortex interaction is accounted for properly. Throughout this paper we therefore use nonlocal, anisotropic London theory, which is valid when $b=B/B_{c2}<0.25$ and $\kappa\gg 1$. Here, κ is the Ginzburg-Landau parameter and B_{c2} is the upper critical field. The region of very low reduced induction $b=B/B_{c2}\ll 1$ is of particular importance in high-T_c superconductors due to their large values of B_{c2}.

The total energy of an arbitrarily distorted system of unpinned vortices may be derived from the anisotropic London equations [10],

$$F=\frac{\Phi_0^2}{8\pi}\sum_{i,j}\int\int dr_j^\alpha dr_i^\beta V_{\alpha\beta}(\mathbf{r}_i-\mathbf{r}_j)\,. \tag{1}$$

Here, $V_{\alpha\beta}(\mathbf{r})$ is the nonlocal interaction potential between any two infinitesimal vortex segments in the system, $(\alpha,\beta)\in(x,y,z)$, and $\Phi_0=2.07\times10^{-7}$ G cm^2 is the flux quantum. Expanding this energy to second order in the displacements $\mathbf{u}(\mathbf{k})$ of the flux lines from their equilibrium positions in the ground state, we find the excess energy due to these displacements,

$$\Delta F=\frac{1}{2}\int\frac{d^3k}{(2\pi)^3}u_\alpha(-\mathbf{k})\Phi_{\alpha\beta}(\mathbf{k})u_\beta(\mathbf{k})\,, \tag{2}$$

where now $(\alpha,\beta)\in(x,y)$ (flux lines along z). The elastic matrix $\Phi_{\alpha\beta}(\mathbf{k})$ is given by [9]

$$\Phi_{\alpha\beta}(\mathbf{k})=\frac{B^2}{4\pi}\sum_{\mathbf{Q}}[f_{\alpha\beta}(\mathbf{k}+\mathbf{Q})-f_{\alpha\beta}(\mathbf{Q})]\,, \tag{3}$$

$$f_{\alpha\beta}(\mathbf{k})=k_z^2\tilde{V}_{\alpha\beta}(\mathbf{k})+k_\alpha k_\beta\tilde{V}_{zz}(\mathbf{k})-2k_zk_\beta\tilde{V}_{z\alpha}(\mathbf{k})\,. \tag{4}$$

The sum runs over the reciprocal-lattice vectors of the FLL in its appropriate ground state. The last term of the tensor $f_{\alpha\beta}(\mathbf{k})$ in Eq. (3), first considered by Sardella [9], vanishes for all $\mathbf{k}$ when $\mathbf{B}\parallel\hat{\mathbf{c}}$; then only one shear modulus of the FLL exists. At oblique angles, however, this term gives rise to an additional anisotropy in the shear stiffness if one goes beyond the local limit $\mathbf{k}\to 0$ discussed in Ref. [11], but does not influence the tilt moduli of Ref. [9].

The above expressions are quite general and make no reference to specific values of the reciprocal-lattice vectors, which should only belong to an equilibrium FLL. For uniaxially anisotropic London superconductors the Fourier-transformed interaction tensor $\tilde{V}_{\alpha\beta}(\mathbf{k})$ is given by [9,10]

$$\tilde{V}_{\alpha\beta}(\mathbf{k})=\frac{\exp(-2g)}{1+\Lambda_1k^2}\left[\delta_{\alpha\beta}-\frac{\Lambda_2q_\alpha q_\beta}{1+\Lambda_1k^2+\Lambda_2q^2}\right], \tag{5}$$

where $\Lambda_1=\lambda_{ab}^2$, $\Lambda_2=\lambda_c^2-\lambda_{ab}^2$, $\mathbf{q}=\mathbf{k}\times\hat{\mathbf{c}}$, λ_{ab} and λ_c are the magnetic penetration depths parallel and perpendicular to the basal a-b plane, respectively, and ξ_{ab} and ξ_c are the corresponding coherence lengths. One has $\lambda_c/\lambda_{ab}=\xi_{ab}/\xi_c=(M_z/M)^{1/2}$, where M_z/M is the mass anisotropy. The cutoff factor in Eq. (4) contains $g=\xi_{ab}^2q^2+\xi_c^2(\mathbf{k}\cdot\hat{\mathbf{c}})^2$, which means that the lattice sum is elliptically cut off at Q vectors of the order of the core size. In the isotropic case this cutoff was shown to reproduce the results of the Ginzburg-Landau theory [5]. For uniaxial anisotropy and not too small $b \gg 1/2\kappa^2$, the equilibrium FLL predicted by [11] has reciprocal-lattice vectors $\mathbf{Q}_{mn} = n\mathbf{Q}_1 + m\mathbf{Q}_2$, where $\mathbf{Q}_1 = 2\pi(\sqrt{3}\hat{\mathbf{y}} + \gamma^2\hat{\mathbf{x}})/\sqrt{3}a\gamma$, $\mathbf{Q}_2 = 4\pi\gamma\hat{\mathbf{x}}/\sqrt{3}a$, $a^2 = 2\Phi_0/\sqrt{3}B$, and $\gamma^4 = \cos^2\theta + M/M_z \times \sin^2\theta$. Here, θ is the angle of the induction $\mathbf{B}$ away from the $\hat{\mathbf{c}}$ axis of the uniaxial superconductor.

The various elastic moduli of the FLL, derivable from Eqs. (2) and (3), are central quantities in the statistical mechanics and dynamics of the FLL and hence deserve special attention. In particular, the tilt modulus $c_{44}(\mathbf{k})$ and shear moduli are crucial in theories of thermal fluctuations [2-4] and collective pinning of the FLL [12]. The bulk modulus $c_{11}(\mathbf{k})$ normally plays a less prominent role, entering the theory of collective flux creep at $T > 0$ [13] but not the collective pinning theory at $T = 0$ [12]: The thermally activated "jumping volume" depends on the bulk modulus, whereas the static "correlated volume" does not.

A detailed discussion of dispersive tilt moduli of the FLL in anisotropic superconductors has been given elsewhere [8,9]. Their main term originates from the overlap of the vortex fields, has Lorentzian dispersion, and is *positive* at all $\mathbf{k}$. Hence, nonuniform tilt waves do not induce a structural instability of the FLL. This is a general result, independent of the specific FLL *structure*.

Usually, it is assumed that the *shear modulus* of the FLL is essentially *dispersionless* in the dominating part of the Brillouin zone (BZ). Given the importance of the dispersion of the tilt moduli and the large contribution of k values close to the BZ boundary to the thermal fluctuations of the FLL [3], it is fair to check to what extent the equally important shear moduli really are dispersionless. These moduli depend on the structure of the FLL, and yield important information about its *stability*. For an isotropic superconductor, the shear modulus and its *geometric dispersion* were calculated numerically in Ref. [5] from the elastic matrix $\Phi_{\alpha\beta}(\mathbf{k})$, using the definitions $c_{66}(k) = \Phi_{xx}(0,k,0)/k^2$ and $c_{66}(k) = \Phi_{yy}(k,0,0)/k^2$, which are obvious from comparison of Eq. (3) with the expression for the elastic matrix in continuum theory,

$$\Phi_{\alpha\beta}(\mathbf{k}) = [c_{11}(\mathbf{k}) - c_{66}(\mathbf{k})]k_\alpha k_\beta + \delta_{\alpha\beta}[c_{66}(\mathbf{k})(k_x^2 + k_y^2) + c_{44}(\mathbf{k})k_z^2]\,. \tag{6}$$

In isotropic superconductors, the assumption $c_{66}(k) \approx c_{66}(0)$ is indeed quite reasonable for $k < 0.3k_{\mathrm{BZ}}$, where k_{BZ} is the radius of the circularized Brillouin zone, $k_{\mathrm{BZ}}^2 = 4B\pi/\Phi_0$. For the case $\theta = 0$ this finding remains true even in uniaxially anisotropic superconductors. For $\theta \neq 0$ there are two shear moduli, $c_{66}^{(e)}$ and $c_{66}^{(h)}$ (easy and hard) [11]. These two moduli may be extracted from the elastic matrix $\Phi_{\alpha\beta}(\mathbf{k})$ as

$$c_{66}^{(e)}(k) = \frac{\Phi_{xx}(0,k,0)}{k^2}, \quad c_{66}^{(h)}(k) = \frac{\Phi_{yy}(k,0,0)}{k^2}\,. \tag{7}$$

This may again be seen by comparing Eq. (3) with the Fourier transform of the general elastic energy of a FLL of rigid vortices (since $k_z = 0$ for pure shear) when also a torsion term describing the coupling of the FLL to the underlying uniaxial crystal is included [11].

The shear moduli $c_{66}^{(e)}(\theta)$ and $c_{66}^{(h)}(\theta)$ as computed from Eq. (6) at the zone center $\mathbf{k} = 0$ agree with the results of Ref. [11], where a different cutoff scheme to truncate the lattice sum at the vortex core was used. The results for $M_z/M = 2$, 5, and 25, $b = 0.0001$, and $\kappa = 50$ are shown in the inset of Fig. 1. For $\mathbf{k} = 0$, both $c_{66}^{(e)}(\mathbf{k})$ and $c_{66}^{(h)}(\mathbf{k})$ remain positive for all $\theta \in [0, \pi/2]$. The small value of $c_{66}^{(e)}(\theta)$ for $\mathbf{k} = 0$ and $\theta \approx \pi/2$ is responsible for the existence of a whole class of *nearly degenerate* hexagonal vortex structures with one vortex per unit cell [14,15].

We next consider the shear moduli at *finite* values of $\mathbf{k}$. A surprising feature that we find is the *pronounced dispersion* of $c_{66}^{(e)}(\mathbf{k})$ when $\theta \neq 0$. This is shown in Fig. 1 for parameters $\kappa = 50$, $b = B/B_{c2} = 0.0001$, and $M_z/M = 3600$. Note that in this case $c_{66}^{(e)}(\mathbf{k})$ changes sign at $k_y\gamma/Q_{10} \approx 0.62$, when $\theta = 3\pi/8$. Using the same parameters as above, but $M_z/M = 25$, no change of sign in $c_{66}^{(e)}(\mathbf{k})$ is seen at any angle. The hard modulus $c_{66}^{(h)}(\mathbf{k})$ is only weakly dispersive and remains positive down to the lowest fields ($b = 0.00001$) that we have considered.

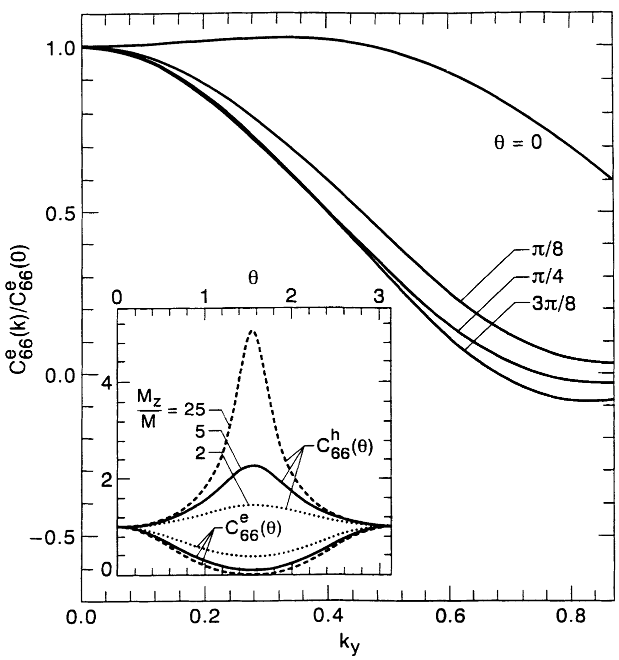

FIG. 1. Dispersion of $c_{66}^{(e)}(\mathbf{k})/c_{66}^{(e)}(\mathbf{k}=0)$ at $\theta = 0$, $\pi/8$, $\pi/4$, and $3\pi/8$, with $\kappa = 50$, $M_z/M = 3600$, and $b = B/B_{c2} = 0.0001$ (rigid flux lines, $k_z = 0$). Note change of sign in $c_{66}^{(e)}(k)$ for $k_y\gamma/Q_{10} \approx 0.62$ at $\theta = 3\pi/8$, signaling a structural instability of the FLL. Inset: $c_{66}^{(e)}(\theta)$ and $c_{66}^{(h)}(\theta)$ at $\mathbf{k} = 0$, normalized to their values at $\theta = 0$, for three mass anisotropies $M_z/M = 2$, 5, and 25, at $b = 0.0001$ and $\kappa = 50$.

The reciprocal-lattice vectors Q_{mn} which we use in calculating the matrix $\Phi_{\alpha\beta}(\mathbf{k})$ and structure-dependent elastic moduli, given below Eq. (4), represent the *global minimum* of a class of variational solutions obtained by *uniform* deformation of trial lattice structures [14,15]. This is the reason why the structure-dependent elastic moduli at $\mathbf{k}=0$ are found to be positive at all angles. As we have seen, $c_{66}^{(e)}(\mathbf{k})$ may become negative at finite $\mathbf{k}$ when θ and M_z/M are sufficiently large and b is sufficiently small. This finding hints at a *structural instability with respect to periodic shear* of the FLL defined by the above-given Q_{mn}.

The origin of the strong and weak dispersion of $c_{66}^{(e)}(\mathbf{k})$ and $c_{66}^{(h)}(\mathbf{k})$, respectively, when $\theta\neq 0$, may be understood qualitatively by considering rigid vortices ($k_z=0$) in the limit of small but finite $\mathbf{k}$. Using Eq. (6), we obtain to leading order in $\mathbf{k}$,

$$c_{66}^{(e)}(\mathbf{k})-c_{66}^{(e)}(0)\sim k^2\sum_{\mathbf{Q}}Q_x^2\frac{\partial^4\tilde{V}_{zz}(\mathbf{Q})}{\partial Q_y^4}, \tag{8}$$

and similarly for $c_{66}^{(h)}(\mathbf{k})-c_{66}^{(h)}(0)$ with x,y indices interchanged. The anisotropic part of $\tilde{V}_{zz}(\mathbf{Q})\sim-(\lambda_c^2-\lambda_{ab}^2)Q_x^2\sin^2\theta/(1+\lambda_{ab}^2Q_x^2+\lambda_\theta^2Q_y^2)(1+\lambda_{ab}^2Q^2)$, with $\lambda_\theta^2=\lambda_{ab}^2\sin^2\theta+\lambda_c^2\cos^2\theta$. Thus, $\tilde{V}_{zz}(\mathbf{Q})$ will depend more strongly on Q_y than on Q_x at large $\mathbf{Q}$ when $\theta\approx\pi/2$ and $M_z/M\gg 1$, and the correction to the isotropic result is larger for $c_{66}^{(e)}(\mathbf{k})$ than for $c_{66}^{(h)}(\mathbf{k})$ in very anisotropic superconductors. The latter essentially retains its weak dispersion at $\theta=0$, which is the same as for the isotropic case.

Given the above results, we further investigate the stability of the FLL by considering its strongly dispersive normal modes. Regardless of the symmetry of the FLL or the orientation of the induction $\mathbf{B}$, the FLL always has precisely two normal modes since only displacements *perpendicular* to the flux lines have physical significance. The normal modes $\Omega^{\pm}(\mathbf{k})$ of the FLL are found by diagonalizing the matrix $\Phi_{\alpha\beta}(\mathbf{k})$. At $\theta=0$, the mode $\Omega^-(\mathbf{k})$ corresponds to a *transverse* phonon mode, which in the continuum limit $\mathbf{k}_\perp\ll K_{10}=4\pi/\sqrt{3}a$ is given by

$$\Omega^-(\mathbf{k})=c_{66}(\mathbf{k})k_\perp^2+c_{44}(\mathbf{k})k_z^2. \tag{9}$$

The hard mode $\Omega^+(\mathbf{k})$ in this geometry corresponds to a *longitudinal* mode which, however, goes soft at $\mathbf{k}=0$. This is due to screening of the magnetic field by supercurrents, and a resulting exponentially small interaction potential at large enough distances. In the continuum limit, we find

$$\Omega^+(\mathbf{k})=c_{11}(\mathbf{k})k_\perp^2+c_{44}(\mathbf{k})k_z^2. \tag{10}$$

Here, the bulk modulus $c_{11}(\mathbf{k})$ of the FLL [3,5] is Lorentzian dispersive, as is the tilt modulus $c_{44}(\mathbf{k})$, due to the long-range interaction between flux lines. Since $c_{11}(\mathbf{k})\gg c_{66}(\mathbf{k})$ for $k<K_{10}/2$, particularly at very low inductions, the transverse mode is the dominant mode of fluctuations of the FLL at $\theta=0$. Both modes $\Omega^{\pm}(\mathbf{k})$ remain hard in the entire BZ away from the zone center.

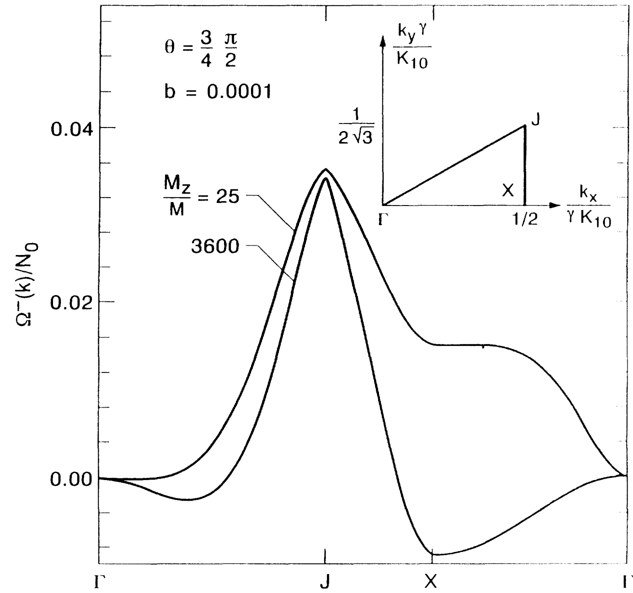

FIG. 2. Normal mode $\Omega^-(\mathbf{k})/N_0$ along three symmetry directions in the BZ for rigid flux lines ($k_z=0$) and mass anisotropies $M_z/M=25$ and 3600 at $\theta=3\pi/8$, with $N_0=B^2/4\pi$. We have used $b=B/B_{c2}=0.0001$, and $\kappa=50$. The normal mode is plotted with k_x in units of $K_{10}\gamma$ and k_y in units of K_{10}/γ, with $\gamma=(\cos^2\theta+M/M_z\sin^2\theta)^{1/4}$, and $K_{10}=4\pi/\sqrt{3}a$.

This is expected from our discussion of $c_{66}^{(e)}(\mathbf{k})$ at $\theta=0$, which demonstrated that the FLL is robust against nonuniform shear deformations in this geometry, as is also the case for tilt and compressional deformations [9].

We now turn to the more interesting situation where $\theta\neq 0$. From our consideration of the modulus $c_{66}^{(e)}(\mathbf{k})$ we are led to consider $\Omega^-(\mathbf{k})$ at $\theta=3\pi/8$; $\Omega^+(\mathbf{k})$ remains hard, and will not be considered further. In Fig. 2, we show $\Omega^-(\mathbf{k})$ at $b=0.0001$, $\kappa=50$ for $M_z/M=25$ and 3600. The most important feature is that this mode *becomes completely soft at finite* $\mathbf{k}$ *vectors in the Brillouin zone* when $M_z/M=3600$, but not for $M_z/M=25$. Further, in Fig. 3 we show $\Omega^-(\mathbf{k})$ for the parameters $M_z/M=3600$, $\kappa=50$, and $\theta=3\pi/8$ for various values of $b\in[0.0001,0.0004]$. While the mode is soft at finite $\mathbf{k}$ for $b=0.0001$ and 0.0002, this is not the case for the largest inductions. These results show that the instabilities of a hexagonal FLL only develop at very low inductions in very anisotropic superconductors provided also that the vortices are tilted away from the $\hat{\mathbf{c}}$ axis. *It is not necessary to invoke surface effects or boundary conditions to see these instabilities.*

In preparation for the numerics, it is discovered that the value of $\Omega^-(\mathbf{k})/(B^2/4\pi)$ is controlled by the vortex-field overlap parameter $\gamma_0\equiv\lambda_{ab}^2K_{10}^2=4\pi b\kappa^2/\sqrt{3}$. Structural instabilities of the FLL at too large values of γ_0 are not possible, since substantial overlap of vortex fields renders the effective intervortex interaction uniformly repulsive. In this regime of larger inductions $0.0002\ll b<0.2$ we therefore expect a stable hexagonal FLL at

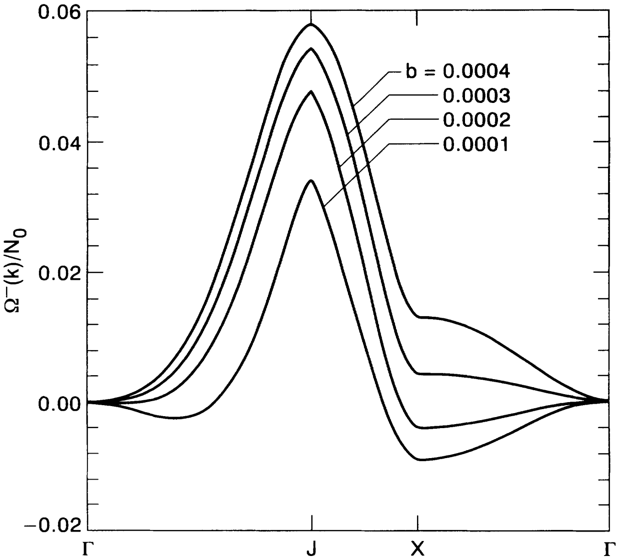

FIG. 3. Same as Fig. 2, for one value of $M_z/M=3600$ with reduced induction $b=B/B_{c2}=0.0001$, 0.0002, 0.0003, and 0.0004. Only at the two lowest inductions is $\Omega^-(\mathbf{k})$ soft for finite **k**.

all angles θ. This is *consistent* with recent results of Ref. [8], which in this field regime treated the nonlocal elasticity at oblique angles of the induction by scaling transformations of the isotropic case. In particular, the thermal fluctuations of the vortices (obtained by integrating $[\Omega^-(\mathbf{k})]^{-1}$ over the BZ) were found to be finite.

Recently, FLL structures were investigated theoretically for the case where the vortices were slightly inclined with respect to the easy *a-b* plane [14]. A class of nearly degenerate solutions were found ($\theta \approx \pi/2$), yielding FLLs with a rhombic unit cell highly compressed along the direction of the easy plane, of which the FLL found in Ref. [15] comprises the global minimum. The calculations of Refs. [14,15] considered, by assumption, only uniform ($\mathbf{k}=0$) flux distributions. However, the instability we find, at *finite* **k**, implies a vortex ground state of a *different* nature than those discussed in Refs. [14,15]. A particular possibility is one where the vortices form a FLL with a basis. In general, however, instabilities will be found at wave vectors which are not rational fractions of the reciprocal-lattice vectors of a distorted hexagonal lattice, allowing incommensurate flux-density waves to form.

In summary, we have discussed the structural instability of a class of hexagonal FLLs in uniaxial superconductors at oblique orientations of **B** in the extreme low-induction regime. The instability is induced by nonuniform (finite **k**) shear deformations of the FLL. Since they are found at finite **k** in the first BZ and are brought about by the surprisingly strong dispersion of the easy shear modulus $c_{66}^{(c)}(\mathbf{k})$, they can only be detected through the use of *nonlocal* elasticity theory. The precise determination of the correctly reconstructed ground state of unpinned rigid vortices, at oblique orientations of **B**, is a highly nontrivial problem. Its solution will require nonlinear terms in the elastic energy to be added, obtained from a further expansion of the total energy, Eq. (1). The novel type of ground state is likely to be a FLL with a basis or, more generally, a flux-density wave. The reconstruction of ground states that we have found for $M_z/M=3600$ may be related to the exotic vortex structures observed in $Bi_{2.2}Sr_2Ca_{0.8}Cu_2O_8$ [6]. For $M_z/M=25$, we find that a conventional distorted hexagonal FLL is stable for $b=B/B_{c2}>0.00001$ at all angles $\theta=\angle(\mathbf{B},\hat{\mathbf{c}})$. This means that a barrier must exist for the reconstruction of the hexagonal lattice for these parameters. Our main point is that anisotropic London theory does provide a framework for discussing flux-line lattices with exotic vortex structures, not only conventional Abrikosov lattices.

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