Generalized London free energy for high-T_c vortex lattices

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(Received 21 August 1996)

We generalize the London free energy to include fourfold anisotropies that could arise from d-wave pairing or other sources in a tetragonal material. We use this simple model to study vortex lattice structure and discuss neutron scattering, scanning tunneling microscopy, Bitter decoration, and muon-spin-rotation experiments. [S0163-1829(97)50402-4]

The London free energy provides a very simple way of studying the vortex lattice in an extreme type-II superconductor. The conventional isotropic model[1] predicts a hexagonal vortex lattice with an arbitrary orientation relative to the ionic lattice. Recent neutron scattering[2] and scanning tunneling microscopy[3] (STM) experiments on high-T_c compound $YBa_2Cu_3O_{7-\delta}$ (YBCO) revealed vortex lattices with centered rectangular symmetry and a specific orientation with respect to the ionic lattice. It has been proposed that this effect can arise from additional quartic derivative terms in the Ginzburg-Landau (GL) free energy[4–7] or, alternatively, from including two or more order parameters (such as d and s) in the GL free energy with derivative mixing terms reflecting the ionic lattice symmetry.[8–11] Such models predict interesting effects in the behavior of the various order parameters in the vortex lattice. However, these models contain a large number of unknown parameters and are rather cumbersome to work with numerically. Another approach[12,13] to the macroscopic effects of d-wave pairing takes into account the generation of quasiparticles near the gap nodes due to current flow and thermal excitation. This leads to a nonlinear relationship between supercurrent and superfluid velocity which becomes singular at $T\to 0$.

The purpose of this paper is to present a simple and general approach to these effects based on a generalization of the London free energy to include anisotropy of fourfold symmetry, characteristic of a tetragonal ionic lattice. The number of new parameters is far smaller than in the GL approach (a reasonable model contains only one new parameter) and numerical simulations are considerably easier. It provides a useful model to study vortex lattice structure, pinning by twin boundaries, and the magnetic-field distribution measured in muon-spin-rotation (μSR) experiments. The model is suitable to study the intermediate field region $H_{c1}\ll H\ll H_{c2}$ which is experimentally most relevant but traditionally difficult to handle within the GL theory. Furthermore, this approach can be extended to $T=0$ where GL theory breaks down and the supercurrent becomes singular.

We now present a derivation of the generalized London model, starting from a GL free-energy density with both d and s order parameters:[8,14,15]

$$f=\alpha_s|s|^2+\alpha_d|d|^2+\gamma_s|\vec{\Pi}s|^2+\gamma_d|\vec{\Pi}d|^2+f_4+h^2/8\pi + \gamma_v[(\Pi_y s)^*(\Pi_y d)-(\Pi_x s)^*(\Pi_x d)+\text{c.c.}]. \tag{1}$$

Here $\vec{\Pi}\equiv -i\nabla - e^*\vec{A}/\hbar c$ and f_4 contains the quartic terms. We shall consider a case of a d-wave superconductor in which s identically vanishes in zero magnetic field. In finite field ($H>H_{c1}$) a small s component with a highly anisotropic spatial distribution is nucleated in the vicinity of a vortex giving rise to nontriangular equilibrium lattice structures.[9,10] Our strategy will be to simplify free energy (1) by integrating out this s component in favor of higher-order derivative terms in d. In this process some short length-scale information on the order parameter is lost but the magnetic-field distribution is described accurately. Using its Euler-Lagrange equation s can be expressed to the leading order in $(1-T/T_c)$ as

$$s=(\gamma_v/\alpha_s)(\Pi_x^2-\Pi_y^2)d. \tag{2}$$

Substituting this into f gives the leading derivative terms in d of the form

$$f=\gamma_d[|\vec{\Pi}d|^2-(\gamma_v^2/\gamma_d\alpha_s)|(\Pi_x^2-\Pi_y^2)d|^2]+\cdots. \tag{3}$$

Various additional corrections to the free energy are obtained from integrating out s more accurately, taking into account the $\gamma_s|\vec{\Pi}s|^2$ term and quartic terms. However, these all involve higher powers of $\vec{\Pi}$ or other terms that will not concern us. The coefficient of the second term has dimensions of (length)^2; we will write it in the form $\epsilon\xi^2/3$ where $\epsilon\equiv 3(\alpha_d\gamma_v^2/\alpha_s\gamma_d^2)$ is a dimensionless parameter which controls the strength of the s-d coupling and $\xi\equiv\sqrt{\gamma_d/|\alpha_d|}$ is the GL coherence length. We henceforth assume $\epsilon\ll 1$. As we remark below, neutron scattering and STM experiments probably support this assumption. We note that a term of the form $|(\Pi_x^2-\Pi_y^2)d|^2$ could arise without invoking s-d mixing from a systematic derivation of higher order terms in the GL free energy starting with a BCS-like model and taking into account the square symmetry of the Fermi surface.[4–6,16]

The free energy of Eq. (3) is not bounded below, exhibiting runaway behavior for rapidly varying d fields. This is in fact cured by keeping additional higher derivative terms that also arise from integrating out s. Stability occurs for $\gamma_v^2 < \gamma_s \gamma_d$. In fact, the approximation of Eq. (3) will be sufficient for our purposes, yielding a local minimum which we expect would become a global minimum upon including the additional terms.

We now assume that the penetration depth $\lambda \gg \xi$. We may then assume that $|d(\vec{r})| \approx d_0$, the zero-field equilibrium value, almost everywhere in the vortex lattice, except within a distance of $O(\xi)$ of the cores. This gives the London free energy,

$$f_L = (1/8\pi)(\vec{B})^2 + \gamma_d d_0^2 \{ \vec{v}^2 - (\epsilon \xi^2/3) \times [(v_x^2 - v_y^2)^2 + (\partial_y v_y - \partial_x v_x)^2] \}, \tag{4}$$

written in terms of the superfluid velocity,

$$\vec{v} \equiv \vec{\nabla}\theta - (e^*/\hbar c)\vec{A}, \tag{5}$$

where θ is the phase of d.

The corresponding London equation, obtained by varying f_L with respect to $\vec{A}$, is

$$\frac{c}{4\pi}\vec{\nabla}\times\vec{B} = \left(\frac{2e^*}{\hbar c}\right)\gamma_d d_0^2 \{ \vec{v} - \tfrac{2}{3}\epsilon\xi^2 [(\hat{y}v_y - \hat{x}v_x)(v_y^2 - v_x^2) - (\hat{y}\partial_y - \hat{x}\partial_x)(\partial_y v_y - \partial_x v_x)] \}. \tag{6}$$

For many purposes it is very convenient to express $\vec{v}$ in terms of $\vec{B}$ and its derivatives, and then substitute this expression for $\vec{v}$ back into f_L, giving an explicit expression for f_L as a functional of $\vec{B}$ only. For $\epsilon = 0$ this gives

$$\vec{v}^{(0)} = \vec{\nabla}\times\vec{B}/B_0, \tag{7}$$

where $B_0 \equiv \phi_0/2\pi\lambda^2$ is of order H_{c1} ($\phi_0 \equiv 2\pi\hbar c/e^*$ is the flux quantum) and

$$f_L^0 = (1/8\pi)[\vec{B}^2 + \lambda_0^2(\vec{\nabla}\times\vec{B})^2]. \tag{8}$$

Here the penetration depth, for $\epsilon = 0$ is $\lambda_0^{-2} = 8\pi\gamma_d(e^* d_0/\hbar c)^2$. It is presumably not possible to solve Eq. (6) in closed form for $\vec{v}$ as a function of $\vec{B}$ for $\epsilon \neq 0$. However, this can be done readily in a perturbative expansion in ϵ. The first order correction is

$$\vec{v}^{(1)} = (2\epsilon\xi^2/3)\{ (\hat{y}v_y^{(0)} - \hat{x}v_x^{(0)})[(v_y^{(0)})^2 - (v_x^{(0)})^2] - (\hat{y}\partial_y - \hat{x}\partial_x)(\partial_y v_y^{(0)} - \partial_x v_x^{(0)}) \} \tag{9}$$

with $\vec{v}^{(0)}$ given by Eq. (7). The London free-energy density, up to $O(\epsilon)$ is then

$$f_L = f_L^0 + \frac{\epsilon\lambda_0^2\xi^2}{8\pi}[4(\partial_x\partial_y B)^2 + ((\partial_x B)^2 - (\partial_y B)^2)^2/B_0^2]. \tag{10}$$

Note that we could have arrived at a similar conclusion by simply writing down all terms allowed by symmetry in f_L, expanding in number of derivatives and powers of B. Square anisotropy is first possible in the fourth derivative terms. In principle, we should also include all isotropic terms to order B^4 and ∇^4. However, assuming that these have small coefficients, they will not be important. This result can also be obtained from considering generation of quasiparticles near gap nodes in a d-wave superconductor,[12] in a range of temperature and field where the supercurrent can be Taylor expanded in the superfluid velocity.[17] More generally, the quadratic and quartic terms in Eq. (10) have independent coefficients.

The corresponding London equation is obtained by varying f_L with respect to $\vec{B}(\vec{r})$. For B along the z direction one obtains

$$[1 - \lambda_0^2\nabla^2 + 4\epsilon\lambda_0^2\xi^2(\partial_x\partial_y)^2]B - \epsilon Q[B] = 0, \tag{11}$$

where

$$Q[B] = 2\lambda_0^2\xi^2 B_0^{-2}[(\partial_x^2 - \partial_y^2)B + \partial_x B\partial_x - \partial_y B\partial_y] \times [(\partial_x B)^2 - (\partial_y B)^2] \tag{12}$$

is the nonlinear term arising from the last term in Eq. (10).

To get a feeling for the effect of the extra terms, consider a weak field which depends only on x or else only on $(x+y)$. The solution of the linearized London equation [(11) without the last term] gives an exponentially decaying field with $\lambda = \lambda_0$ for variation along the x axis but $\lambda = \lambda_0\sqrt{[1 + (1 - 4\epsilon\xi^2/\lambda_0^2)^{1/2}]/2}$, for variation at 45° to the crystal axis. The penetration depth is longer along the crystal axis.

To determine vortex lattice structure we insert source terms $\Sigma_j \rho(\vec{r} - \vec{r}_j)$ at the vortex core positions, $\vec{r}_j$, on the right-hand side of Eq. (11). The source terms reflect the topological winding of the phase angle and the reduction of the order parameter in the core.[1] A commonly used phenomenological form is[18]

$$\rho(\vec{r}) = (\phi_0/2\pi\xi^2)e^{-r^2/2\xi^2}. \tag{13}$$

It is straightforward to solve these equations numerically for the vortex lattice by an iterative method. We find that the quartic term makes a negligible contribution. (Contrary to naive expectation, it does not become more important with increasing applied field because the field becomes nearly constant in the vortex lattice when the applied field is large.) Thus to an excellent approximation one may neglect $Q[B]$ in the London equation (11) and the magnetic field may be written explicitly as

$$B(\vec{r}) = \overline{B}\sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}e^{-k^2\xi^2/2}}{1 + \lambda_0^2 k^2 + 4\epsilon\lambda_0^2\xi^2(k_x k_y)^2}. \tag{14}$$

Here the sum is over all wave vectors in the reciprocal lattice and $\overline{B}$ is the average field. The lattice constant is determined by the condition that $\overline{B}\Omega = \phi_0$ where Ω is the area of the unit cell. The lattice symmetry is determined by minimizing the Gibbs free-energy $g_L = f_L - H\overline{B}/4\pi$. We find that the flux lattice has centered rectangular symmetry, with principal axes aligned with the ionic crystal lattice, with an angle β between unit vectors which depends on ϵ and the magnetic field. An example of such a centered rectangular lattice is

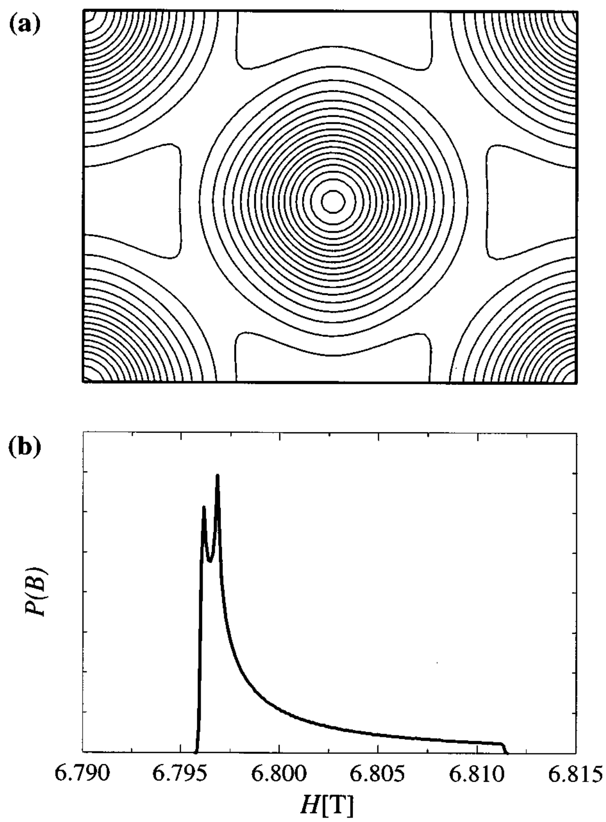

FIG. 1. (a) Distribution of magnetic field in a vortex lattice for $\epsilon=0.3$ and $H=6.8$ T, leading to an angle of $\beta\simeq 74°$. We use $\lambda_0=1400$ Å and $\kappa\equiv\lambda_0/\xi=68$. (b) Corresponding μSR line shape.

shown in Fig. 1(a). In agreement with earlier results within GL (Ref. 10) and Eilenberger[11] formalisms, individual vortices are elongated along the crystalline axes. Figure 2(a) shows the dependence of Gibbs free energy on β for various values of ϵ at fixed applied field $H=400B_0\simeq 6.8$ T. For $\epsilon=0$ minimum occurs for $\beta_{\rm MIN}=60°$, corresponding to a hexagonal lattice. As ϵ increases $\beta_{\rm MIN}$ continuously increases and for sufficiently large ϵ, the flux lattice becomes tetragonal with $\beta_{\rm MIN}=90°$. For $\beta_{\rm MIN}\neq 90°$, there are always two solutions, related by a 90° rotation, in which the long axis of the centered rectangle is aligned with either the x or y axis. The degeneracy is much larger for $\epsilon=0$, when the flux lattice may have an arbitrary orientation relative to the ionic crystal lattice.

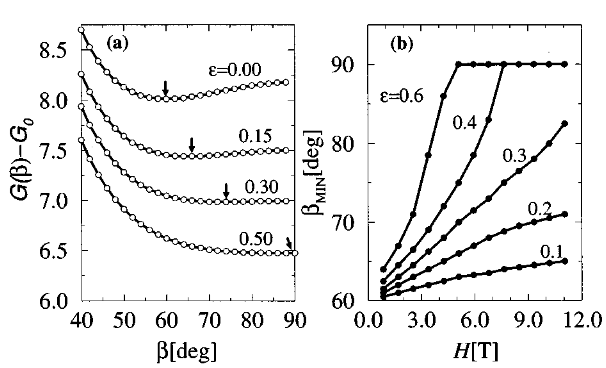

FIG. 2. (a) Gibbs free energy as a function of β for the same parameters as Fig. 1 and various values of ϵ. Arrows indicate positions $\beta_{\rm MIN}$ of the minima and $G_0\equiv -H^2/8\pi$. (b) Equilibrium angle $\beta_{\rm MIN}$ as a function of H for several values of ϵ.

Dependence of $\beta_{\rm MIN}$ on the applied field for various values of ϵ is displayed in Fig. 2(b). Clearly the anisotropic term becomes more important at larger fields. Our perturbative elimination of $\vec{v}$ in favor of B breaks down when ϵ and H are sufficiently large that $\beta_{\rm MIN}$ differs significantly from 60°. Furthermore, we might expect higher-order corrections to Eq. (4) to be important in this regime. By fitting Fig. 2(b) to experimental data on tetragonal materials such as $Tl_2Ba_2CuO_{6+d}$ (once such data become available) one can directly assess the magnitude of ϵ, the only unknown parameter in the model.

Our analysis can be easily extended to take into account effective mass (i.e., penetration depth) anisotropy. In a simple one-component GL model, the derivative term is generalized to

$$f=\sum_{i=x,y,z}\gamma_i|\Pi_i d|^2. \tag{15}$$

We restrict our attention to fields along the z axis. Then the anisotropy can be removed by a rescaling of the x coordinate and a corresponding rescaling of the magnetic field. The coherence length and penetration depth anisotropies are the same: $\xi_y/\xi_x=\lambda_x/\lambda_y$. We will make the simplifying assumption that the higher derivative and mixed derivative terms in f are also simply modified by a rescaling by a common factor. It then follows that the flux lattice shape is obtained by stretching along the x axis by the factor λ_x/λ_y. We now obtain two possible vortex lattices, both of centered rectangular symmetry, aligned with the ionic lattice, with different angles, β. (Relaxing our simplifying assumption may split the degeneracy between these two lattices.) On the other hand, when $\epsilon=0$, we may rotate the hexagonal lattice by an arbitrary angle before stretching. This gives an infinite set of oblique lattices with arbitrary orientation.

To compare theory with YBCO we should take into account twin boundaries which may also tend to align the vortex lattice by pinning vortices to the twin boundaries, at $\pm 45°$ to the x axis. This effect competes with alignment to the ionic lattice which we have been discussing. Only in the special case of a square vortex lattice does a line of vortices occur at $\pm 45°$. If this is not the case, and if pinning by twin boundaries is significant, then we should expect that the vortex lattice will align with the ionic lattice far from twin boundaries but will be deformed in the vicinity of a twin boundary in an effort to align itself with the twin boundary. On the other hand, for $\epsilon=0$, the vortex lattice would remain aligned with the twin boundaries everywhere except within vortex lattice domain boundaries which necessarily exist roughly midway between the twin boundaries.

Neutron-scattering experiments on YBCO (Ref. 2) suggest that the vortex lattice is well-aligned with the twin boundaries and is close to being centered rectangular (the ratio of lattice constants is about 1.04) with $\beta\approx 73°$, with weak dependence on H. This corresponds to a rotation away from alignment with the ionic lattice by 9°. Four different orientational domains, related by reflection in the (1,1,0) axis and 90° rotation were reported. These results can be rather well fitted[19] by the basic London model ($\epsilon=0$) with mass anisotropy. For $\lambda_x/\lambda_y=1.5$, a value roughly consistent with infrared and microwave experiments, this lattice has about the right shape. Taking into account the two crystallographic domains (related by interchanging λ_x and λ_y) there are all together four vortex lattice domains, as seen experimentally. The experimental fact that the vortex lattice appears to be well aligned with the twin boundaries suggests that the tendency to align with the ionic lattice is small. No evidence for a bending of the vortex lattice (by 9°) into alignment with the ionic lattice far from the twin boundaries has so far been found.

STM imaging of the YBCO vortex lattice[3] also suggests that the (highly disordered) lattice has approximately centered rectangular symmetry with $\beta\approx 77°$. However, no evidence for the 9° tilt into alignment with the twin boundaries was reported. Considering the observed anisotropy of the vortex cores it has been concluded that the mass anisotropy alone cannot account for the measured 77° angle of the vortex lattice. It has been suggested that a mechanism related to the internal symmetry of the order parameter (such as the one discussed in the present work) needs to be invoked in order to reconcile these observations.

Low-field Bitter decoration data on YBCO (Ref. 20) show vortex lattice geometry with a very small distortion from hexagonal, consistent with a much smaller anisotropy $\lambda_x/\lambda_y=1.11-1.15$. One may be tempted to attribute this apparent field dependence of β to the effects discussed above in connection with Fig. 2(b). An alternative explanation is a poor quality of samples used in the Bitter decoration experiments that may have resulted in partial washing out of the a-b plane anisotropy.[21]

μSR experiments measure the field distribution $P(B)=(1/\Omega)\int\delta[B-B(\vec{r})]dxdy$. This is shown in Fig. 1(b). For $\beta\neq 60°$, $B(\vec{r})$ has two inequivalent saddle points leading to two peaks in $P(B)$. $P(B)$ is unaffected by effective-mass anisotropy, as can be shown by the rescaling transformation, mentioned above. Existing μSR experiments show only a single peak,[22] but broadening due to the finite muon lifetime or other effects might possibly obscure the second peak.

The weak-field dependence of β, the alignment with twin boundaries in the neutron-scattering experiments, and the single peak in $P(B)$ suggest that ϵ is small in YBCO and that the normal London model, together with twin boundary pinning, provides a good fit to the data. STM and Bitter decoration data on the other hand seem to favor finite ϵ and weak pinning to twin boundaries. Further experimental work, preferably on untwinned YBCO or other tetragonal superconductors, will probably be necessary to clarify the importance of square lattice anisotropy in high-T_c superconductors. It is our hope that the present model will serve as a useful tool for interpretation of such experiments.

The general approach to vortex lattices introduced here may be extended to low temperatures, but then the free energy takes a quite different form which is nonanalytic in B at $T\rightarrow 0$.[12,17]

We would like to thank A. J. Berlinsky, R. E. Kiefl, and J. E. Sonier for helpful discussions. This research was supported by NSERC, the CIAR, and NSF Grant No. DMR-9415549 (M.F.).

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