# Minimum-energy vortex configurations in anisotropic superconductors

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In a type-II superconductor, the optimal vortex configuration is the one that minimizes the free energy for a given value of **B**, the spatial average of the magnetic field. Using anisotropic London theory, we compare the free energy of two very different configurations: (I) a lattice of vortex lines parallel to **B** and (II) a combination of a lattice of lines parallel to  $\hat{\mathbf{c}}$  and a lattice of lines parallel to  $\hat{\mathbf{a}}$ , producing the same **B** as in (I). For large enough anisotropy, configuration (II) can have the lower free energy, for a wide range of **B**.

#### I. INTRODUCTION

The structure of the vortex lattice in highly anisotropic type-II superconductors is a topic that has received much theoretical attention in recent years, chiefly due to interest in the high- $T_c$  oxide compounds. When the average magnetic field **B** is not parallel to one of the crystal symmetry axes, finding the configuration of vortices that minimizes the free energy can be a nontrivial task. For example, at low *B* vortex "chain" phenomena turn out to be important.<sup>1-4</sup>

Several recent papers have explored the idea that a lattice of vortices, with each vortex line parallel to **B**, is not necessarily the optimal configuration. Daemen *et al.*,<sup>5</sup> using London theory, show that when the sample is a finite slab, a mixture of two types of vortices, neither one parallel to **B**, can have a lower free energy. Bulaevskii, Ledvij, and Kogan,<sup>6</sup> using the Lawrence Doniach model, claim that when **B** is almost parallel to the *a-b* plane, a "combined lattice" consisting of vortices parallel to  $\hat{c}$  and vortices parallel to  $\hat{a}$  can be optimal. Sardella and Moore<sup>7</sup> perform a stability analysis on a lattice of vortex lines parallel to **B**, and find that in some cases an unstable mode exists.

In this paper we use the London theory in an infinite medium; thus none of our results depend on boundary effects or on additional physics added by the Lawrence Doniach model. Our goal is to minimize the free energy at fixed **B**. We compare two possibilities.

Case I. An array of vortex lines parallel to **B**, arranged in the Bravais lattice shown in Fig. 1.

Case II. A lattice of vortex lines parallel to  $\hat{\mathbf{c}}$  plus a lattice of vortex lines parallel to  $\hat{\mathbf{a}}$ , producing the same **B** as in case I.

We find that for large enough anisotropy case II can have a lower free energy for a whole range of angles and field strengths. Of course there are many other interesting states to consider besides cases I and II. In this paper we simply want to make clear that case I is not always the best, even in a simple London theory calculation with no boundary effects.

#### **II. LONDON THEORY**

To do our calculation we use the London formalism as described in our previous paper.<sup>4</sup> We treat an anisotropic superconductor, with mutually perpendicular symmetry axes  $\hat{a}$ ,  $\hat{b}$ , and  $\hat{c}$ ; the effective mass tensor is given by

$$M_{ij} = M_c \hat{c}_i \hat{c}_j + M_a (\hat{a}_i \hat{a}_j + \hat{b}_i \hat{b}_j) , \qquad (1)$$

normalized so that det  $(M) = M_c M_a^2 = 1$ . The average penetration depth is  $\lambda$ , and an anisotropy parameter  $\gamma$  is defined by

$$\gamma = (M_c / M_a)^{1/2} . (2)$$

In this paper we are only interested in the case  $\gamma > 1$ . The free energy is given by

$$F = \frac{1}{8\pi} \int d^3x \left[ h^2 + \lambda^2 (\nabla \times \mathbf{h}) \vec{M} (\nabla \times \mathbf{h}) \right] \,. \tag{3}$$

One crucial result, which can easily be seen using (3), is that the interaction energy between a vortex line parallel to  $\hat{c}$  and a vortex line parallel to  $\hat{a}$  is zero. Thus when we calculate the free energy for case II, we can simply add together the energy of each vortex lattice. So for either case I or case II we need the energy density of a lattice of vortex lines, parallel to an arbitrary axis which we denote by  $\hat{z}$ . We take  $\hat{z}$  to be at an angle  $\theta$  with respect to the  $\hat{c}$ 



FIG. 1. The vortex line Bravais lattice in the xy plane.

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$$\hat{\mathbf{z}} = \hat{\mathbf{c}} \cos\theta + \hat{\mathbf{a}} \sin\theta , \qquad (4)$$

$$\hat{\mathbf{x}} = -\hat{\mathbf{c}}\sin\theta + \hat{\mathbf{a}}\cos\theta , \qquad (5)$$

$$\hat{\mathbf{y}} = \hat{\mathbf{b}}$$
 (6)

vortices are located at the point  $\mathbf{R} \pm \boldsymbol{\beta}$ , where  $\boldsymbol{\beta}$  is given by

basis, in the xy plane. The lattice vectors are given by

$$eta = rac{a}{4} \mathbf{\hat{x}} + rac{L}{4} \mathbf{\hat{y}}$$
 .

For case II we need to combine the answers for  $\theta = 0^{\circ}$  and  $\theta = 90^{\circ}$ .

The vortices form a Bravais lattice, with a two-point

The free energy density is then given by<sup>4</sup>

 $\mathbf{R} = n_1 a \mathbf{\hat{x}} + n_2 L \mathbf{\hat{y}};$ 

$$F(a,L,\theta) = \frac{\Phi_0^2}{2\pi a^2 L^2} \sum_{\{\mathbf{G}\}} \phi(\mathbf{G}) \frac{[1 + \lambda_1^2 G^2 (1 + \varepsilon \cos^2 \theta)] \cos^2(\mathbf{G} \cdot \beta)}{[1 + \lambda_1^2 G^2] [1 + \lambda_1^2 G_y^2 (1 + \varepsilon) + \lambda_1^2 G_x^2 (1 + \varepsilon \cos^2 \theta)]}$$
(9)

Here, the reciprocal lattice vectors G are given by

$$\mathbf{G} = n_1 \frac{2\pi}{a} \mathbf{\hat{x}} + n_2 \frac{2\pi}{L} \mathbf{\hat{y}} .$$
 (10)

The average magnetic field is parallel to  $\hat{z}$ , and given by

$$\frac{1}{aL} \int \int_{\text{cell}} dx \, dy \, h_z = 2\Phi_0 \frac{1}{aL} \,. \tag{11}$$

We have introduced a cutoff function  $\phi(\mathbf{G})$ , since otherwise the sum over  $\mathbf{G}$  diverges at large  $|\mathbf{G}|$ . This reflects the breakdown of London theory at short length scales. We follow the suggestion of Brandt,<sup>8</sup> and use an anisotropic Gaussian

$$\phi(\mathbf{G}) = \exp\{-\alpha [G_x^2 \xi_x^2 + G_y^2 \xi_y^2]\} .$$
(12)

Here  $\alpha$  is a numerical parameter, of the order of unity, and the coherence lengths are defined by



FIG. 2. Free energy as a function of *B*, for case I and case II. The magnetic field tilting angle is  $\beta = 60^{\circ}$ . Parameter values are  $\kappa = 60$ ,  $\alpha = 0.02$ , and  $\gamma = 100$ . The two curves intersect at  $\log_{10}(\lambda^2 B / 2\Phi_0) \approx 0.03$ , which is indicated by the cross.

$$\frac{\xi_x^2}{\xi_y^2} = \cos^2\theta + \frac{1}{\gamma^2}\sin^2\theta \tag{13}$$

and

$$\xi_{y}^{2} = \gamma^{2/3} \frac{\lambda^{2}}{\kappa^{2}}$$
 (14)

Here  $\kappa$  is an averaged Ginzburg-Landau parameter. We will usually take  $\kappa = 60$  and  $\alpha = 0.02$ .

We define  $\mathcal{F}(B,\theta)$  in the following way:

$$\mathcal{F}(B,\theta) = \min_{a,L,aL = 2\Phi_0/B} F(a,L,\theta) .$$
(15)

That is, we adjust a and L to minimize (9), subject to the condition that  $B = 2\Phi_0/aL$ .

#### **III. RESULTS**

We now express the energy densities for case I and case II in terms of the  $\mathcal{F}(B,\theta)$  of Eq. (15). We take the mag-



FIG. 3. Free energy as a function of *B*, for case I and case II. The magnetic field angle is  $\beta = 60^{\circ}$ . Parameter values are  $\kappa = 60$ ,  $\alpha = 0.02$ , and  $\gamma = 5$ .

(7)

(8)

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FIG. 4. Phase diagram in the  $\gamma$ -B space. In the region labeled II, configuration II has the lower free energy; in the region labeled I, configuration I has the lower free energy. The magnetic field angle is  $\beta = 60^{\circ}$ , while the other parameters are given by  $\alpha = 0.02$  and  $\kappa = 60$ .



FIG. 6. The free energy difference,  $\mathcal{F}_{I} - \mathcal{F}_{II}$ , as a function of the angle  $\beta$ . Curves for two different values of *B* are shown. Parameter values are  $\kappa = 60$  and  $\alpha = 0.02$ .

For case I, then, we have

$$\mathcal{F}_{\mathbf{I}}(\boldsymbol{B},\boldsymbol{\beta}) = \mathcal{F}(\boldsymbol{B},\boldsymbol{\beta}) \ . \tag{18}$$

For case II we have

$$\mathcal{F}_{\mathrm{II}}(B,\beta) = \mathcal{F}(B\cos(\beta),\theta=0^{\circ}) + \mathcal{F}(B\sin(\beta),\theta=90^{\circ}) .$$
(19)

So the expression in (19) is the sum of two terms: a vor-



FIG. 7. Magnified version of Fig. 6, showing the region from  $\beta = 80^{\circ}$  to  $\beta = 90^{\circ}$  in more detail. For both curves the free energy difference reaches zero at  $\beta = 90^{\circ}$ , as it should.



$$\mathbf{B} = B_a \mathbf{\hat{a}} + B_c \mathbf{\hat{c}} = B \sin\beta \mathbf{\hat{a}} + B \cos\beta \mathbf{\hat{c}} , \qquad (16)$$

$$B = \sqrt{B_a^2 + B_c^2} \ . \tag{17}$$



FIG. 5. This figure illustrates the effect of changing the cutoff parameter  $\alpha$  on the  $\gamma$ -B phase diagram. Two phase boundaries are shown, one for  $\alpha = 0.02$  and one for  $\alpha = 0.005$ . Other parameter values are  $\beta = 60^{\circ}$  and  $\kappa = 60$ .

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In Fig. 2 we show a plot of  $\mathcal{F}_{I}$  and  $\mathcal{F}_{II}$  as functions of *B*, for  $\beta = 60^{\circ}$  and  $\gamma = 100$ . The noteworthy feature is that  $\mathcal{F}_{II}$  is actually slightly lower than  $\mathcal{F}_{I}$  up to  $\log_{10}(\lambda^2 B/2\Phi_0) \approx 0.03$ . Figure 3 shows the same plot for  $\gamma = 5$ . At this much lower value for the anisotropy parameter,  $\mathcal{F}_{I}$  is always lower. Finally in Fig. 4 w show the phase diagram in the  $\gamma$ -*B* space, with  $\beta = 60^{\circ}$ . There is a large region, at higher  $\gamma$  and lower *B*, where  $\mathcal{F}_{II}$  is lower than  $\mathcal{F}_{I}$ . We thus find, perhaps surprisingly, that the combination of a 0° vortex lattice and a 90° vortex lattice can have the lower free energy, at fixed **B**.

We can test the sensitivity of our result to the cutoff parameter. In Fig. 5, we show the phase diagram, for  $\beta = 60^{\circ}$ , for two different values of the cutoff parameter  $\alpha$ . Changing  $\alpha$  by a factor of 4 simply causes a small shift in the phase diagram.

It is also of interest to investigate the range of angle  $\beta$ over which  $\mathcal{F}_{II}$  is lower than  $\mathcal{F}_{I}$ . In Fig. 6 we plot  $\mathcal{F}_{I} - F_{II}$  as a function of  $\beta$ , for fixed  $\gamma$  and  $|\mathbf{B}|$ . We see that  $\mathcal{F}_{II}$  is lower over a wide range of angles, for the two values of  $|\mathbf{B}|$  chosen. We also note that the two curves display interesting structure near 90°; this structure is shown in more detail on the expanded plot of Fig. 7.

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IV. DISCUSSION

Our results show that, in the framwork of a welldefined London theory with a cutoff, a combination of two perpendicular vortex lattices can have a lower free energy than a single vortex lattice with the same **B**. This provides another example of the surprising features arising from vortices in anisotropic superconductors.

As can be seen from Fig. 1, at  $\gamma = 100$  case II is lower in free energy than case I by only a small amount. It is therefore important to go beyond London theory, and treat the vortex energetics with a more accurate theory; in particular, an approach which handles vortex core effects more carefully, such as the Ginzburg-Landau theory, should be applied. We hope to turn to this work in the future.

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