# Minimum-energy vortex configurations in anisotropic superconductors

G. Preosti and Paul Muzikar

Department of Physics, Purdue University, West Lafayette, Indiana 47907

(Received 4 June 1993)

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 Band (II) a combination of a lattice of lines parallel to  $\hat{c}$  and a lattice of lines parallel to  $\hat{a}$ , 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.

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. $1 - 4$ 

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  $\bf{B}$  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  $\hat{c}$  plus a lattice of vortex lines parallel to  $\hat{a}$ , 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. The vortex line Bravais lattice in the xy plane.

#### I. INTRODUCTION **II. LONDON THEORY**

To do our calculation we use the London formalism as described in our previous paper. $4$  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

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

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

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

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  $\hat{c}$ 



## 9922 G. PREOSTI AND PAUL MUZIKAR

$$
basis: basis: basic basic basic basic basic basic basic white white white white vertices vector size given by basic white white white value vector size time value value
$$

$$
\hat{\mathbf{z}} = \hat{\mathbf{c}} \cos \theta + \hat{\mathbf{a}} \sin \theta , \qquad (4) \qquad \mathbf{R} = n_1 a \hat{\mathbf{x}} + n_2 L \hat{\mathbf{y}} ;
$$

$$
\hat{\mathbf{x}} = -\hat{\mathbf{c}}\sin\theta + \hat{\mathbf{a}}\cos\theta \tag{5}
$$

$$
\hat{\mathbf{y}} = \mathbf{\hat{b}} \tag{6}
$$

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

$$
\beta = \frac{a}{4}\mathbf{\hat{x}} + \frac{L}{4}\mathbf{\hat{y}}.
$$

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>

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

Here, the reciprocal lattice vectors  $G$  are given by

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

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

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

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

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

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°. 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

$$
\xi_y^2 = \gamma^{2/3} \frac{\lambda^2}{\kappa^2} \tag{14}
$$

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

We define  $\mathcal{J}(B,\theta)$  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  $\mathcal{J}(B,\theta)$  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.

 $(7)$ 

 $(8)$ 

### MINIMUM-ENERGY VORTEX CONFIGURATIONS IN ...







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

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

For case II we have

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

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



FIG. 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° and  $\kappa$  = 60.

 $log_{10}(\lambda^2B/2\Phi_0)$ 

 $\overline{1}$ 

 $-2$ 

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

netic field **B** to be

300

225

 $~150$ 

75

 $\Omega$  $-3$   $\beta = 60^{\circ}$ 

 $\kappa = 60$ 

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

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

 $\alpha = .02$ 

 $\alpha = .005$ 

 $\circ$ 

 $\overline{1}$ 

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°. 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°, 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  $|B|$  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.

- <sup>1</sup>A. I. Buzdin and A. Yu. Simonov, Physica C 175, 143 (1991).
- <sup>2</sup>A. M. Grishin, A. Yu. Martynovich, and S. V. Yampol'skii, Zh. Eksp. Teor. Fiz. 97, 1930 (1990) [Sov. Phys. JETP 70, 1089 (1990).
- <sup>3</sup>L. L. Daemen, L. J. Campbell, and V. G. Kogan, Phys. Rev. B 46, 3631 (1992).
- 4G. Preosti and P. Muzikar, Phys. Rev. B 47, 8831 (1993).

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.

#### **ACKNOWLEDGMENTS**

This work was supported by the National Science Foundation under Grant No. DMR88-09854 through the Science and Technology Center for Superconductivity, and by DOE Grant No. DE-FG02-90ER45427 through the Midwest Superconductivity Consortium.

- 5L. L. Daemen, J.J. Campbell, A. Yu. Simonov, and V. G. Kogan, Phys. Rev. Lett. 70, 2948 (1993).
- L. N. Bulaevskii, M. Ledvij, and V. G. Kogan, Phys. Rev. B 46, 366 (1992).
- 7E. Sardella and M. A. Moore (unpublished).
- E. H. Brandt, Physica C 195, <sup>1</sup> (1992).