Vortex Lattices in Cubic Superconductors

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Nonlocal corrections to London equations are employed to describe a variety of vortex lattices seen through neutron scattering in cubic crystals of V_3Si with large κ. Within this model the observed symmetries of vortex lattices and their coupling to the underlying crystal are reproduced. Predicted lattice structures are field dependent in agreement with the data. [S0031-9007(97)03649-1]

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The recently renewed interest in the vortex lattices (VL) as reflecting on the magnetic structure of vortices, their interactions, and the symmetry of the underlying order parameter [1–9] prompted us to review a rich pool of data on VL's in conventional superconductors. The hexagonal VL (made of equilateral triangles) is seldom seen even in cubic materials. Only the low field decoration experiments (in which the intervortex spacing exceeds the penetration depth) usually show this structure predicted by the Ginzburg-Landau (GL) or London (L) theories. VL's seen in small angle neutron scattering experiments (SANS) on cubic crystals are distorted triangular (or square, in some situations) with parameters depending on both temperature and applied magnetic field. Extensive data on cubic Nb, PbTl, and PbBi are summarized by Schelten and Obst [10], and by Christen *et al.* [11]. The latter group have also studied V_3Si, the cubic material with relatively large GL parameter κ [12]. Related to these are new SANS data on borocarbides (e.g., $ErNi_2B_2C$) with the field along [001] in which the square lattice is observed in high fields [13].

Since the GL or L theories incorporate the crystal anisotropy via the second rank mass tensor m_{ik}, within these approaches the cubic crystals should behave as isotropic, i.e., VL's should always be hexagonal. Attempts were made to incorporate the nonlocal effects which correspond to higher order derivatives in the GL free energy expansion, to explain the VL distortions [12,14,15]. These, however, were only partially successful as the later data analysis has shown [11,12]. This is not surprising since one could not expect the terms designed to correct the GL energy *near* the critical temperature T_c to provide an adequate description of the SANS data taken as a rule far from T_c and from the upper critical field H_{c2}.

Being simpler than the GL, the London approach has an advantage of applicability at all T's. However, the approach fails at distances of the order ξ, the coherence length. This shortcoming does not matter for VL structures, provided the intervortex spacing exceeds the core size ξ substantially. Such a situation arises in materials with large κ in fields well under the H_{c2}. Thus, the idea of developing the nonlocal corrections to the L theory for description of VL's at low T's is more attractive than the similar idea within the GL framework.

These corrections have recently been derived to address the problem of low-T magnetization in high-T_c materials [16]. We reproduce here the main points of this work. We then use the nonlocal corrections to analyze in detail the data [12] on VL's in V_3Si and show that our approach not only predicts correctly all structures observed, but provides the VL parameters and their *field* dependence close to the observed experimentally.

The nonlocality in superconductors is caused by a finite size ξ_0 of Cooper pairs: The current $\mathbf{j}(\mathbf{r})$ is determined by the vector potential $\mathbf{A}$ within a domain $\sim\xi_0$ around $\mathbf{r}$ [17]. Instead of local relations between $\mathbf{j}$ and $\mathbf{A}$ of the GL or L approaches, the microscopic theory provides an integral equation with a kernel $\hat{Q}(\mathbf{r})$ extending to distances $\sim\xi_0$; in Fourier space this relation is of the form $\mathbf{j}(\mathbf{k}) = \hat{Q}(\mathbf{k})\mathbf{A}(\mathbf{k})$ [18]. In the GL domain where $\xi(T) \gg \xi_0$, or far from the vortex cores, the nonlocal corrections vanish.

Deriving the L equations from the microscopic theory, one assumes that the currents small relative to the depairing value do not suppress the order parameter $|\Delta|$. Only the phase θ changes in space and provides the flux quantization. In fact, the small current case is the only one for which the kernel $\hat{Q}$ is known [18]. The derivation based on the Eilenberger theory is given, e.g., in Ref. [16]:

$$j_i(\mathbf{k}) = -[4\pi e^2 N(0) T \Delta_0^2/c] a_l(\mathbf{k}) \times \sum_{\omega>0} \frac{\beta'}{\beta_0^2} \left\langle \frac{v_i v_l}{\beta'^2 + \hbar^2(\mathbf{v}\cdot\mathbf{k})^2/4} \right\rangle. \quad (1)$$

Here, $\mathbf{a} = \mathbf{A} + \phi_0\nabla\theta/2\pi$, and ϕ_0 is the flux quantum; $\mathbf{v}$ is the Fermi velocity, $\Delta = \Delta_0 e^{i\theta}$, $N(0)$ is the density of states at the Fermi level per one spin; $\hbar\omega = \pi T(2n+1)$ with an integer n; $\langle\cdots\rangle$ stands for the average over the Fermi surface. Further, $\beta_0^2 = \Delta_0^2 + \hbar^2\omega^2$ and $\beta' = \beta_0 + \hbar/2\tau$ with τ being the scattering time due to nonmagnetic impurities; summation is implied over

repeated subscripts. Equation (1) is explicitly gauge invariant and holds for any anisotropic Fermi surface.

Equation (1) yields *local* London relation $\mathbf{j} \propto \mathbf{a}$, if one disregards the $\mathbf{k}$-containing term in the denominator. We expand the denominator in powers of $(\mathbf{v}\cdot\mathbf{k})^2$ and keep only the first order correction:

$$\frac{4\pi}{c} j_i = -\frac{1}{\lambda^2}\,(m_{ij}^{-1} - \lambda^2 n_{ijlm} k_l k_m) a_j\,. \tag{2}$$

Here

$$\begin{aligned} \frac{1}{\lambda^2} &= \frac{16\pi^2 e^2 N(0) T \Delta_0^2 \langle v^2\rangle}{3c^2} \sum_{\omega>0} \frac{1}{\beta_0^2 \beta'}\,, \\ m_{ij}^{-1} &= \frac{3\langle v_i v_j\rangle}{\langle v^2\rangle}\,, \\ n_{ijlm} &= \frac{4\pi^2 e^2 \hbar^2 N(0) T \Delta_0^2}{c^2} \langle v_i v_j v_l v_m\rangle \sum_{\omega>0} \frac{1}{\beta_0^2 \beta'^3}\,. \end{aligned} \tag{3}$$

We defined λ so as to have the correct isotropic limit and m_{ij} to have a convenient property $\det m_{ij} = 1$. The tensor $\hat{n}$, symmetric in all indices, can also be written as

$$n_{ijlm} = \frac{3\hbar^2 \langle v_i v_j v_l v_m\rangle}{4\langle v^2\rangle \Delta_0^2 \lambda^2}\,\gamma, \qquad \gamma = \frac{\Delta_0^2 \sum \beta_0^{-2} (\beta')^{-3}}{\sum \beta_0^{-2} (\beta')^{-1}}\,. \tag{4}$$

The quantity $\gamma(T,\tau)$ was evaluated in Ref. [16]; in the clean limit $\gamma = 2/3$ at $T = 0$. Scattering suppresses γ; in the dirty limit $\gamma \to (\tau\Delta_0/\hbar)^2 \to 0$, i.e., nonlocal effects vanish. Thus, $n \sim \xi_0^2/\lambda^2 \sim \kappa^{-2}$ in the clean case and of the order $(v\tau/\lambda)^2$ for dirty materials.

With $\hat{n} = 0$, Eq. (2) is the standard L equation [19]. Being dependent on the shape of the Fermi surface, the fourth-rank tensor $\hat{n}$ couples supercurrents with the crystal even in cubic materials which, within the local L theory, should behave isotropically. From now on, we focus on the cubic case in which $m_{ij} = \delta_{ij}$, whereas $\hat{n}$ in the crystal frame X, Y, Z has two independent components n_{XXXX} and n_{XXYY}; to evaluate these one needs Fermi surface averages of products of Fermi velocities, i.e., one turns to the band structure of the material in question.

For V_3Si, the averages were obtained from full potential linearized augmented plane wave method [20] using the local density approximation. The cubic A15 lattice constant of V_3Si of 4.72 Å was used. For V, the 3*s* and 3*d* orbitals were treated as semicore states, for which extra local orbitals were included in the basis set [21]. We obtain

$$\begin{aligned} \langle v^2\rangle &= 2.94 \times 10^{14}\,(\mathrm{cm/sec})^2\,, \\ \langle v_X^4\rangle &= 3.42 \times 10^{28}\,(\mathrm{cm/sec})^4\,, \\ \langle v_X^2 v_Y^2\rangle &= 0.656 \times 10^{28}\,(\mathrm{cm/sec})^4\,. \end{aligned} \tag{5}$$

We can now evaluate $\hat{n}$ provided Δ_0, λ, and τ are given. Of these three, only the penetration depth is established reliably: $\lambda = 1060$ Å [12]. We then lump all these parameters in one:

$$n_{ijlm} = C \frac{\langle v_i v_j v_l v_m\rangle}{\langle v^2\rangle^2}\,, \qquad C = \frac{3\hbar^2 \langle v^2\rangle \gamma}{4\Delta_0^2 \lambda^2}\,, \tag{6}$$

where C is to be determined from fitting one of the data sets. We then use this value of C to analyze the rest of the data. With the averages (5) we have

$$n_1 = n_{XXXX} = 0.395C, \quad n_2 = n_{XXYY} = 0.0758C\,. \tag{7}$$

Validity of the truncation procedure which led to Eq. (2) central to our model, sets a restriction on the C value. Indeed, since the major role in the VL problem belongs to $k \sim 2\pi/a_0$ with a_0 being the intervortex spacing, the nonlocal correction in Eq. (2) is small if $(2\pi\lambda/a_0)^2 n \ll 1$ or if

$$C \ll a_0^2/\lambda^2 \sim H_{c1}/B\,, \tag{8}$$

where H_{c1} is the lower critical field.

In experiments [12] on V_3Si, the field was applied in the (110) plane, which is the crystal symmetry plane (see Fig. 1 of Ref. [12]). We denote this plane as xz and look for VL's having (110) as a symmetry plane. Thus, the VL unit cell is a rhombus with one of the diagonals along x in the (110) plane. There are other symmetries in the four available data sets with fields along [110], [111], [112], and [001]; we will consider them case by case.

We now apply Eq. (2) to a vortex along z. To find the field component h_z (the only one needed for evaluating intervortex interaction $\phi_0 h_z/4\pi$), we first invert Eq. (2) to isolate $\mathbf{a}$, and then use the flux quantization condition, $\mathrm{curl}\ \mathbf{a} = \mathbf{h} - \phi_0 \hat{z}\,\delta(\mathbf{r})$. We utilize the smallness of nonlocal corrections to obtain after straightforward algebra:

$$\begin{aligned} h_z(\mathbf{k}) &= \frac{\phi_0}{1 + \lambda^2 k^2 + \lambda^4 (N_{xx} k_y^2 + N_{yy} k_x^2 - 2N_{xy} k_x k_y)}\,, \\ N_{ij} &= n_{ijlm} k_l k_m\,, \qquad k_z = 0\,. \end{aligned} \tag{9}$$

Note that for all cases of interest here, components of $\hat{n}$ can contain only even numbers of y's (and x's) due to the symmetry $y \to -y$. For a particular field orientation, one has to transform $\hat{n}$ from the crystal frame where it is given by Eq. (7) to the frame xyz with z along the vortex axes, and x being situated in the (110) plane of the crystal. We will skip here details of these standard transformations providing only the results.

The free energy density of a VL directed along z is

$$F = B^2 \sum_{\mathbf{q}} h_z(\mathbf{q})/8\pi\phi_0\,, \tag{10}$$

where B is the magnetic induction and h_z of Eq. (9) is taken at wave vectors $\mathbf{k} = \mathbf{q}$ forming a proper reciprocal lattice [22]. The equilibrium VL at a given $\mathbf{H}$ corresponds to the minimum of $G = F - \mathbf{BH}/4\pi$. Note that only for [112] case $\mathbf{BH} \neq BH$.

We start with $\mathbf{H} \parallel [001]$. In this case the vortex system xyz is rotated 45° relative to the crystal frame XYZ: $n_{xxxx} = n_{yyyy} = (n_1 + 3n_2)/2, n_{xxyy} = (n_1 - n_2)/2$. The VL vectors are $m\mathbf{b}_1 + n\mathbf{b}_2$ with integers m, n; $\mathbf{b}_1 = b(\hat{\mathbf{x}}\sin\beta_1 + \hat{\mathbf{y}}\cos\beta_1), \mathbf{b}_2 = b(-\hat{\mathbf{x}}\sin\beta_1 + \hat{\mathbf{y}}\cos\beta_1)$; b is the side of the isosceles triangle, and $2\beta_1 = \beta$ is the apex angle: $b = \sqrt{\phi_0/B\sin\beta}$. The reciprocal lattice is $q_x = \pi(m-n)/b\sin\beta_1,\ q_y = \pi(m+n)/b\cos\beta_1$.

The sum in Eq. (10) is formally convergent; see Eq. (9). Still, our theory is valid outside the vortex core, and we have to introduce a cutoff at $q_{\max} \sim 1/\xi$. To avoid unphysical sensitivity of the sum to a choice of the summation domain, we introduce $\exp(-q^2\xi^2)$ in the summand, thus making the sum a smooth function of parameters β and B [23]. The minimization of G is done by randomly sampling variational parameters (Monte Carlo). Positions of minima in $G(\beta)$ are not sensitive to a particular cutoff in the field range of interest here.

For the field $H = 4020\,\mathrm{G}$ along [001] (used in Ref. [12]) we take the experimental value $\beta = 58°$ and vary the Gibbs energy relative to C; the sum in Eq. (10) is cut taking $\xi = \lambda\sqrt{C/5}$ (for the clean case $3\pi^2\gamma/4 \approx 5$). The minimum is achieved at $C = 4.83 \times 10^{-3}$. This value of C will be used in all the rest of data analyses. Note that $H_{c1}/B \approx 8 \times 10^{-2}$ and the condition (8) is satisfied. Calculating $G(\beta)$ for this field orientation, we find two minima of the same depth at $\beta = 58°$ and 122°; see Fig. 1. The second minimum corresponds to the same VL rotated 90° relative to that with $\beta = 58°$. This is expected since $\hat{z}$ is the fourfold symmetry axis for this case. These two structures are seen in SANS as two coexisting domains [12]. Figure 1 shows that the square VL aligned with the crystal axes corresponds to the maximum of G.

The above analysis is based on (110) as a symmetry plane for VL's. For $\mathbf{H} \parallel [001]$, one could also consider VL's with the symmetry plane (100). We find local minima of G for the isosceles triangle as a half-unit cell with the base at [100] and $\beta = 62°$ or 118°. The maximum of G corresponds to the square VL rotated 45° relative to the crystal. However, at fields less than a certain H^* (in this case $H^* \sim 4$ kG), all these structures have higher energies than those discussed above. For $H > H^*$, the situation flips: The triangular VL with a base at [100] becomes stable (while triangles based at [110] become metastable). With the field further increasing, the angular distance between the minima of $F(\beta)$ drops along with the reduction in the value of $G(90°)$; at a certain $H = H_s$ the minima merge into a single minimum at 90°, i.e., the 45°-rotated square becomes stable. We find $H_s \approx 3\,\mathrm{T}$ in V_3Si; this is not a reliable estimate since at fields that high, the first nonlocal corrections may not suffice.

The situation just described is probably realized in borocarbides where the 45°-rotated square VL is seen in large [001] fields in SANS [13,24,25], and in the scanning tunneling [26]. Moreover, the small field decoration experiments show a triangular VL [24] similar to what the model predicts for V_3Si. More work is needed to evaluate the transition field H_s in these compounds.

Analyzing data for other field orientations, it is convenient to write the denominator in Eq. (9) as

$$1 + \lambda^2 q^2 + \lambda^4 (n_{xxyy} q^4 + d q_x^2 q_y^2), \qquad d = n_{xxxx} + n_{yyyy} - 6 n_{xxyy}. \tag{11}$$

One can verify that in the isotropic case $d = 0$; thus $d \neq 0$ is responsible for the anisotropy.

For $\mathbf{H} \parallel [111]$, we find $n_{xxyy} = n_1/6 + n_2/2$, while $d = 0$. Thus, F takes the isotropic form and $\beta = 60°$ while the VL orientation within the crystal is arbitrary. Experiment [12] shows $\beta = 60°$ with one of the triangle sides in (110) plane; the orientational degeneracy of our model may be removed by higher order terms in the nonlocal expansion (2) or by any other weak interaction [27].

For $\mathbf{H} \parallel [112]$, $\mathbf{B}$ is not parallel to $\mathbf{H}$. The misalignment of the two, however, is very small, and in the lowest order can be disregarded. We find $n_{xxyy} = (n_1 + n_2)/3$ and $d = (18n_2 - 7n_1)/12$. The energy G is minimized by β shown in Fig. 2 for a few values of H; the base of the triangle is along $[11\bar{1}]$ as is seen in SANS [12]. We find, however, that these VL's can be 90°-rotated with no change in G. It remains to be seen whether or not the $\mathbf{B}, \mathbf{H}$ misalignment removes this degeneracy.

For $\mathbf{H} \parallel [110]$, we have $n_{xxyy} = n_2$ and $d = 3(n_1 - 3n_2)/2$. If H is between 1 and 10 kG we obtain minima of G for the triangle base **a** at [001], or $[\bar{1}10]$; the first is seen in SANS. The calculated β depends on H and is

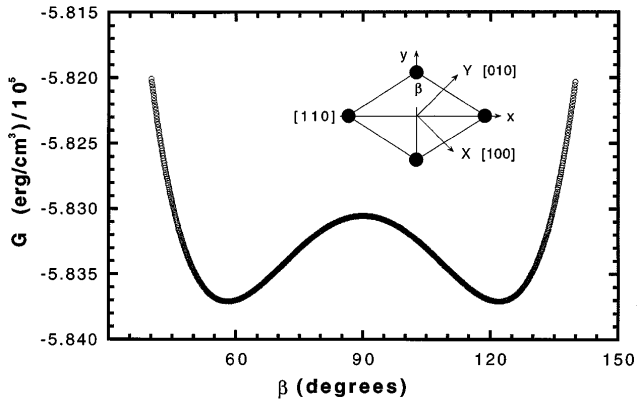

FIG. 1. The Gibbs energy vs the apex angle β shown in the inset.

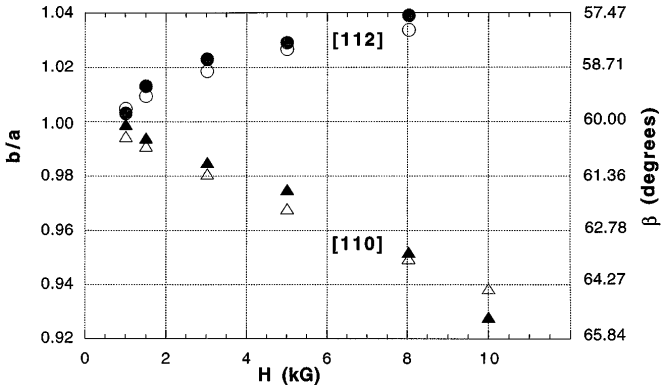

FIG. 2. The side-to-base ratio b/a (or the apex angle β) vs applied fields along [112] (circles) and [110] (triangles). Solid markers are for the data, open ones are calculated.

shown in Fig. 2. As H decreases, $\beta \to 60°$ as expected since the nonlocal effects vanish at large distances.

For the data shown in Fig. 2 the disagreement between the theory and the data is less than 2%. The mismatch in high fields might be due to the increasing sensitivity of the results to a particular cutoff, which is weak in fields under ~10 kG. Still, the agreement is remarkable: Forcing only one data point to the theory, we reproduce actual geometries of VL's and their field dependence. Thus the nonlocal effects indeed play an important role in forming VL's in V_3Si [28]. The method, however, should be justified in each application. In particular, one should check that κ is not close to one. Otherwise, the domain of applied fields for which the intervortex spacing $a_0 \gg \xi$ shrinks to a narrow region near H_{c1}, i.e., there is no room for any version of the L approach.

One should also keep in mind that magnetoelastic interactions can be relevant for VL's. These arise due to a small difference in specific volumes of the normal material in vortex cores and the superconducting phase in the rest of the sample (see [27], and references therein). We estimated that for V_3Si these interactions can be disregarded relative to nonlocal corrections to the free energy.

Finally, we comment on efforts to show that VL's observed in YBCO are due to unconventional symmetries of the order parameter. For the field along $\hat{c}$, the VL consists of isosceles triangles with $\beta \simeq 73°-77°$ [3,4]. This structure can be reproduced using the GL theory for the $d_{x^2-y^2}$ order parameter [2,6–9]. However, as the variety of VL's observed in Nb [10,11], PbTl, PbBi [10], and V_3Si discussed here, clearly demonstrates, it is difficult to establish a simple relation between the order parameter symmetry and a particular VL structure since the latter is sensitive to the temperature, field value, and orientation even in s-wave materials.

In conclusion, we have shown that nonlocal corrections to London equations describe correctly the SANS data on VL's in cubic V_3Si. For the first time, it is shown that the VL structure is field dependent. The work can be applied to recent SANS and scanning tunneling data on VL's in borocarbides [13,25,26].

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