# Vortex-induced strain and flux lattices in anisotropic superconductors

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(Received 4 January 1995)

Strains in superconductors that accompany vortex nucleation and arise due to the difference in the specific volumes of the superconducting and normal phases are evaluated. The strain in anisotropic materials causes an extra intervortex interaction, which is long range as compared to a stronger but finite-range London force. In materials with a strong pressure dependence of superconductivity (such as $NbSe_2$) the strain-induced interaction affects the structure of the flux lattices. For the field parallel to the $c$ axis of $NbSe_2$ the flux lattice is locked on the crystal, a fact that cannot be explained either by London or by harmonic elastic interactions. The possible role of anharmonic elastic interactions of vortices for this case is discussed.

## I. INTRODUCTION

There is a puzzling disagreement between predictions of the London theory[1] and the flux-line lattices (FL) observed in single crystals of $NbSe_2$ in the scanning tunneling experiments (STM),[2] decoration,[3] and in small angle neutron scattering.[4] For any angle $\theta$ between the magnetic field and the $c$ crystal axis (except $\theta = 0°, 90°$), the London energy is minimum for the structure $(A)$, and maximum for $(B)$ shown in Fig. 1; see Ref. 5. In all experiments in tilted fields, only the structure $(B)$ is seen. When the field is along $c$, the hexagonal vortex lattice is locked on the crystal, whereas the London theory does not distinguish between different orientations of the FL within the crystal. This suggests that factors other than London interaction of vortices are at play.

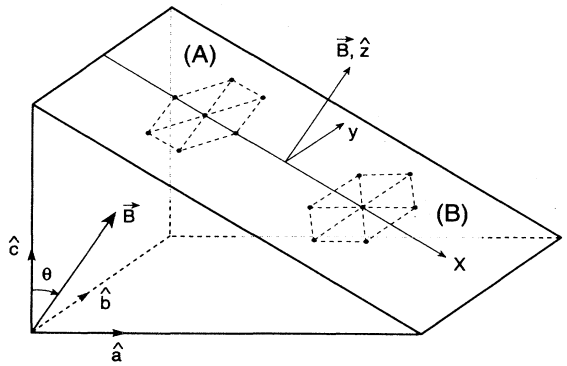


FIG. 1. The cros-section $xy$ perpendicular to the field $\mathbf{B}$ of the crystal with principal directions $a, b, c$; $\mathbf{B}$ forms angle $\theta$ with the $c$ axis. Vortex axes are along $z$. The axis $y$ is along $b$, whereas $x$ is along the projection of $c$ onto the $xy$ plane. For an arbitrary vortex orientation within the crystal (except the principal directions), the flux-line lattices $(A)$ and $(B)$ have the minimum and maximum London energies, respectively (in materials with the coherence length ratio $\xi_{ab}/\xi_c > 1$). The structure $(B)$ is seen in the decoration, neutron scattering, and in most of the STM experiments with $NbSe_2$.

The elastic strain caused by vortices in superconducting crystals was discussed about 20 years ago as a source of pinning[6,7] and as a possible reason[8] for observed correlations between FL and crystal lattices[9] (for further references, see Ref. 10). Recently, the kinetic energy of "deformable" crystals collateral to vortex motion has been associated with vortex inertia.[11] Early discussions dealt mostly with cubic Nb and its alloys. With highly anisotropic superconductors taking the central stage, much stronger FL-crystal interactions may have broader implications and deserve careful treatment.

In this paper, we study in some detail the strain-induced interaction of vortices in anisotropic materials and show that the interaction is *long range* [similar to the interaction of two-dimensional (2D) dipoles in the $1/R^2$ dependence on the intervortex distance $R$, but different from the latter in the angular behavior]. For a FL with the vortex density $B/\phi_0$ ($B$ is the magnetic induction and $\phi_0$ is the flux quantum), the macroscopic energy density due to this interaction is shown to be of the order

$$F_{\rm int} \sim \lambda \left( \frac{\phi_0 B}{16\pi^2 \lambda_L^2 T_c} \frac{\partial T_c}{\partial p} \right)^2 . \qquad (1)$$

Here $\lambda$ stands for the order-of-magnitude estimate of elastic moduli ($10^{12}$ erg/cm$^3$), $\lambda_L$ is the London penetration depth, and $\partial T_c/\partial p$ is the pressure derivative of the critical temperature (typically, $10^{-10}$ K cm$^3$/erg). We note that London energies for different FL's in intermediate fields, $H_{c1} \ll B \ll H_{c2}$, differ by $(\phi_0/\lambda_L^2)^2$ with a small

 

numerical factor $\sim 10^{-7}$; see Ref. 1. Direct comparison shows that in materials with a strong pressure dependence of $T_c$ and not very high critical temperature (as $NbSe_2$), the energy (1) may play a dominant role in forming FL structures.

It is worth noting that for $H_{c1} \ll B \ll H_{c2}$, due to the long-range interaction, the elastic energy is proportional to $B^2$, while the London energy is linear in $B$. Moreover, in this domain, differences in London energies for different FL's are practically field independent. Therefore, as far as the FL's are concerned, the elastic interactions become more significant at greater inductions.

## II. ELASTIC INTERACTION OF VORTICES

We begin with isotropic materials. Within standard notation,[12] the elastic energy density reads

$$F = \lambda u_{ll}^2/2 + \mu u_{ik}^2 , \tag{2}$$

where $u_{ik}$ is the strain tensor, and $\lambda, \mu$ are Lamé coefficients; summation over double indices is implied. The stress tensor $\sigma_{ik} = \partial F/\partial u_{ik} = \lambda u_{ll}\delta_{ik} + 2\mu u_{ik}$, and the equilibrium condition $\partial\sigma_{ik}/\partial x_k \equiv \sigma_{ik,k} = 0$ is given by

$$\lambda u_{ll,i} + 2\mu u_{ik,k} = 0 . \tag{3}$$

Let us consider vortex nucleation prior to which the superconductor has been strain free. We model the vortex core as a normal ($N$) cylinder of radius $\xi$, the coherence length, surrounded by the superconducting ($S$) phase with the normalized order parameter $|\psi| = 1$. Nucleation of the normal core causes stress, since the $N$ phase has larger specific volume $V_n$ than $V_s$. The relative volume change $\zeta$ is related to the pressure dependence of the condensation energy or of the thermodynamic critical field $H_c$ (see, e.g., Ref. 13):

$$\zeta = \frac{V_n - V_s}{V_s} = \frac{H_c}{4\pi}\frac{\partial H_c}{\partial p} , \tag{4}$$

typically, $\zeta \sim 10^{-7}$–$10^{-5}$.

We take the vortex direction as $z$. The displacement $\mathbf{u} = (u_x, u_y, 0)$ is radial in the plane $xy$, i.e., $\mathrm{curl}\,\mathbf{u} = 0$ or $\mathbf{u} = \nabla\chi$, and $u_{\alpha\beta} = \chi_{,\alpha\beta}$; the Greek subscripts acquire only $x$ and $y$ values here and throughout the text. The equilibrium condition (3) takes the form $\lambda\chi_{,\beta\beta\alpha} + 2\mu\chi_{,\alpha\beta\beta} = 0$ with the first integral $\chi_{,\beta\beta} \equiv \nabla^2\chi = \mathrm{const}$. Boundary conditions, however, for the core interior and for the $S$ phase around are different. In the core center $\mathbf{u} = \mathbf{0}$, and we obtain

$$\mathbf{u}_n = -\gamma_n\mathbf{r}, \quad u_{\alpha\beta}^{(n)} = -\gamma_n\delta_{\alpha\beta} , \tag{5}$$

where $\mathbf{r} = (x, y)$. In the $S$ phase, $\mathbf{u}_s = \mathbf{0}$ at infinity, and

$$\mathbf{u}_s = \frac{\gamma_s\xi^2\mathbf{r}}{r^2}, \quad u_{\alpha\beta}^{(s)} = \frac{\gamma_s\xi^2}{r^2}\left(\delta_{\alpha\beta} - \frac{2}{r^2}x_\alpha x_\beta\right); \tag{6}$$

$\xi^2$ is introduced for convenience.

The constants $\gamma_n$ and $\gamma_s$ are to be determined from the boundary conditions at the core surface $r = \xi$. One of these relates $\gamma$'s to the coefficient $\zeta$ of Eq. (4). To find this relation, note that had the $N$ core been "extracted" from the $S$ environment, it would have expanded in a *stress-free* situation from the actual radius $\xi$ to a $\xi_n > \xi$, whereas the "hole" in $S$ would have contracted to $\xi_s < \xi$; see Ref. 14. This means that $u_n(\xi) = \xi - \xi_n = -\gamma_n\xi$, whereas $u_s(\xi) = \xi - \xi_s = \gamma_s\xi$. On the other hand, $\pi(\xi_n^2 - \xi_s^2) = 2\zeta\pi\xi_s^2/3$ (the area expansion factor is $\frac{2}{3}$ of the bulk coefficient $\zeta$) or $\xi_n - \xi_s = \zeta\xi/3$. Hence one can exclude auxiliary quantities $\xi_n$ and $\xi_s$ to obtain $\gamma_n + \gamma_s = \zeta/3$. The second equation for $\gamma$'s is provided by equating stresses at the $N$ and $S$ sides of the core surface at $r = \xi$. We then obtain

$$\gamma_n = \frac{\zeta\mu}{3(\lambda + 2\mu)} , \quad \gamma_s = \frac{\zeta(\lambda + \mu)}{3(\lambda + 2\mu)} . \tag{7}$$

The strain energy of a vortex can now be estimated; it is of the order $\xi^2\zeta^2\lambda$. The ratio of elastic energy associated with a vortex to the London line energy is of the order $\xi^2\zeta^2\lambda/H_{c1}\phi_0 \sim \zeta^2\lambda/H_c^2$. Usually, this ratio is small.

Let us now turn to the question of intervortex interaction. For two parallel vortices, 1 and 2, the total strain $u_{\alpha\beta} = u_{\alpha\beta}^{(1)} + u_{\alpha\beta}^{(2)}$. Substitute this in Eq. (2) to obtain $F = F_1 + F_2 + F_{12}$, where $F_1$ and $F_2$ are the energy densities of 1 and 2 taken separately, and

$$F_{12} = \lambda u_{\beta\beta}^{(1)}u_{\alpha\alpha}^{(2)} + 2\mu u_{\alpha\beta}^{(1)}u_{\alpha\beta}^{(2)} \tag{8}$$

is the interaction part.

For anisotropic materials,

$$F = \lambda_{iklm}u_{ik}u_{lm}/2 \tag{9}$$

and the equilibrium conditions are $\lambda_{iklm}u_{lm,k} = 0$ or in terms of the displacement $\mathbf{u}$: $\lambda_{iklm}u_{m,kl} = 0$.[12] For vortices along $z$, indices $m, k, l$ acquire only $x, y$ values.

The displacement field $\mathbf{u}$ outside cores has the core expansion as a source. To find $\mathbf{u}$ for a system of well-separated vortices ($r \gg \xi$), we consider cores as point sources. Then, similar to the thermal expansion of anisotropic bodies subject to point heat sources,[12] one has to add a term

$$\eta_{\alpha\beta}u_{\alpha\beta}\sum_v \delta(\mathbf{r} - \mathbf{r}_v) \tag{10}$$

to the free-energy density for the sources at $\mathbf{r}_v$. Here $\eta_{\alpha\beta}$ is a 2D symmetric tensor, a characteristics of the material in the plane perpendicular to the vortex axis. The equilibrium conditions now read

$$\lambda_{\alpha\mu\nu\beta}u_{\beta,\mu\nu} = -\eta_{\alpha\beta}\partial_\beta\sum_v \delta(\mathbf{r} - \mathbf{r}_v). \tag{11}$$

In the isotropic case $\eta_{\alpha\beta} = \eta\delta_{\alpha\beta}$ and $\lambda_{\alpha\beta\mu\nu} = \lambda\delta_{\alpha\beta}\delta_{\mu\nu} + \mu(\delta_{\alpha\mu}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\mu})$. Solving Eq. (11) (by Fourier transform) we obtain the correct isotropic result, Eqs. (6) and (7), provided

$$\eta = -2\pi\xi^2\zeta(\lambda + \mu)/3 . \tag{12}$$

Thus $\eta$ is proportional to the core area $S = \pi\xi^2$ (see, Ref. 15).

In an anisotropic situation, the coefficient $\zeta$ becomes a 3D tensor ($\zeta_{ii} = \zeta$). Besides, the core is no longer a circle, and in general, $T_c$ and $H_c$ depend on the direction of the applied stress.[16–18] For a given vortex direction $z$ within the crystal, $\eta_{\alpha\beta}$ transforms as a 2D tensor under coordinate transformations in the plane $xy$ which leave the core area $S$ unchanged. Therefore, to construct $\eta_{\alpha\beta}$ we are left with 2D tensors $\zeta_{\mu\nu}$ and $\lambda_{\alpha\beta\mu\nu}$. One can check that the combination

$$\eta_{\alpha\beta} = -S\zeta_{\mu\nu}\lambda_{\alpha\beta\mu\nu} \tag{13}$$

has a correct isotropic limit (12).

The equilibrium Eq. (11) can be solved in the Fourier space following the general idea of Ref. 19:

$$\begin{aligned} &G^{-1}_{\alpha\beta}u_\beta = f_\alpha\,,\\ &G^{-1}_{\alpha\beta} = \lambda_{\alpha\mu\nu\beta}k_\mu k_\nu\,,\\ &f_\alpha = i\eta_{\alpha\beta}k_\beta\sum_v \exp(-i\mathbf{k}\cdot\mathbf{r}_v)\,, \end{aligned} \tag{14}$$

where $G_{\alpha\beta}$ is the elastic Green's function: $u_\alpha = G_{\alpha\beta}f_\beta$. The total energy is

$$\mathcal{F} = \frac{1}{2}\lambda_{\alpha\beta\gamma\delta}\int d^2\mathbf{r}u_{\alpha\beta}u_{\gamma\delta} + \eta_{\alpha\beta}\sum_v u_{\alpha\beta}(\mathbf{r}_v), \tag{15}$$

where $u_{\alpha\beta}$ is the strain caused by all vortices.

Let us evaluate now the interaction $\mathcal{F}_{12}$ of two vortices, one at $\mathbf{r} = \mathbf{0}$ and another at $\mathbf{r} = \mathbf{R}$:

$$\mathcal{F}_{12} = \lambda_{\alpha\beta\mu\nu}\int d^2\mathbf{r}u^{(1)}_{\alpha\beta}(\mathbf{r})u^{(2)}_{\mu\nu}(\mathbf{r}) + 2\eta_{\alpha\beta}u^{(1)}_{\alpha\beta}(\mathbf{R}), \tag{16}$$

where we make use of $u^{(1)}_{\alpha\beta}(\mathbf{R}) = u^{(2)}_{\alpha\beta}(0)$. In the Fourier space

$$\mathcal{F}_{12}(\mathbf{R}) = -\int\frac{d^2\mathbf{k}}{(2\pi)^2}e^{i\mathbf{k}\cdot\mathbf{R}}\eta_{\mu\alpha}\eta_{\nu\beta}G_{\mu\nu}k_\alpha k_\beta\,. \tag{17}$$

The relation $\lambda_{\alpha\mu\nu\beta}G_{\beta\gamma}k_\mu k_\nu = \delta_{\alpha\gamma}$ [see Eq. (14)] and the symmetry of $\lambda_{\alpha\beta\mu\nu}$ with respect to $\alpha \leftrightarrow \beta$ and $\mu \leftrightarrow \nu$ have been used.

Inverting $G^{-1}_{\alpha\beta}$ of Eq. (14), we have in the isotropic case

$$G_{\alpha\beta} = \frac{1}{\mu k^2}\left(\delta_{\alpha\beta} - \frac{\lambda+\mu}{\lambda+2\mu}\frac{k_\alpha k_\beta}{k^2}\right). \tag{18}$$

Substitute this in (17) to see that $\mathcal{F}_{12} = 0$ for any finite $R$. Thus, there is no strain-induced interaction of parallel vortices in isotropic materials (in the harmonic approximation of elasticity; see Ref. 20).

In a coordinate frame with $z$ along the vortex axis, the 2D tensor $\lambda_{\alpha\beta\gamma\delta}$ has a maximum of six independent components: $\lambda_{xxxx}$, $\lambda_{xxxy}$, $\lambda_{xxyy}$, $\lambda_{xyxy}$, $\lambda_{xyyy}$, and $\lambda_{yyyy}$. If the vortex axis $z$ happens to lie in one of the crystal symmetry planes, one can choose the intersect of this plane with $xy$ as, e.g., the $y$ axis; then all $\lambda_{\alpha\beta\gamma\delta}$ with an odd number of $x$'s turn zero, leaving four nonzero components. This is the case for the hexagonal symmetry for which the crystal is elastically isotropic in the $ab$ plane. The same is true for a "uniaxial body" isotropic in the $ab$ plane: irrespective of the vortex direction, $zc$ is the symmetry plane. For different crystallographic systems one easily identifies situations (proliferating with increasing symmetry) for which four moduli suffice (in the cubic case, of course, this number is reduced to three). Thus, the case of four 2D moduli covers perhaps the largest number of situations of interest.

We now evaluate the strain-induced interaction between two parallel vortices for such a situation. The energy density is

$$F = \frac{1}{2}(\lambda_1 u^2_{xx} + \lambda_2 u^2_{yy}) + \lambda_3 u_{xx}u_{yy} + 2\lambda_4 u^2_{xy}\,, \tag{19}$$

where $\lambda_{xxxx}$, $\lambda_{yyyy}$, $\lambda_{xxyy}$, and $\lambda_{xyxy}$ are abbreviated to $\lambda_1$, $\lambda_2$, $\lambda_3$, and $\lambda_4$, respectively. Tensor $G_{\alpha\beta}$ is given by

$$\begin{aligned} &G_{xx}\Delta = G^{-1}_{yy} = \lambda_4 k_x^2 + \lambda_2 k_y^2\,,\\ &G_{xy}\Delta = -G^{-1}_{xy} = -(\lambda_3+\lambda_4)k_x k_y\,,\\ &G_{yy}\Delta = G^{-1}_{xx} = \lambda_1 k_x^2 + \lambda_4 k_y^2\,,\\ &\Delta = \lambda_4(\lambda_1 k_x^4 + \lambda_2 k_y^4) + (\lambda_1\lambda_2 - \lambda_3^2 - 2\lambda_3\lambda_4)k_x^2 k_y^2. \end{aligned} \tag{20}$$

Since for a uniaxial crystal $\zeta_{xy} = 0$, $\eta_{\alpha\beta}$ is diagonal with eigenvalues $\eta_1, \eta_2$. The elastic interaction of two vortices then reads

$$\mathcal{F}_{12}(\mathbf{R}) = -\int\frac{d^2\mathbf{k}}{(2\pi)^2}e^{i\mathbf{k}\cdot\mathbf{R}}\frac{N}{\Delta}\,, \tag{21}$$

where $N = \eta_1^2 k_x^2 G^{-1}_{yy} + \eta_2^2 k_y^2 G^{-1}_{xx} - 2\eta_1\eta_2 k_x k_y G^{-1}_{xy}$. The integration over $k_x$ is done evaluating residues of $\Delta$ in the lower (for $x > 0$) half-plane of the complex $k_x$; the integral over $k_y$ is known. We obtain

$$\mathcal{F}_{12}(\mathbf{R}) = \frac{A}{R^2}\mathcal{G}(\varphi)\,, \tag{22}$$

where $R = \sqrt{x^2+y^2}$ and $\varphi = \tan^{-1}(y/x)$ give the position of the second vortex (for the first at the origin). The constant prefactor is

$$\begin{aligned} &A = \frac{\eta_2^2}{2\pi\lambda_1(D_1^2 - D_2^2)},\quad D^2_{1,2} = (P \pm \sqrt{P^2 - 4Q})/2,\\ &P = \frac{\lambda_2}{\lambda_4} - \frac{\lambda_3^2}{\lambda_1\lambda_4} - \frac{2\lambda_3}{\lambda_1},\quad Q = \frac{\lambda_2}{\lambda_1}\,. \end{aligned} \tag{23}$$

The angular dependence of $\mathcal{F}_{12}$ is given by a dimensionless function:

$$\begin{aligned} &\mathcal{G} = \mathcal{G}_2 - \mathcal{G}_1\,,\\ &\mathcal{G}_{1,2} = \Lambda_{1,2}\frac{(D^2_{1,2}+1)\cos^2\varphi - 1}{[(D^2_{1,2}-1)\cos^2\varphi + 1]^2}\,,\\ &\Lambda_{1,2} = \frac{D^2_{1,2}\Lambda - (\rho D^2_{1,2}+1)^2}{D_{1,2}},\quad \rho = \frac{\eta_1}{\eta_2}, \end{aligned} \tag{24}$$

and $\Lambda = (\lambda_1 + \rho^2\lambda_2 - 2\lambda_3\rho)/\lambda_4$. Equations (23) and (24) hold provided $P^2 - 4Q > 0$, the condition to be checked dealing with a particular material (in the isotropic case

$P^2 - 4Q = 0$). If this condition is not met, the solution should be replaced by another one that will be discussed elsewhere.

Thus, the strain-induced interaction of vortices is long range: it changes as $R^{-2}$, i.e., slow as compared to the exponential decay of the London interaction. Clearly, the angular behavior of the interaction, $\mathcal{G}(\varphi)$, can be studied only in one quadrant. One can see that $\int_0^{\pi/2} \mathcal{G}(\varphi)d\varphi = 0$. Besides, the boundary values, $\mathcal{G}(0) = \Lambda_2/D_2^2 - \Lambda_1/D_1^2$ and $\mathcal{G}(\pi/2) = \Lambda_1 - \Lambda_2$, are of the same sign or not, depending on the constants involved. This means that $\mathcal{G}(\varphi)$ changes sign once or twice within the quadrant. Since $\mathcal{G}$ determines the sign of interaction $\mathcal{F}_{12}$, the behavior of $\mathcal{G}$ is physically relevant.

The potential $\mathcal{F}_{12}$ is reminiscent of the dipole-dipole interaction in electrostatics: for two equal 2D dipoles $d\hat{x}$, $\mathcal{F}_d = d^2(2\cos^2\varphi - 1)/R^2$. This, however, turns zero only once in a quadrant. The angular dependence of $\mathcal{F}_{12}$, on the other hand, is sensitive to the relative values of the elastic constants as well as to the vortex orientation in a quite complicated way [as is evident from Eqs. (24)] An example of this complexity is seen in Fig. 2, where $\mathcal{F}_{12}(x, y)$ for $NbSe_2$ is plotted in the first quadrant of the $xy$ plane for vortices at $\theta = 60°$.

Given the intervortex interaction, we can evaluate its part in the energy of a flux-line lattice by summing up all pairwise contributions. The macroscopic energy density of elastic interaction can then be written as the interaction of the vortex at the origin with all others, multiplied by their number density:

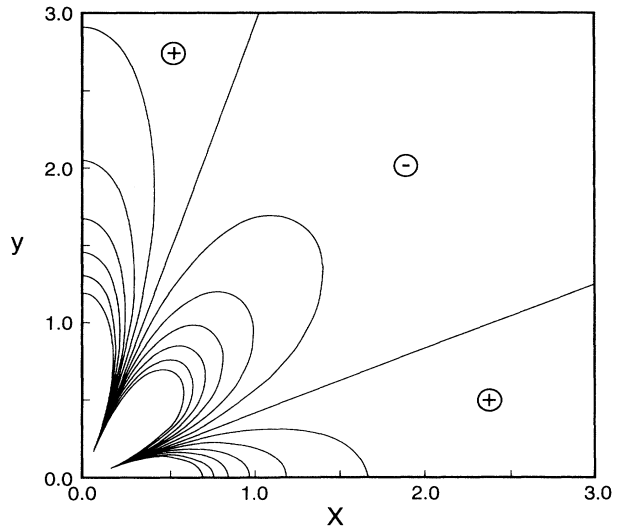


FIG. 2. Strain induced interaction $\mathcal{F}_{12}$ of vortices for $NbSe_2$. One vortex is placed at the origin, the second is at $(x, y)$. Vortices are tilted at $\theta = 60°$ relative to the $c$ axis. Coordinates $x, y$, and $z$ (perpendicular to the figure) are the same as in Fig. 1. Contours $\mathcal{F}_{12}(x, y) = \text{const}$ are shown in the first quadrant of the plane $xy$. The coordinates $x$ and $y$ are in units $(2\Phi_0/\sqrt{3}B)^{1/2}$; $B = 5$ kG. Straight lines correspond to $\mathcal{F}_{12} = 0$; adjacent contours differ by $\Delta\mathcal{F}_{12} = 10^{-13}$ erg/cm.

$$F_{\text{int}} = \frac{B}{\phi_0} A \sum_{mn}{}' \frac{\mathcal{G}(\varphi_{mn})}{R_{mn}^2}; \tag{25}$$

positions $\mathbf{R}_{mn}$ form a 2D lattice, $\varphi_{mn}$ are the corresponding azimuthal angles, and the prime indicates that the term $m = n = 0$ is skipped. Since all $R_{mn}^2 \propto \phi_0/B$, we have $F \propto (B/\phi_0)^2$, the direct result of the long-range interaction. The order-of-magnitude estimate of the energy (25) is given in Eq. (1). An alternative form of this estimate is

$$F_{\text{int}} \sim \lambda\zeta^2(B/H_{c2})^2. \tag{26}$$

We note that the estimate $F_{\text{int}} \sim \lambda\zeta^2$ of Ref. 8, being independent of the vortex density, cannot be correct.

The 2D sum $\sum' R_{mn}^{-2}$ diverges logarithmically. Due to cancellation caused by the angular function $\mathcal{G}$ (the average of which is zero) the sum (25) converges. The result for $F_{\text{int}}$, however, depends on the shape of the summation domain chosen. This is a direct consequence of the long-range dipole-type interaction in question. As in the case of the dipole-dipole interaction in magnetic materials, the elastic interaction of vortices yields the shape-dependent contribution to the total energy. Fortunately, the *difference* in $F_{\text{int}}$ for two different FL's is shape independent since the contribution of large distances to the sum (25) is sensitive only to the density of vortices rather than to their arrangement. Hence, evaluating $F_A - F_B$ we can choose any summation domain which provides for the cancellation mentioned above. Having this in mind, we take the domain of summation over $m$ and $n$ so as to assure the circular shape in the plane $xy$; then contribution of large $R$'s (where the sum can be replaced with an integral) vanishes. In doing so we disregard possible effects of sample surfaces, which may turn out to be considerable: the convergence of the sum (25) up to three significant digits is achieved when $m, n$ reach $10^2$–$10^3$, i.e, on *macroscopic* distances. The shape and surface effects of the long-range interaction in question call for a separate consideration.

### A. Flux lattice of $NbSe_2$ in tilted fields

We apply now the results obtained to the hexagonal $NbSe_2$. To address major features of FL's in this material we consider it as "uniaxial," so that the potential $\mathcal{F}_{12}$ developed above applies. For vortices along $z$ at an angle $\theta$ relative to the sixfold axis $c$, one has to find the 2D moduli in the plane $xy$. The $xyz$ frame is obtained from $abc$ by rotation $\theta$ about $y = b$; transforming $\lambda_{iklm}$ from the crystal frame $abc$ to $xyz$ we have

$$\begin{aligned}
\lambda_1 &\equiv \lambda_{xxxx} = C_{11}\cos^4\theta + (2C_{13} + 4C_{44})\sin^2\theta\cos^2\theta \\
&\quad + C_{33}\sin^4\theta, \quad \lambda_2 \equiv \lambda_{yyyy} = C_{11}, \\
\lambda_3 &\equiv \lambda_{xxyy} = C_{12}\cos^2\theta + C_{13}\sin^2\theta, \\
\lambda_4 &\equiv \lambda_{xyxy} = \frac{1}{2}(C_{11} - C_{12})\cos^2\theta + C_{44}\sin^2\theta\,.
\end{aligned} \tag{27}$$

The moduli $C_{ij}$ (common notation for $\lambda_{iklm}$ in principal axes) are estimated in Ref. 21 from the phonon-dispersion

curves by employing certain theoretical models; we take the average of the values thus obtained: $C_{11} = 1.47$, $C_{12} = 0.38$, $C_{13} = 0.11$, $C_{33} = 0.53$, and $C_{44} = 0.174 \times 10^{12}$ erg/cm$^3$.

Similarly, one obtains $\zeta_{\alpha\beta}$:

$$\zeta_{xx} = \zeta_{ab}\cos^2\theta + \zeta_c\sin^2\theta, \quad \zeta_{yy} = \zeta_{ab}\,, \tag{28}$$

where (see Ref. 22)

$$\zeta_{ab} \simeq \frac{H_c^2(0)}{4\pi T_c}\frac{\partial T_c}{\partial p_{ab}}\,, \quad \zeta_c \simeq \frac{H_c^2(0)}{4\pi T_c}\frac{\partial T_c}{\partial p_c}\,, \tag{29}$$

and $H_c(0)$ is the low-temperature limit of $H_c(T)$. To estimate $\eta_{xx}$ and $\eta_{yy}$ we use the $T_c$ dependence on unidirectional stress $p_c$ along the $c$ axis in the *low* stress limit:[16] $\partial T_c/\partial p_c = 5.3 \times 10^{-10}$ K cm$^3$/erg. Combining this with $\partial T_c/\partial p \approx 0.46 \times 10^{-10}$ K cm$^3$/erg for the hydrostatic compression,[17] we estimate $\partial T_c/\partial p_{ab}$ as $-2.4 \times 10^{-10}$ K cm$^3$/erg. Using $T_c = 7.2$ K, the low-temperature value of $H_c \approx 1.4$ kG, and Eq. (13) we obtain the needed $\zeta$'s and $\eta$'s.

With these input parameters, we are now able to evaluate the interaction energy of two FL's shown in Fig. 1. The lattice vectors for the cases $(A)$ and $(B)$ given in units of $(2\phi_0/\sqrt{3}B)^{1/2}$ are:[1]

$$R_x^{(A)} = \gamma(n + m/2), \quad R_y^{(A)} = \sqrt{3}m/2\gamma\,;$$
$$R_x^{(B)} = \sqrt{3}\gamma n/2\,, \qquad R_y^{(B)} = (n/2 + m)/\gamma. \tag{30}$$

Further, $\gamma^4 = \Gamma^{-2}\sin^2\theta + \cos^2\theta$ and $\Gamma \approx 3.1$ for $NbSe_2$. The core area $S = \phi_0/H_{c2}(\theta) = 2\pi\xi_{ab}^2\gamma^2$ for a uniaxial material; $\xi_{ab} \simeq 80$ Å. Doing the sum in Eq. (25) for $B = 5$ kG we obtain $F_A(\theta)$ and $F_B(\theta)$. The energy $F_B(\theta)$ is shown by the dashed line in Fig. 3; the lower solid line shows the difference $F_B - F_A$. Hence, the strain-induced interaction prefers the FL $(B)$, which is seen experimentally.[2–4]

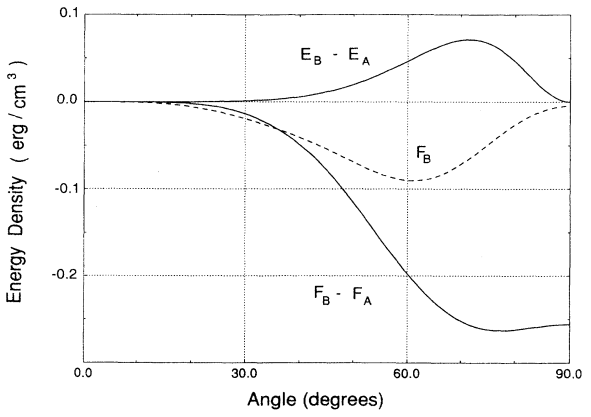


FIG. 3. The energy density $F_B$ of the structure $(B)$ as a function of the angle $\theta$ between the field direction and the $c$ axis of $NbSe_2$ (dashed line). The solid lines show the differences of the elastic $(F_B - F_A)$ and London $(E_B - E_A)$ energy densities.

These energies are to be compared with the *difference* in London energies $E$ for the structures $(A)$ and $(B)$. Although the London energy in high fields is given by a logarithmically divergent sum over the reciprocal lattice,[1] the difference $E_B - E_A$ is fast convergent. At $T \approx 5$ K (as in Ref. 4), the in-plane London penetration depth $\lambda_{ab} \approx 5000$ Å, and we obtain $E_B - E_A$ shown in Fig. 3 by the upper solid line. One sees that notwithstanding the London preference for the structure $(A)$, the elastic interactions in $NbSe_2$ win, resulting in the observed FL $(B)$.

### B. Flux lattice of $NbSe_2$ for $\mathbf{B} \parallel \hat{c}$

Clearly, the elastic interaction described above cannot be responsible for the locking of the FL in $NbSe_2$ on a certain crystal direction observed in sufficiently large fields along the $c$ axis:[2,3] in this case, the 2D tensor $\lambda_{\alpha\beta\mu\nu}$ is isotropic and the strain-induced interaction is absent.

However, in a treatment based on the standard elasticity we neglect the anharmonic terms in the energy expansion. The first such term is of the form $\lambda^{(a)}_{\alpha\beta\gamma\delta\mu\nu}u_{\alpha\beta}u_{\gamma\delta}u_{\mu\nu}$. It can be shown that the six-rank material tensor $\hat{\lambda}^{(a)}$ for a hexagonal crystal is *not isotropic* even for $\mathbf{B} \parallel \hat{c}$; Ref. 23. Since for the field parallel to the sixfold crystal axis both London and harmonic elastic interactions are degenerate with respect to different orientations of hexagonal FL's, the effect mentioned may well be caused by anharmonic strains induced by vortices.

There is no point in detailed derivation of these extra interactions because we have no data on actual values of $\hat{\lambda}^{(a)}$. Still, the anharmonic contribution to the energy can be estimated by observing that Eq. (1) can be written as $F_{\rm int} \sim \lambda U^2$, where $U$ is an estimate for the strain within the FL cell. In other words, $U$ is given by the expression in parentheses of Eq. (1). Then,

$$F_{\rm int}^{(a)} \sim \lambda^{(a)}\left(\frac{\phi_0 B}{16\pi^2\lambda_L^2 T_c}\frac{\partial T_c}{\partial p}\right)^3. \tag{31}$$

Since $F_{\rm int}^{(a)} \propto B^3$, in sufficiently small fields the anharmonic effects should give way to whatever weak pinning that is always present even in "perfect" crystals.

The latter is estimated for a *weak* collective pinning[24] as

$$F_p \sim \frac{H_c^2}{\lambda_L\xi^2\Gamma^2}\left(\frac{a_0 j_c}{j_0}\right)^3. \tag{32}$$

Here, $a_0 = \sqrt{\phi_0/B}$ is the FL cell size, and $j_0 = cH_c/3\sqrt{6}\pi\lambda_L \approx 3 \times 10^7$A/cm$^2$ is the depairing current density. The critical current density $j_c$ for the crystals of $NbSe_2$ studied[4] is field dependent: $j_c \approx j_{c0}B_0/B$ with $j_{c0} \approx 40$ A/cm$^2$ and $B_0 \approx 2$ kG. Hence, the pinning energy increases with the falling field: $F_p \propto B^{-9/2}$.

Equating $F^{(a)}$ to $F_p$, we obtain a crude estimate of the crossover field $B_c$ under which the pinning should dominate:

$$B_c^{15/2} \sim \frac{\lambda_L^5 H_c^2}{\lambda^{(a)}\Gamma^2}\left(\frac{16\pi^2 T_c}{\phi_0^{1/2}\partial_p T_c}\frac{j_{c0}B_0}{j_0}\right)^3. \quad (33)$$

With the numbers available and taking $\lambda^{(a)} \sim \lambda \sim 10^{12}$ erg/cm$^3$, we estimate $B_c \sim 1000$ G. This is not far from the experimental estimate of 100 G for this field.[3]

## III. DISCUSSION

There is yet another observation which may possibly be explained by anharmonic interactions: increasing the tilt angle $\theta$ from $\mathbf{B} \parallel \hat{c}$, one sees the structure ($B$) being gradually established with increasing $\theta$.[2] Qualitatively, this should be so: although the harmonic interactions are absent at $\theta = 0$, they take over the anharmonic terms when the angle increases. Actual evaluation of this interplay should involve more than just comparison of two given FL structures; one has to find the ground-state structure in the presence of both the London and the full elastic interactions. This calculation does not seem feasible: suffice it to mention that the moduli $\lambda^{(a)}$ are not known.

Among other materials for which application of the interaction potential discussed above is of interest, we point to $YBa_2Cu_3O_7$. As is seen in Eq. (1), high $T_c$ suppresses the elastic interactions, still the stress dependence of $T_c$ in this material is strong and highly anisotropic.[18] The potential developed here may not apply, however, because of a peculiar set of elastic constants[25] which yields a negative parameter $P^2-4Q$ [see the discussion after Eq. (24)]. We will present the proper potential elsewhere.

One should mention that the relative role of vortex-induced strain and of other possible contributions to the anisotropic intervortex interaction were the subject of intensive discussion in the early 1970's. The anisotropy of the gap $\Delta$ has been removed from the list of major factors for the coupling between FL's and the crystal, since it was established experimentally that the FLL in Nb crystals is stable with respect to the increasing impurity concentration that smears out the gap anisotropy (see the review by Schelten in Ref. 26 and references therein).

Among other factors, a major role belongs to nonlocal effects in superconductors with anisotropic Fermi surfaces, the question discussed by Takanaka.[26] He derived terms of higher order in gradients of the order parameter in the Ginzburg-Landau energy functional, which provide corrections to GL equations beyond the standard "mass-tensor" approximation.[27] Although Takanaka's formalism applies only near $T_c$ or in the immediate vicinity of $H_{c2}$ (while the decoration or neutron-scattering techniques imply $H \ll H_{c2}$), he showed that some FL's seen in cubic crystals correlate with the model predictions.

A quantitative comparison of Takanaka's results with those presented here is difficult because they are derived for different field domains. In fact, Takanaka dismissed any role for the elastic interactions referring to the paper by Roger *et al.*,[28] who incorporated the Fermi surface anisotropies simply by replacing the density of states $N(0)$ at the Fermi level in the expression for the London penetration depth, $\lambda_L^{-2} \propto N(0)$, with the anisotropic density of states $N(\mathbf{k}_F)$. This procedure is hard to justify, however, because only quantities integrated over the Fermi surface, such as $N(0)$, enter BCS-type formulas for the penetration depth (see, e.g., Ref. 27).

One can roughly estimate the role of higher-order derivatives at *arbitrary* temperatures by examining the structure of the general nonlocal BCS relation between the current $\mathbf{j}$ and the vector potential $\mathbf{A}$ in the Fourier space:

$$j_i(\mathbf{k}) = -\frac{4\pi e^2 N(0) T\Delta^2}{c}\sum_{\omega>0}\frac{\beta+\hbar/2\tau}{\beta^2} \times\left\langle\frac{v_i v_j}{(\beta+\hbar/2\tau)^2+(\hbar\mathbf{v}\cdot\mathbf{k}/2)^2}\right\rangle A_j(\mathbf{k}). \quad (34)$$

Here $\omega$ is the Matsubara frequency, $\beta^2 = \Delta^2 + \hbar^2\omega^2$, $\mathbf{v}$ is the Fermi velocity, $\tau$ is the scattering time, and $\langle\cdots\rangle$ stands for the average over the Fermi surface. Equation (34) is the anisotropic version of the BCS result which holds in small fields.[29] One can obtain this equation starting with Eilenberger equations and looking for solutions which are small perturbations to the zero-field case.

Note that in the clean limit ($\tau \to \infty$), the term containing $\mathbf{v}\cdot\mathbf{k}$ is of the order $\xi_0^2 k^2$ relative to the first one in the denominator of Eq. (34) where $\xi_0 = \xi(T=0)$. This is the term responsible for nonlocal corrections to the current (being converted to the real space, it gives rise to higher derivatives of $\mathbf{A}$ in the current-field relation). The major $k$'s contributing to the FL energy are of the order $a^{-1} = \sqrt{B/\phi_0}$, the inverse unit cell size. Since in the field domain of our interest $\xi^2/a^2 \ll 1$, one can expand Eq. (34) in this small parameter and obtain corrections to the London current. Then one estimates corrections to the standard London FL energy density $F_L \approx H_{c1}B/8\pi$ as being of the order

$$\frac{H_{c1}B}{8\pi}\frac{\xi_0^2}{a^2} = \frac{H_{c1}(T)B^2}{16\pi^2 H_{c2}(0)} \quad (35)$$

with a numerical factor of about 0.1 since averages over the Fermi surface (such as $\langle v_i v_k v_l v_m\rangle$ in the first correction term) decrease with the number of $v$'s being averaged.

To estimate relative contributions of the elastic interactions and of the "beyond-London" currents to the FL energies, this quantity is to be compared with the elastic energy (1). We then obtain approximately the same energy due to the nonlocal terms as the elastic energy: the ratio of the latter to the first in $NbSe_2$ $\sim 10^{-1}\lambda H_{c1}H_{c2}(\partial_p T_c/T_c)^2 \sim 1$ at $T \to 0$.

We further observe that for $k \to 0$ (e.g., at large distances from the vortex core) and in the dirty limit ($\tau \to 0$) the term with $\mathbf{v}\cdot\mathbf{k}$ in the denominator of Eq. (34) can be disregarded; then $j_i \propto \langle v_i v_k\rangle A_k$, which is just the anisotropic London equation (the latter is commonly written[27] in terms of the "mass tensor" $m_{ik}^{-1} \propto \langle v_i v_k\rangle$). In other words, in the dirty limit, the current-field relation is local, and there are no corrections from the microscopic theory to the London description beyond the

standard mass tensor approach. One can expect that in materials with a short mean-free path, our estimate (35) will be further suppressed. As we have mentioned, the same FL-crystal correlations in the cubic Nb are observed in dirty crystals as well as in clean. This suggests that in these crystals, the nonlocal corrections could not be a major factor in forming FL's. Similarly, for a "moderately clean" $NbSe_2$, the estimate (35) should be reduced by impurities and by raising $T$'s. This would lean the balance in favor of elastic interactions as the most important. A quantitative comparison, however, is still to be done.

Concluding, we have shown that the vortex-induced strain in anisotropic superconductors results in extra intervortex interaction, which may well compete with London energies in determining the equilibrium flux-line arrangement. This interaction is *long range* (it goes as $R^{-2}$) and has an angular dependence sensitive to details of elastic properties of a particular crystal, to the stress dependence of $T_c$, and to the vortex orientation. Most of the experimental information on flux lattices in $NbSe_2$ can be understood if this interaction is taken into account.

## ACKNOWLEDGMENTS

The authors thank D. Bishop, P. Gammel, H. Hess, J. Clem, and A. Khachaturyan for informative and useful discussions. The work was supported by the Office of Basic Energy Sciences of the DOE and in part by NSF Grants No. DMR9307581 and PHY89-04035.

[1] L. J. Campbell, M. M. Doria, and V. G. Kogan, Phys. Rev. B **38**, 2439 (1988).
[2] H. F. Hess, C. A. Murray, and J. V. Waszzak, Phys. Rev. Lett. **69**, 2138 (1992); Phys. Rev. B **50**, 16 528 (1994).
[3] C. A. Bolle *et al.*, Phys. Rev. Lett. **71**, 4039 (1993).
[4] P. L. Gammel *et al.*, Phys. Rev. Lett. **72**, 278 (1994).
[5] At $\theta = 0$, both $A$ and $B$ structures reduce to hexagons rotated with respect to each other and belonging to a continuum of hexagons of the same energy. The degeneracy exists also at $\theta = 90°$: $A$ and $B$ belong to a continuum of now different FL's of the same energy, the question discussed in Ref. 1 within the London model and by K. G. Petzinger and G. A. Warren in the Ginzburg-Landau domain [Phys. Rev. B **42**, 2023 (1990)].
[6] E. G. Kramer and C. L. Bauer, Philos. Mag. **15**, 1189 (1967).
[7] H. Kronmüller and R. Schmucker, Phys. Status Solidi B **57**, 667 (1973); **74**, 261 (1976).
[8] H. Ullmaier, R. Zeller, and P. H. Dederichs, Phys. Lett. **44A**, 331 (1973).
[9] B. Obst, Phys. Status Solidi B **45**, 467 (1971); J. Schelten, H. Ullmaier, and W. Schmatz, *ibid.* **48**, 649 (1971); U. Essmann, Physica **55**, 83 (1971).
[10] A. M. Campbell and J. E. Evetts, Adv. Phys. **21**, 199 (1972).
[11] E. Šimánek, Phys. Lett. A **154**, 309 (1991); M. Coffey, Phys. Rev. B **49**, 9774 (1994); J. Low Temp. Phys. **96**, 81 (1994); **97**, 181 (1994).
[12] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* (Pergamon, New York, 1986).
[13] D. Shoenberg, *Superconductivity* (Cambridge University Press, Cambridge, 1952), p. 74; L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon, New York, 1984), Chap. 6.
[14] Our procedure is similar to that for nucleation of a new phase during phase transformations in crystals: A. G. Khachaturyan, *Theory of Structural Transformations in Solids* (Wiley, New York, 1983).
[15] For $\lambda_L \gg \xi$, it is better to define the core area as $S = \phi_0/H_{c2} = 2\pi\xi^2$ so that the core "radius" is $\xi\sqrt{2}$; see J. R. Clem, J. Low Temp. Phys. **18**, 427 (1975).
[16] M. A. Obolenskii *et al.*, Fiz. Nizk. Temp. **15**, 984 (1989) [Sov. J. Low Temp. Phys. **15**, 544 (1989)].
[17] T. F. Smith, J. Low Temp. Phys. **6**, 171 (1972); T. Sambongi, *ibid.* **18**, 139 (1975).
[18] U. Welp *et al.*, Phys. Rev. Lett. **69**, 2130 (1992).
[19] I. M. Lifshitz and L. N. Rosenzveig, Zh. Eksp. Teor. Fiz. **17**, 783 (1947).
[20] In a more realistic model of the vortex core, without a sharp boundary between the $N$ and $S$ phases, this interaction exists even in the isotropic case. However, it is short range (of the order $\xi$) and is practically absent at distances of interest here.
[21] J. L. Feldman, Phys. Rev. B **25**, 7132 (1982).
[22] Estimating $dH_c(T)/dp = [dH_c(T)/dT_c](dT_c/dp)$, one can use $H_c(T) \approx H_c(0)(1 - T^2/T_c^2)$ and $dH_c(0)/dT_c \approx H_c(0)/T_c$. Then, $dH_c(T)/dT_c \approx [H_c(0)/T_c]f(t)$, where $f$ is a slow function of the reduced temperature: $f(0) = 1$, $f(1) = 2$.
[23] In the isotropic case the six-rank tensor $\hat{\lambda}$ has three independent components (Ref. 12). For $\mathbf{B} \parallel \hat{c}$ of a hexagonal crystal, this number is 6 (use the method of Ref. 12).
[24] G. Blatter *et al.*, Rev. Mod. Phys. **66**, 1125 (1994); Ch. 4. In our case the "bundle size" $R_c > \lambda_L\Gamma$.
[25] E. Zouboulis *et al.*, Physica C **190**, 329 (1992); Ming Lei *et al.*, Phys. Rev. B **47**, 6154 (1993).
[26] *Anisotropy Effects in Superconductors*, edited by H. Weber (Plenum, New York, 1977).
[27] L. P. Gor'kov and T. K. Melik-Barkhudarov, Zh. Eksp. Teor. Fiz. **45**, 1493 (1963) [Sov. Phys. JETP **18**, 1031 (1964)]; C. Caroli, P. G. deGennes, and J. Matricon, Phys. Kondens. Materie **1**, 176 (1963).
[28] M. Roger, R. Kahn, and J. M. Delrieu, Phys. Lett. **50A**, 291 (1974).
[29] J. Bardin, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957); E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics* (Pergamon, New York, 1980), Pt. 2.