ON NEUTRON DIFFRACTION FROM VORTICES IN UNIAXIAL SUPERCONDUCTORS

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The London approach is used to obtain the neutron scattering form factor of a vortex in a uniaxial layered superconductor. The form factor depends upon the direction of the scattering vector within the crystal. The structure of the vortex lattice is determined in the same approximation for any orientation of the vortices in the crystal.

1. As was shown first by Takanaka [1], a transverse component $\boldsymbol{h}_{\mathrm{tr}}$ of the magnetic field arises in a vortex of an anisotropic type II superconductor (unless the vortex orientation coincides with one of the principal crystal directions). The field $\boldsymbol{h}_{\mathrm{tr}}$ is not necessarily small; e.g., for a vortex at 45° to the layers of $NbSe_2$, $\langle h_{\mathrm{tr}}^2\rangle \approx 0.25\,\langle h_z^2\rangle$, where h_z is the usual axial field [2,3]. The field $\boldsymbol{h}_{\mathrm{tr}}$, therefore, should be observable in a neutron scattering experiment, which is done usually in low fields where vortices are well separated. For $NbSe_2$, the Ginzburg–Landau parameter κ is of order 10, so that a wide region of low fields exists, where the London approximation can give a reasonable accuracy in evaluation of the form factor for the neutron scattering.

The anisotropic London equations [4] read in general cartesian coordinates [2]:

$$h_i = \lambda^2 m_{kl} e_{lsi} e_{ktj} \frac{\partial^2 h_j}{\partial x_s\, \partial x_t} + \phi_0 \hat{z}_i \sum_\nu \delta(\boldsymbol{r} - \boldsymbol{r}_\nu). \qquad (1)$$

Here e_{ikl} is the Levi-Civita tensor. The phenomenological dimensionless mass tensor m_{kl} is normalized using the mean mass $\bar{M} = (M_1 M_2 M_3)^{1/3}$, where M_i are the eigenvalues of the dimensional mass tensor M_{kl}. The mean penetration depth λ is defined here in terms of $\bar{M}$ in the same way as the penetration depth of an isotropic material in terms of the isotropic mass. For a uniaxial crystal $m_1 = m_2$; in the case of a layered uniaxial material $m_1 = m_2 < m_3$, where m_3 is the mass in the direction normal to the layers; note that $m_1^2 m_3 = 1$. The unit vector $\hat{z}$ points in the direction of vortices; the magnetic flux in this direction is quantized. The corresponding singularities are taken into account by the last term of eq. (1), where ϕ_0 is the flux quantum, and $\boldsymbol{r}_\nu$ are the loci of the vortex cores in the plane normal to $\hat{z}$.

In the system of the crystal principal axes the mass tensor is diagonal. Let θ be the angle between the vortex direction z and the principal axis Z normal to the layers (see fig. 1). We choose the (x, y, z) frame as the most convenient for our problem: no physical quantity depends on z for a vortex situated along z. In this frame

$$m_{xx} = m_1 \cos^2\theta + m_3 \sin^2\theta, \quad m_{xy} = m_{yz} = 0,$$

$$m_{yy} = m_1, \quad m_{zz} = m_1 \sin^2\theta + m_3 \cos^2\theta, \qquad (2)$$

$$m_{xz} = (m_1 - m_3) \sin\theta \cos\theta .$$

Eq. (1) now reads ($\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$):

$$h_x = \lambda^2 [m_{zz} \nabla^2 h_x - m_{xz}(\partial^2 h_z/\partial y^2)],$$

$$h_y = \lambda^2 [m_{zz} \nabla^2 h_y + m_{xz}(\partial^2 h_z/\partial x\, \partial y)], \qquad (3)$$

$$h_z = \lambda^2 (m_1\, \partial^2 h_z/\partial x^2 + m_{xx}\, \partial^2 h_z/\partial y^2 - m_{xz}\, \nabla^2 h_x) + \phi_0 \sum_\nu \delta(\boldsymbol{r} - \boldsymbol{r}_\nu).$$

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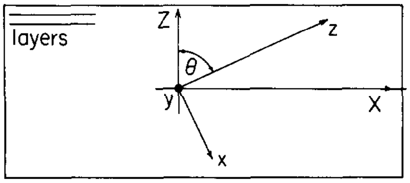

Fig. 1. The X, Y and Z are the principal axes of the crystal. The vortex is directed along the z axis.

2. The form factor $F(\boldsymbol{k})$ for neutrons scattered by the magnetic field $\boldsymbol{h}(\boldsymbol{r})$ of an isolated vortex, is defined by $|F(\boldsymbol{k})|^2 = |\boldsymbol{h}(\boldsymbol{k})|^2/\phi_0^2$, where $\boldsymbol{k}$ is the scattering vector and $\boldsymbol{h}(\boldsymbol{k})$ is the Fourier transform of $\boldsymbol{h}(\boldsymbol{r})$; $F(0) = 1$ under the normalization chosen. The vector $\boldsymbol{h}(\boldsymbol{k})$ is easily obtained from eq. (3):

$$h_x(\boldsymbol{k}) = -h_y(\boldsymbol{k})k_y/k_x = \phi_0\lambda^2 m_{xz}k_y^2/d,$$
$$h_z(\boldsymbol{k}) = \phi_0(1 + \lambda^2 m_{zz}k^2)/d, \tag{4}$$

$$d = (1 + \lambda^2 m_1 k_x^2 + \lambda^2 m_{xx}k_y^2)(1 + \lambda^2 m_{zz}k^2) - \lambda^4 m_{xz}^2 k^2 k_y^2. \tag{5}$$

We have after some elementary algebra:

$$F(\boldsymbol{k}) = [(1 + \lambda^2 m_{zz}k^2)^2 + \lambda^4 m_{xz}^2 k^2 k_y^2]^{1/2}/d. \tag{6}$$

Eqs. (6), (2) and (5) determine the dependence of F upon the vortex orientation θ and upon the value and the direction of the scattering vector $\boldsymbol{k}$. This result can be experimentally verified.

In the simplest case when vortices are normal to the layers ($\theta = 0$, $m_{xx} = m_1$, $m_{zz} = m_3$, $m_{xz} = 0$), we have the known result [5] : $F(\boldsymbol{k}) = (1 + \lambda^2 m_1 k^2)^{-1}$. Here all vortex currents are in the layers, i.e., the mass m_1 is the only one relevant. The vortex is cylindrically symmetric so that F is independent of the $\boldsymbol{k}$ direction.

If the vortex axes are in the layer plane ($\theta = \pi/2$, $m_{xx} = m_3$, $m_{zz} = m_1$, $m_{xz} = 0$), $F(\boldsymbol{k}) = (1 + \lambda^2 m_1 k_x^2 + \lambda^2 m_3 k_y^2)^{-1}$. We see that F depends upon the $\boldsymbol{k}$ orientation even in this simple situation. Note also that for an arbitrarily directed vortex, the general expression for $F(\boldsymbol{k})$ given by eqs. (6) and (5), reduces to a simpler one at the particular orientation $k_y = 0$: $F(k_x, 0) = (1 + \lambda^2 m_1 k_x^2)^{-1}$.

3. Neutron diffraction makes it possible to see the structure of the vortex lattice. We consider this problem in the intermediate field region where the intervortex spacing L obeys $\xi \ll L \ll \lambda$ (ξ is the coherence length); we follow the method of ref. [5] . For a periodic array of vortices, $\boldsymbol{h}(\boldsymbol{r})$ is a periodic function. Its Fourier components h_{iG} are given by eqs. (4), where the continuous vector $\boldsymbol{k}$ is replaced by the discrete set of reciprocal lattice vectors $\boldsymbol{G}$, and ϕ_0 is replaced by the induction $B = N\phi_0$ (N is the number density of vortices). The London free energy

$$\mathcal{F} = \int (h^2 + \lambda^2 m_{ik}\, \mathrm{curl}_i \boldsymbol{h}\, \mathrm{curl}_k \boldsymbol{h})/8\pi$$
$$= \sum_{\boldsymbol{G}} (|h_{iG}|^2 + \lambda^2 m_{ik} j_{iG} j_{kG}^*)/8\pi,$$

where $\boldsymbol{j} = \mathrm{curl}\, \boldsymbol{h}$. Using $j_{xG} = \mathrm{i}G_y h_{zG}$, $j_{yG} = -\mathrm{i}G_x h_{zG}$, $j_{zG} = \mathrm{i}(G_x h_{yG} - G_y h_{xG})$, and h_{iG} of eqs. (4) and (5), we obtain after simple manipulations

$$8\pi\mathcal{F} = B^2 \sum_{\boldsymbol{G}} (1 + \lambda^2 m_{zz}G^2)/d(\boldsymbol{G}). \tag{7}$$

The denominator $d(\boldsymbol{G})$ can be transformed to the more convenient form

$$d = (1 + \lambda^2 m_{zz}G_x^2 + \lambda^2 m_3 G_y^2)(1 + \lambda^2 m_1 G^2) \tag{8}$$

with the help of the identities: $m_{xx}m_{zz} - m_{xz}^2 = m_1 m_3$, $m_{xx} + m_{zz} = m_1 + m_3$ that follow from eqs. (2). In all terms of the sum (7) except that of $\boldsymbol{G} = 0$, $\lambda^2 G_{x,y}^2 \gg 1$ because $|G|_{\min} \approx L^{-1}$. Therefore,

$$8\pi\mathcal{F} = B^2 + (B^2 m_{zz}/\lambda^2 m_1)\sum{}' (m_{zz}G_x^2 + m_3 G_y^2)^{-1}, \tag{9}$$

where $\Sigma' = \Sigma_{\boldsymbol{G}\neq 0}$.

Note that the (x, z) plane (see fig. 1) has to be a symmetry plane for the vortex lattice, because it is a symmetry plane of the crystal and of the external field [‡1]. If the anisotropy would have vanished, this plane would have to coincide with one of the two essentially different symmetry planes of the equilateral triangular lattice (s_1, z) or (s_2, z) (see fig. 2a). This

[‡1] Strictly speaking, the external field is symmetric with respect to the combined operation $\sigma_{xz}\cdot R$, where σ_{xz} is the reflection plane (x, z) and R is the time inversion. The crystal is symmetric with respect to σ_{xz} and R separately, i.e., the $\sigma_{xz}\cdot R$ is the common symmetry element of both the field and the crystal. Thus, the magnetic structure of the vortex lattice cannot change under $\sigma_{xz}\cdot R$.

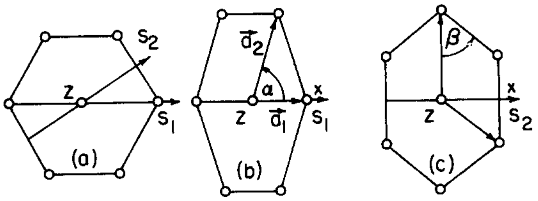

Fig. 2. (a) The (s_1, z) and (s_2, z) planes are the symmetry planes of the equilateral triangular lattice of the isotropic case. (b) The $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are the primitive cell vectors; the (s_1, z) plane coincides with (x, z). (c) The alternative structure; the (s_2, z) plane coincides with (x, z).

means that we have only two possible lattices in our case [6]; they are shown in figs. 2b, c.

Consider first the situation of fig. 2b and denote the primitive cell vectors as $\boldsymbol{a}_1 = x\hat{x}$, $\boldsymbol{a}_2 = \frac{1}{2}x\hat{x} + y\hat{y}$. Then, the reciprocal lattice is given by

$$G_{pq} = (2\pi/S)[py\hat{x} + (q - \tfrac{1}{2}p)x\hat{y}],$$

where the cell area $S = xy = \phi_0/B$. The free energy (9) transforms now to

$$8\pi\mathcal{F} = B^2 + (\phi_0^2 m_{zz}/4\pi^2\lambda^2 m_1)$$

$$\times \sum_{pq}{}' [m_{zz}p^2y^2 + m_3(q - \tfrac{1}{2}p)^2x^2]^{-1},$$

where Σ'_{pq} means that p and q cannot be zero simultaneously.

Under fixed B, the free energy has a minimum with respect to possible changes in a lattice structure. Because $xy = \phi_0/B = \text{const.}$, we have only one variational parameter in the problem. We can choose it as $t = y/x = \frac{1}{2}\tan\alpha$, where α is the angle between $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ (see fig. 2b). Then the variable part (Σ') of the free energy is proportional to

$$t\sum{}' [(m_{zz}/m_3)t^2p^2 + (q - \tfrac{1}{2}p)^2]^{-1}. \qquad (10)$$

In the isotropic case all masses are equal, and the last sum $t\Sigma'[t^2p^2 + (q - \frac{1}{2}p)^2]^{-1}$ is a minimum for the equilateral triangular lattice, i.e., at $t_0 = \frac{1}{2}\tan 60° = \frac{1}{2}\sqrt{3}$. The sum (10) depends upon $t(m_{zz}/m_3)^{1/2}$ as a parameter; therefore, it is a minimum at $t(m_{zz}/m_3)^{1/2} = \frac{1}{2}\sqrt{3}$ or for

$$\tan\alpha = (3m_3/m_{zz})^{1/2}. \qquad (11)$$

For a lattice of vortices normal to the layers ($\theta = 0$, $m_3 = m_{zz}$), this gives $\alpha = 60°$ as it should be. For a lattice in the layer plane ($\theta = \pi/2$, $m_{zz} = m_1$), $\tan\alpha = (3m_3/m_1)^{1/2}$ yields $\alpha \approx 80°$ in the case of $NbSe_2$, where $m_3/m_1 \approx 11$ according to ref. [3]. Formula (11) gives the angle α as a function of the vortex orientation θ in the crystal via $m_{zz}(\theta)$ [see eq. (2)].

For the second alternative lattice (fig. 2c), a similar argument gives

$$\tan\beta = (3m_{zz}/m_3)^{1/2}, \qquad (12)$$

where β is shown in fig. 2c. In $NbSe_2$, the angle β changes from $60°$ at $\theta = 0$ to $\approx 27.6°$ at $\theta = \pi/2$.

A straightforward comparison shows that the free energies (9) of the two lattices considered are equal. This degeneracy, however, might be just a feature of the London approximation. A better theory or an experiment may show that one of the structures is more stable ‡2.

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‡2 Dobrosavljević and Raffy [7] argue that the two structures are of the same free energy in the field region near H_{c2}. However, as was pointed out in ref. [6], "only one kind of flux line lattice (that of fig. 2c) is observed in experiment".

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