Simple Ginzburg-Landau Theory for Vortices in a Crystal Lattice

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We study the Ginzburg-Landau model with a nonlocal quartic term as a simple phenomenological model for superconductors in the presence of coupling between the vortex lattice and the underlying crystal lattice. In mean-field theory, our model is consistent with a general oblique vortex lattice ranging from a triangular lattice to a square lattice. This simple formulation enables us to study the effect of thermal fluctuations in the vortex liquid regime. We calculate the structure factor of the vortex liquid nonperturbatively and find Bragg-like peaks with fourfold symmetry appearing in the structure factor even though there is only a short-range crystalline order. [S0031-9007(97)03333-4]

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It is of great interest to study vortex lattice structure and correlations in superconductors in the presence of coupling between the vortex lattice and the underlying crystal lattice. Various experimental probes including neutron diffraction [1], Bitter decoration [2], and scanning tunneling microscopy [3,4] have been used to reveal a range of vortex lattice structures from the usual triangular lattice to a general oblique lattice and a square lattice oriented along a specific direction of the crystal axis. An important feature of these structures is the emergence of the fourfold symmetry representing the symmetry of the underlying crystal lattice. This effect of the crystal lattice on the vortex lattice is found to be dependent upon the external field in such a way that a triangular vortex lattice is observed at low fields, while at higher fields a square lattice is observed [4].

In order to study the vortex lattice structure, one usually uses a Ginzburg-Landau (GL) phenomenological theory. Since the usual GL theory is rotationally invariant, one needs additional terms that break this symmetry to account for the appearance of the fourfold symmetric vortex lattice structure. The conventional way to include this effect is to introduce terms quadratic in the order parameter in the GL free energy with fourth order derivatives [4–6]. The observed fourfold symmetric vortex lattice structure can be explained within these formalisms. However, the equations involved in these theories are very difficult to handle even at the linearized level where one has to resort to approximate or numerical methods.

In this paper we propose a much simpler phenomenological model for vortices in a crystal lattice. Our model is the usual GL theory for a one-component complex order parameter, except that the term quartic in the order parameter, $\Psi(\mathbf{r})$ is *nonlocal*. We consider the situation where the effect of the underlying crystal on the order parameter symmetry can be summarized into an appropriate form for the nonlocal interaction potential. The vortex lattice structure is determined within our model without much calculational effort. We find that the fourfold symmetric vortex lattice structure can be modeled with the appropriate choice of a minimal number of parameters describing the nonlocal quartic interaction. The a-b plane anisotropy found in high-temperature superconductors is also incorporated in our model in the usual way through second order gradient terms. We believe that this model captures the same physics as in the higher derivative approaches of Ref. [4–6], but is just much simpler to handle calculationally.

One feature of our simple formulation is that it allows a study of the effect of thermal fluctuations in the vortex liquid regime. This would be quite impossible in the conventional formulations. We apply the nonperturbative method developed by us in Ref. [7] to calculate the structure factor of the vortex liquid, which is measured in neutron scattering experiments. One of the main results of the present work is that one can observe in the structure factor the ring patterns expected for a liquid state but broken up into Bragg-like peaks. This suggests that even in the vortex liquid state where there is a short-range crystalline order, a weak fourfold symmetric coupling to the underlying crystal may produce the spots observed in neutron scattering experiments and usually attributed to the formation of the vortex crystal state.

The model we study in this paper is based on the GL free energy with a nonlocal quartic interaction for a two-dimensional superconductor in a magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$,

$$F[\Psi] = \int d^2\mathbf{r}\left(\frac{\hbar^2}{2m_x}|D_x\Psi|^2 + \frac{\hbar^2}{2m_y}|D_y\Psi|^2 + \alpha|\Psi(\mathbf{r})|^2\right) + \frac{\beta}{2} \times \int d^2\mathbf{r}_1\, d^2\mathbf{r}_2 |\Psi(\mathbf{r}_1)|^2 g(\mathbf{r}_1 - \mathbf{r}_2)\, |\Psi(\mathbf{r}_2)|^2, \quad (1)$$

where α, β are phenomenological parameters, m_x the effective mass in the x direction, m_y in the y direction, and $\mathbf{D} = -i\nabla - (e^*/\hbar c)\mathbf{A}$. The a-b plane anisotropy is represented by the ratio of the effective masses. For later use, we define $\sigma \equiv (m_x/m_y)^{1/4}$. The only difference between our model and the usual GL theory is the nonlocal quartic interaction term represented here by a

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general function $g(\mathbf{r}) = g(x, y)$, which is equal to the delta function $\delta^{(2)}(\mathbf{r})$ for the usual local GL theory.

One reason we study the two-dimensional version of the model in this paper is that one can easily apply the nonperturbative method in Ref. [7] to calculate the vortex liquid structure factor. But, more importantly, as noted by one of us [8], the phase correlation length parallel to the field direction in a bulk superconductor grows exponentially as one approaches zero temperature. When this length scale becomes comparable to or larger than the sample size in the low-temperature regime, the system effectively behaves as a two-dimensional thin film with phase coherence across the sample and a very low effective temperature [8]. We note that most of the experiments mentioned earlier are performed in this regime, and we expect that they can be described by the present model when the parameter α is set to large negative values, i.e., low temperatures.

A nonlocal quartic interaction as in (1) appeared in the renormalization group study [9] of this system near its upper critical dimension. Even if one starts from a local theory, renormalization always drives the quartic term into an effective nonlocal one. It is not our aim here to derive an explicit form of $g(\mathbf{r})$ from a microscopic theory. Instead, we take (1) as our starting point for the phenomenological description of superconductors in the presence of an interaction between the vortex lattice and the crystal lattice, and show that the variety of vortex lattice structures observed in experiments can be explained using a very simple form of $g(\mathbf{r})$.

The main ingredient one has to incorporate into the phenomenological construction of $g(\mathbf{r})$ is the presumed fourfold symmetry of the underlying crystal. (Generalizations to other crystal symmetries are, of course, possible.) In the present work, we construct $g(\mathbf{r})$ such that it contains a term with explicit fourfold symmetry in addition to a rotationally symmetric term. Thus, we take for the Fourier transform $\tilde{g}(\mathbf{k}) \equiv \int d^2\mathbf{r}\, g(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$,

$$\tilde{g}(\mathbf{k}) = \exp\{-C(k/\mu)^4[1 - \varepsilon\cos 4(\theta + \theta_0)]\}, \qquad (2)$$

where $\mathbf{k} = (k\cos\theta, k\sin\theta)$ and $\mu = \sqrt{e^* B/\hbar c}$ is the inverse magnetic length. In particular, $\tilde{g}(\mathbf{k}) = \exp\{-C[(1-\varepsilon)(k_x^4 + k_y^4) + 2(1+3\varepsilon)k_x^2 k_y^2]/\mu^4\}$ for $\theta_0 = 0$. In (2), we introduced three parameters C, ε, and θ_0 in such a way that the overall constant C controls the strength of the interaction between the vortex lattice and the underlying crystal (note that when $C \to 0$, a local GL theory is recovered), and the dimensionless parameter ε $(0 \le \varepsilon < 1)$ represents the strength of the fourfold symmetric interaction compared to the rotationally symmetric one. As will be discussed later, θ_0 controls the orientation of the vortex lattice with respect to the underlying crystal. This choice for $\tilde{g}$ is certainly not unique. One could use various other forms with a fourfold symmetric term as long as they are positive definite (to ensure the stability of GL theory) and they do not introduce any unphysical nonanalyticity [note that in order to ensure the analyticity of $\tilde{g}(\mathbf{k})$ near $\mathbf{k} = 0$ with the $\cos 4\theta$ term, we need at least k^4 terms in (2)]. But, in the presence of the growing length scale mentioned earlier, we might expect that universality applies and the present form of the nonlocal quartic interaction does not alter the physical results. Note that we measure the wave vectors with respect to the inverse magnetic length. But this is just for convenience in later calculations. A more natural length scale for the nonlocal kernel will be the lattice spacing of the crystal lattice, l_0. Therefore, the dimensionless parameter C which appears in (2) will depend on the ratio of two length scales, i.e., $C \sim (l_0\mu)^4$. As the magnetic field increases, the intervortex spacing, μ^{-1}, gets smaller, so the nonlocal interaction term becomes more important. This qualitative feature of our model is consistent with experimental findings where the fourfold symmetric vortex lattice structure is observed only in the high field regime.

It is convenient to map the free energy functional of Eq. (1) into a form with isotropic gradient terms using the following transformations: $\mathbf{a}(\mathbf{r}') = (a_x(\mathbf{r}'), a_y(\mathbf{r}')) \equiv (\sigma^{-1}A_x(\mathbf{r}), \sigma A_y(\mathbf{r}))$, and $h(\mathbf{r}') \equiv g(\mathbf{r})$, where $\mathbf{r}' = (x', y') \equiv (\sigma x, \sigma^{-1} y)$, or the Fourier transform $\tilde{h}(\mathbf{k}') = \tilde{g}(\sigma k_x', \sigma^{-1} k_y')$. Then Eq. (1) becomes in the new order parameter $\psi(\mathbf{r}') \equiv \Psi(\mathbf{r}) = \Psi(\sigma^{-1}x', \sigma y')$,

$$F[\psi] = \int d^2\mathbf{r}'\left(\frac{\hbar^2}{2m}|\mathbf{D}'\psi|^2 + \alpha|\psi(\mathbf{r}')|^2\right) + \frac{\beta}{2}\int d^2\mathbf{r}_1'\, d^2\mathbf{r}_2' |\psi(\mathbf{r}_1')|^2 h(\mathbf{r}_1' - \mathbf{r}_2') \times |\psi(\mathbf{r}_2')|^2, \qquad (3)$$

where $\mathbf{D}' = -i\nabla' - (e^*/\hbar c)\mathbf{a}(\mathbf{r}')$ and $m = (m_x m_y)^{1/2}$.

Within mean-field theory, the structure of the vortex lattice in our model can be determined in exactly the same way as in Abrikosov's work using the lowest Landau level approximation (LLL) [10]. We look for a periodic solution to the linearized GL equations while restricting the order parameter to the space spanned by the LLL wave functions. In the Landau gauge, $\mathbf{a} = (-By', 0)$, the normalized solution quasiperiodic over the two periodicity vectors, $\mathbf{r}_{\mathrm{I}}' = l(1,0)$, $\mathbf{r}_{\mathrm{II}}' = l(\zeta, \eta)$ is given by [11] $\psi(\mathbf{r}') \sim \phi(\mathbf{r}'|0) \equiv (2\eta)^{1/4}\exp(-\mu^2 y'^2/2)\theta_3[\pi(x' + iy')/l|\zeta + i\eta]$ with the theta function θ_3. The magnetic length μ^{-1} is fixed by the flux quantization condition; $2\pi\mu^{-2} =$ (area of unit cell) $= l^2\eta$. A useful representation for $\phi(\mathbf{r}')$ is [12]

$$|\phi(\mathbf{r}')|^2 = \sum_{m,n=-\infty}^{\infty} (-1)^{mn}\exp(-\mathbf{G}^2/4\mu^2 + i\mathbf{G}\cdot\mathbf{r}'), \qquad (4)$$

where $\mathbf{G} = \mu^2 l(\eta m, n - \zeta m)$ is the reciprocal lattice vector corresponding to the periodicity vectors in the $\mathbf{r}'$ space. The mean-field free energy density is given by $F_{\mathrm{MF}} = -\alpha_H^2/2\beta\beta_A$, where $\alpha_H \equiv \alpha + \hbar e^* B/2mc = 0$ determines the upper critical field $H_{c2}(T)$, and the Abrikosov ratio β_A, which accounts for the contribution from the quartic term, is given by

$$\beta_A = \sum_{m,n} \exp(-\mathbf{G}^2/2\mu^2)\, \tilde{h}(\mathbf{G})\,. \tag{5}$$

In order to find a minimum free energy configuration, one has to minimize β_A.

Since the sum in (5) converges very quickly, it is not difficult to find a configuration that minimizes β_A for given values of C, ε, and θ_0. In the limit where $C \to 0$ (the low-magnetic field regime), one recovers the local GL theory, and β_A attains the familiar minimum value, $1.159\ldots$ for a triangular lattice in the $\mathbf{r}'$ space. Also, since rotational invariance exists in the $\mathbf{r}'$ space when $C \to 0$, the triangular lattice has no preferred orientation with respect to the underlying crystal. When transformed back to the original $\mathbf{r}$ space, it results in a distorted triangular lattice due to the a-b plane anisotropy.

In the high field regime where one cannot neglect the effect of the nonlocal quartic term, the situation is different. Because of the a-b plane anisotropy carried over to $\tilde{h}(\mathbf{k}')$, the system in the $\mathbf{r}'$ space is neither rotationally invariant nor fourfold symmetric. Therefore, the vortex lattice is orientated with respect to the crystal. In our model, the parameter θ_0 specifies the orientation. In general, we obtain an oblique lattice whose form depends on the values of C and ε. In the original $\mathbf{r}$ space, this lattice is further distorted due to the a-b plane anisotropy. To be more specific, we parametrize the periodicity vectors, $\mathbf{r}'_{\mathrm{I}}$ and $\mathbf{r}'_{\mathrm{II}}$, in terms of a centered rectangular lattice for which one can write $\zeta = 1/2$ and $\eta = (1/2)\tan\varphi'$, where φ' is an angle between $\mathbf{r}'_{\mathrm{I}}$ and $\mathbf{r}'_{\mathrm{II}}$. We consider a general case where this lattice is rotated by an angle φ'_0. The resulting lattice can also be regarded as an oblique lattice with two primitive vectors of equal length and an angle $2\varphi'$ (or $\pi - 2\varphi'$) between them. For simplicity we focus on the case where $\theta_0 = 0$. For given C, ε, and $\theta_0 = 0$, we look for φ' and φ'_0 that minimizes β_A. For $\theta_0 = 0$, we find that the minimum free energy configuration always corresponds to $\varphi'_0 = 0$, where one of the primitive vectors, $\mathbf{r}'_{\mathrm{I}}$, coincides with the x' axis. Any other orientation of the vortex lattice can be obtained using different values of θ_0. The angle φ' that gives the minimum free energy changes continuously from $\sim 60°$ corresponding to a distorted triangular lattice to $\sim 45°$ for a distorted square lattice as the fourfold symmetric coupling ε increases from 0 toward 1 for fixed C. We find that for C greater than some value $C_c \sim 0.015$, there exists ε_c which depends on C such that the vortex lattice remains as a distorted square lattice for $\varepsilon > \varepsilon_c$. A similar behavior to this was obtained in Ref. [4]. Now, since the original order parameter $\Psi(\mathbf{r})$ is quasiperiodic with respect to $l(\sigma^{-1}, 0)$ and $l(\sigma^{-1}\zeta, \sigma\eta)$ for $\varphi'_0 = 0$, the oblique lattice in the $\mathbf{r}$ space has an angle φ, where $\tan\varphi = \sigma^{-2}\tan\varphi'$. (This relation becomes more complicated if $\varphi'_0 \neq 0$.) To summarize, within mean-field theory, the structure of the vortex lattice is mainly determined by the anisotropy parameter σ and the fourfold symmetric coupling ε, and the orientation by θ_0. All these parameters can in principle be fixed by experiments which determine the flux lattice structure as a function of the magnetic field.

Thermal fluctuations, which are especially important in high-T_c materials, melt the mean-field vortex lattice into a vortex liquid. For the local theory ($C = 0$), the effect of thermal fluctuations around the mean-field solution was studied by Eilenberger [11] using the orthonormal basis for the LLL wave functions, $\phi(\mathbf{r}|\mathbf{r}_0) = \exp(\mathrm{i}\mu^2 x y_0)\phi(\mathbf{r}|0)$, where $\mathbf{r}_0$ spans one fundamental cell, or $\mathbf{q} = \mu^2(y_0, -x_0)$ belongs to the first Brillouin zone. There are two different modes of excitation, whose energies are denoted by $\epsilon_\pm(\mathbf{q})$. In the long wavelength limit, $q \to 0$, the hard mode behaves as $\epsilon_+(q) = \mathrm{const} + O(q^2)$ while the soft mode takes the form $\epsilon_-(q) = (\alpha_0/2)\,(q^4/\mu^4) + O(q^6)$ as $q \to 0$. The soft mode corresponds to an incompressible shear deformation of the vortex lattice [13] and α_0 can be identified with the shear modulus c_{66} of the triangular lattice.

When terms which break the rotational symmetry are present, the orientation of the vortex lattice is locked to the underlying crystal. Therefore we expect that there exists an excitation energy cost associated with a rigid rotation of the vortex lattice against the crystal lattice. We shall calculate this energy when the coupling to the underlying lattice is very weak, i.e., $C \ll 1$. Following Ref. [11], we first determine the soft mode energy $\epsilon_-(\mathbf{q})$ associated with (1) to the lowest order in C. (We assume $\sigma = 1$ for simplicity.) After lengthy but otherwise straightforward algebra, we obtain the following anisotropic expression:

$$\begin{aligned}\epsilon_-(\mathbf{q}) = \frac{\alpha_0}{2}\,&[(1 + C\alpha_1)\,(q^4/\mu^4) \\ &+ C\varepsilon(\beta_1 q_x^4 + 2\beta_2 q_x^2 q_y^2 + \beta_3 q_y^4)/\mu^4] \\ &+ O(q^6, C^2)\,,\end{aligned} \tag{6}$$

with known *numerical* constants $\alpha_1, \beta_1, \beta_2$, and β_3. This corresponds to a general form of the effective free energy [14] for the displacement $\mathbf{u}$, which should involve the rotation fields, $v_{ij} \equiv (\partial_i u_j - \partial_j u_i)/2$ as well as the usual strain fields, $u_{ij} \equiv (\partial_i u_j + \partial_j u_i)/2$. In our case where the vortex lattice is incompressible and fourfold symmetric, the effective free energy density reduces to

$$\tfrac{1}{2}\{\lambda_1(\partial_x u_x - \partial_y u_y)^2 + 4\lambda_2 u_{xy}^2 + 4\omega v_{xy}^2 + 8\xi u_{xy} v_{xy}\}\,,$$

with four energy constants, $\lambda_1, \lambda_2, \omega$, and ξ. For $C = 0$, one only has the purely elastic part ($\omega = \xi = 0$) and $\lambda_1 = \lambda_2 = c_{66}$. For small C, the shear modulus will have a O(C) correction, and the rotation modulus ω and the coupling ξ between the rotation and strain fields will be proportional to $C\varepsilon$. From (6), we obtain using the method of Ref. [13] $\lambda_1 = c_{66}[1 + C\alpha_1 + C\varepsilon(2\beta_2 - \beta_1 - \beta_3)/4]$, $\lambda_2 = c_{66}(1 + C\alpha_1)$, $\omega = c_{66}C\varepsilon(\beta_1 + \beta_3)/2$, and $\xi = c_{66}C\varepsilon(\beta_1 - \beta_3)/2$.

A useful quantity in studying the effect of thermal fluctuations is the so-called structure factor $\Delta(\mathbf{k})$ of the vortex liquid, which is proportional to the Fourier transform of the density-density correlation function $\langle|\Psi(\mathbf{r})|^2|\Psi(\mathbf{r} + \mathbf{R})|^2\rangle_c$. In the low-temperature regime, the length scale

$l_\perp$ governing the degree of a short-range crystalline order perpendicular to the magnetic field in the vortex liquid becomes very large ($l_\perp \gg l_0$). We expect then that a tiny amount of coupling to the underlying lattice might be able to break the rotational symmetry of the vortex liquid system even though there is only a short-range translational order. For example, a ringlike pattern expected in a structure factor will be broken up into Bragg-like spots even in a liquid state (these spots will not be delta-function peaks, i.e., not true Bragg peaks). This is to be contrasted with the usual explanation of the appearance of Bragg-like spots in neutron diffraction patterns using a phase transition from a vortex liquid state to a vortex lattice state. We can estimate the angular dispersion $\delta\theta$ of these spots using the above discussion on the rotation modulus: Since the energy associated with a rigid rotation by $\delta\theta$ of the crystalline region of area $l_\perp^2$ is given by $l_\perp^2 \omega(\delta\theta)^2$, by equating this to $k_B T$, one finds that

$$(\delta\theta)^2 \sim k_B T/\omega l_\perp^2 = (0.012) k_B T/c_{66} l_\perp^2 C\varepsilon\,, \quad (7)$$

where we have used the numerical values for β_1 and β_3.

As the temperature is raised, according to (7), one needs larger values of $C\varepsilon$ to observe the Bragg-like spots. At moderately low temperatures, an approximation scheme, called the parquet resummation method [7] is accessible for the calculation of the structure factor of the vortex liquid. Using this method, one can explicitly observe a ringlike pattern in the structure factor is broken up into Bragg-like spots as the temperature is lowered. For an isotropic system described by (3), it is straightfoward to apply the parquet resummation method to calculate the structure factor $\Delta'(\mathbf{k}')$ in the $\mathbf{k}'$ space. The only difference compared to the usual local theory is that one starts from the bare quartic potential $\tilde{h}(\mathbf{k}')$ which explicitly breaks the rotational symmetry of the local theory. For the detailed form of the nonperturbative equations one has to solve numerically for Δ', and the reader is referred to Ref. [7] for details. The structure factor in the original space is given simply by $\Delta(\mathbf{k}) = \Delta'(\mathbf{k}')$, where $(k_x', k_y') = (\sigma^{-1} k_x, \sigma k_y)$.

We have calculated $\Delta(\mathbf{k})$ for various values of the parameters, C, ε, and at different temperatures down to $\alpha_T \sim -6.7$, where the temperature is represented by the dimensionless quantity, $\alpha_T \equiv \alpha_H \sqrt{2\pi/\beta\mu^2}$, which goes to $-\infty$ as one approaches zero temperature. Figure 1 shows a contour plot of $\Delta(\mathbf{k})$ at $\alpha_T \simeq -6.3$ for the values of C and ε that correspond to a moderately strong coupling between the vortex lattice and the underlying crystal ($\varepsilon = 0.5$). One can clearly observe four bright spots, which correspond to the nearest peaks in the structure factor, emerging from a ringlike pattern. To observe the next and higher order spots (which will give a structure factor a closer resemblance to that expected for a triangular lattice) one has to obtain the structure factor at lower temperatures. We find in general that, as the coupling between the vortex lattice and the underlying crystal gets weaker, one has to go to lower temperatures to observe the Bragg-like spots.

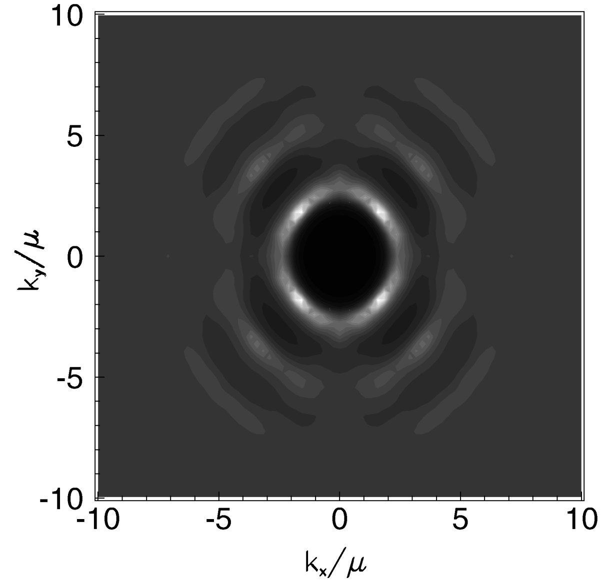

FIG. 1. A contour plot of $\Delta(\mathbf{k})$ at $\alpha_T \simeq -6.3$. The parameters used are $C = 0.01$, $\varepsilon = 0.5$, $\theta_0 = 0$, and $\sigma^{-2} = 1.15$.

This fact is in qualitative agreement with (7) (although the present numerical calculation is not done in the strict weak coupling limit).

In summary, we considered a simple phenomenological model for vortices in a crystal lattice using a nonlocal GL theory. As well as explaining the observed fourfold symmetric vortex lattice structures within mean-field theory, the present model suggests that there is a possibility of observing Bragg-like spots within the vortex liquid regime as a consequence of coupling of the vortices to the underlying crystal.

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