Interpretation of the Neutron Scattering Data on Flux Lattices of Superconductors

D. Chang,[1] C.-Y. Mou,[1] B. Rosenstein,[2] and C. L. Wu[1]

[1]*Center for Theoretical Sciences and Department of Physics, National Tsing Hua University,
Hsinchu, Taiwan, 30043, Republic of China*
[2]*Electrophysics Department, National Chiao Tung University, Hsinchu, Taiwan, 30043, Republic of China*
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Small angle neutron scattering (SANS) experiments are analyzed using a recently developed and properly generalized one-field effective free energy method. In the case of experiment of Keimer *et al.* on YBa$_2$Cu$_3$O$_7$, we show that the fourfold symmetry of the underlying crystal is explicitly broken, but the reflection with respect to the [110] and [1$\bar{1}$0] axes remains a symmetry. The vortex lattice also becomes generally oblique instead of rectangular body centered. An unexpectedly rich phase diagram is described. [S0031-9007(97)04956-9]

There are growing evidences that superconductivity in layered high T_c cuprates is largely due to the $d_{(x^2-y^2)}$ pairing [1] with small mixing of *s*-wave component [2–4]. The unconventional pairing mechanism makes an impact on the single vortex and the vortex lattice structure. Recent studies on the detailed structure of the Abrikosov vortex lattice in YBa$_2$Cu$_3$O$_7$ (YBCO), using small angle neutron scattering (SANS) [5,6] and tunneling spectroscopy [7], show clear deviations from the standard triangular lattice. It is natural to try to explain these deviations theoretically with modified phenomenological Ginzburg–Landau (GL) theory. To investigate *d*-wave superconductors with *s*-wave mixing, Ren *et al.* [8] and Soininen *et al.* [9] both derived an effective GL type theory using two order parameters: *s* and *d*. From this effective action, or more fundamental equations [10], one obtains a characteristic four-lobe structure for an isolated vortex and its associated magnetic field [11]. The fourfold vortex core structure comes into conflict with the high symmetry of the triangular lattice and can distort it at already accessible fields much lower than H_{c2}. The vortex lattices obtained within this approach are basically centered rectangular lattice with chains of vortices oriented along crystalline axes [100] and [010] (see Fig. 1). They spontaneously break the fourfold rotational symmetry (i.e., two different lattices related by 90° rotation), but preserve the reflections with respect to the axes [100] and [010].

These predictions come close to results of some experiments [5,7], but clearly disagree with those of [6]. According to the interpretation given in [6], the centered rectangular vortex lattice gets rotated by 45° with respect to the crystalline axes [see Fig. 2(a)], i.e., the chains of vortices lie along the diagonal directions [110] and [1$\bar{1}$0] instead. A recent theoretical study by Ren *et al.* [12] has considered explicit breaking of the fourfold symmetry within the two field framework. Their results, however, remain qualitatively the same as the case with fourfold symmetry—only centered rectangular nonrotated vortex lattices are obtained. So far, there is no theoretical interpretation for the lattice data observed in [6]. We shall provide such an interpretation in this Letter. Our answer is different from that provided in [6], however, the results can still be derived from the GL theory with proper fourfold symmetry breaking terms.

In this work we adopt a recently developed one-field effective theory, first introduced by Affleck *et al.* [13] in which they work mainly in the London limit, and later by us [14] for static and moving vortex lattices near H_{c2}. Most of the above mentioned results can be reproduced in this much simpler formulation in which only the field *d* is introduced and the theory is based on the following D_{4h} symmetric free energy:

$$F_{\text{eff}}[d] = \frac{1}{2m_d}|\Pi d|^2 - \alpha_d|d|^2 + \beta|d|^4$$
$$- \eta d^*\left(\Pi_y^2 - \Pi_x^2\right)^2 d, \tag{1}$$

where $\Pi = -i\nabla - e^*\mathbf{A}$. The last term which we call F_{4d} parametrizes the breaking of full rotational symmetry down to D_{4h} and can be treated as a perturbation. Near H_{c2}, the linearized equation in the one-field approach can be solved perturbatively in η, which allows one to easily generalize the description of the centered rectangular lattices to the most general oblique lattices [14]. This will be crucial in the present work in which these more general lattices are indeed the ground state in some cases.
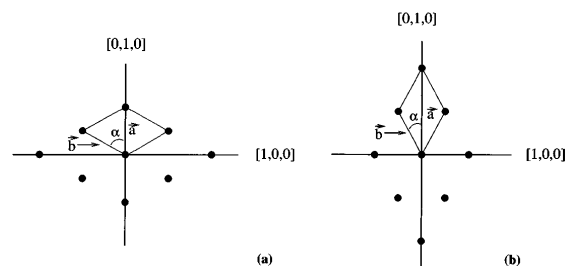

FIG. 1. The body-centered rectangular lattice obtained in the fourfold symmetric case, the two lattices (a) and (b) are related by a rotation of 90° or reflection about the [110] axis.
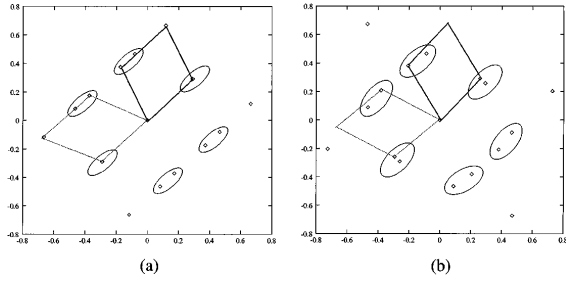
FIG. 2. Keimer *et al.*'s SANS diffraction pattern and two different interpretations. (a) Keimer *et al.*'s interpretation, and (b) the interpretation given in this paper.

Note that the contributions to the coefficient η might not only come from the d-s mixing which always gives a positive η, but also from other sources [14]. The possibility of having negative η will be discussed later. It is also important to realize that since this formulation utilizes only the symmetry properties, it can be applied to the conventional type II superconductors with D_{4h} symmetry as well. In this case, η is proportional to the angular average of products of Fermi velocities on the Fermi surface, describing the deviation of the Fermi surface from a perfect sphere [15]. The effective strength of F_{4d} can be characterized by a dimensionless parameter $\eta' \equiv \eta m_d e^* H$ [14]. Using the free energy in Eq. (1), one finds centered rectangular vortex lattices [see Fig. 1] with the angle α directly related to the coefficient η'. The lattice becomes square when η' exceeds a critical value $\eta'_c = 0.0235$ [14]. This can accommodate the tunneling spectroscopy data of [7] and the SANS data of [5] for YBCO, as well as a recent decoration and neutron scattering data for a low T_c material ErNi$_2$B$_2$C [16]. The analysis presented in [14] indicates that the precise SANS data of [16] unambiguously shows that for large η', the vortex lattice becomes a square one, exhibiting perfect D_{4h} symmetry. The less precise data

of [7] gives an angle $\alpha \approx 54°$, which corresponds to $\eta' \approx 0.019$ and is in the centered rectangular phase. These two experiments on two different samples both seem to show manifestation of D_{4h} symmetric GL free energy and correspond to its two different phases. The transition from the centered rectangular vortex lattice to the square lattice was observed in ErNi$_2$B$_2$C [16] and has not been observed yet in high T_c materials.

In order to explain the data in [6], we now generalize the formalism to include terms which break the D_{4h} symmetry. This can be also motivated by noting that in many high T_c cuprates the D_{4h} symmetry is not exact. For example, the CuO chains in YBCO break the fourfold symmetry down to twofold [12]. Up to (scaling) dimension three, there are two possible terms that break fourfold symmetry: $F_{x^2-y^2} = -\mu d^*(\Pi_y^2 - \Pi_x^2)d$ and $F_{xy} = -\lambda d^*(\Pi_x \Pi_y + \Pi_y \Pi_x)d$. The first term $F_{x^2-y^2}$ describes the asymmetry between [100] and [010] axes and has the reflection symmetries $x \to -x, y \to y$ (σ_x) and $x \to x, y \to -y$ (σ_y). This term has already been considered in [12]. The second term F_{xy}, on the other hand, preserves the reflection symmetry with respect to the [110] and [1$\bar{1}$0] directions, that is, $x \to y, y \to x$ and $x \to -y, y \to -x$. In the BCS theory, the presence of the second term requires that the shape of the Fermi surface also breaks the σ_x and σ_y symmetries. Since this is quite unlikely, we do not expect that it will occur in the conventional superconductors. We will find, however, in the case of Keimer *et al.*'s SANS experiment, the F_{xy} term is required to explain the data.

The method of calculation is quite analogous to that of the η correction explained in [14], so here we just present the result. Let a, b be the two lattice constants and α be the angle between the two basis vectors (Fig. 1). It will be convenient to introduce the complex variable $\zeta \equiv \frac{b}{a}e^{i\alpha} \equiv \rho + i\sigma$. The angle between the vortex lattice and the crystalline lattice will be denoted by φ. The Abrikosov's $\beta_A \equiv \langle |d|^4 \rangle / \langle |d|^2 \rangle$ is then given by

$$\beta_A(\rho, \sigma) = \beta_A^0(\rho, \sigma) + \frac{\sqrt{\sigma}}{4} \operatorname{Re}\left\{ \left[\sum_{n'=-\infty}^{\infty} \exp(-2\pi i\zeta^* n'^2) \right] \left[\sum_{n=-\infty}^{\infty} \exp(2\pi i\zeta n^2) G(n) \right] + \left(n \to n + \frac{1}{2}, n' \to n' + \frac{1}{2} \right) \right\}, \tag{2}$$

where $\beta_A^0(\rho, \sigma)$ can be found in a standard textbook or in [14]. All the three anisotropic corrections are collected in the prefactor

$$G(n) = \eta' e^{4i\varphi}(64\pi^2\sigma^2 n^4 - 48\pi\sigma n^2 + 3)$$
$$+ 4\mu' e^{2i\varphi}(8\pi\sigma n^2 - 1)$$
$$+ 4\lambda' e^{2i(\varphi + \pi/4)}(8\pi\sigma n^2 - 1), \tag{3}$$

where $\mu' \equiv \mu m_d, \lambda' = \lambda m_d$.

The term $F_{y^2-x^2}$ in the effective energy preserves the symmetries of the centered rectangular lattice and is

therefore not expected to produce interesting qualitative effects, so we will drop the μ' term in the following discussions; however, it is understood that in making quantitative comparison with data, the μ' term may have to be included. The remaining correction to β_A summarized in $G(n)$ has two parts: the first one comes from the fourfold symmetric term F_{4d} and has $e^{4i\varphi}$ angular dependence. The second one has $e^{2i(\varphi + \pi/4)}$ angular dependence and comes from F_{xy}. It is this conflict between the two contributions that gives rise to the observed diffraction pattern. Either F_{4d} or F_{xy} alone

will give reflection invariant lattices, i.e., rectangular body centered lattice aligned along [100] or [110], respectively. The lattice structure is determined by minimizing β_A with respect to ρ, σ, and φ numerically. One obtains generally nonrectangular oblique vortex lattices. It differs markedly from the D_{4h} symmetric case.

Figure 2(b) shows the diffraction pattern and the corresponding lattice structure that we obtained at $\eta' = 0.019, \lambda' = 0.04$. (Note that in 2D the reciprocal lattice is nothing but a rotation of $90°$ of the real lattice.) In one of the diffraction patterns, Fig. 2(a), one sees clearly two large peaks in the [110] direction and four weaker points on both sides of the [110] line, giving totally ten points. This was interpreted in Ref. [6] as a nearly rectangular lattice with one of the basis vectors lying on [110], together with its reflected version. (Presumably, the two lattice orientations are degenerate ground state and show up simultaneously as different domains in the sample.) The points on the [110] line then coincide and produce constructive interference. In comparison, in the previous calculations, because the reflection symmetries σ_x and σ_y are preserved, one always obtained rectangular lattices which are aligned to either [100] or [010]. They possess twofold symmetry and upon reflection one is unable to produce different lattices. As a result, there will be only six points on the diffraction pattern and one cannot account for the data.

We notice an important difference here: The off diagonal points (the four weaker points) are not really on the line parallel to [110] as Keimer *et al.* claimed. One might hope to tune the parameters such that when the two points on [110] merge into one, the off diagonal points will align themselves as well, but this is not the case. In fact, they will also merge with each other, and there will be no splitting anymore. If one looks carefully at their contour plot it is possible to tell the difference. Furthermore, the lattice we obtained is not rectangular; this is consistent with their possibly 5% difference between the length of the two primitive basis vectors.

The vortex lattice phase diagram in the (η', λ') plane is presented in Fig. 3. Since changing the sign of λ' only reverses the roles of [110] and [1$\bar{1}$0] axes, it suffices to show only the positive λ'. First, consider the D_{4h} symmetric case with $\lambda' = 0$. Then $\eta' = 0$ corresponds to the conventional triangular lattice with no special orientations. For $\eta' < \eta_c'$ the lattice is centered rectangular aligned to [100] and [010] with double degeneracy (related by reflection about [110]). Increasing η' elongates lattices along either [100] or [010] so that when $\eta' > \eta_c'$, the two degenerate lattices both becomes square and the full D_{4h} symmetry is restored.

For $\lambda' > 0$, there are three phases and two phase transition lines. The lattice, compared to the corresponding $\lambda' = 0$ case, can in general be thought of as resulting from a deformation in the [110] direction. (For $\lambda' < 0$, the corresponding deformation will be in the [1$\bar{1}$0] direc-
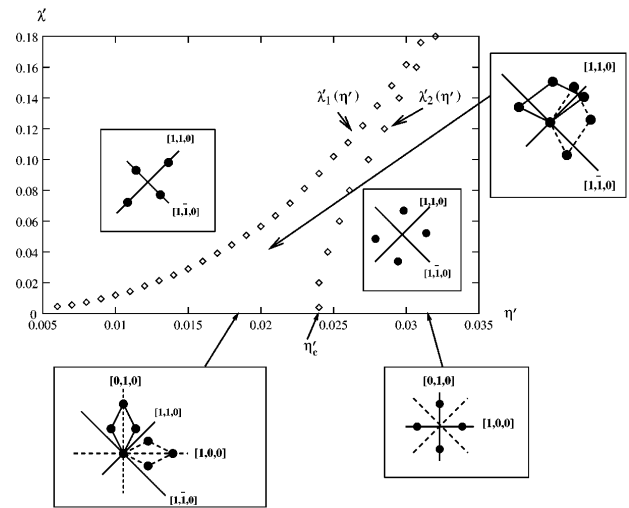

FIG. 3. The phase diagram for the vortex lattice structure as a function of the fourfold anisotropy parameter η' and the twofold anisotropy parameter λ'.

tion.) The lattice is centered rectangular for smaller values of η', while it is rectangular (not centered) for larger values of η'. Symmetry of the unique ground state in each of these two cases is larger than that of the free energy. There is, however, no direct phase transition between them. Instead, in the region between these two phases bounded by $\lambda_1'(\eta')$ and $\lambda_2'(\eta')$, there is a less symmetric phase in which ground states are doubly degenerate. This comes from a nontrivial competition between F_{4d} and F_{xy}. The two degenerate lattices are also related by the reflection about [110] and are generally oblique. We see that the data in [6] can be fitted into this phase. The transition line $\lambda_1'(\eta')$ starts from the origin and monotonically increases with η', while $\lambda_2'(\eta')$ starts from $(\eta_c', 0)$ and also increases monotonically. $\lambda_2'(\eta')$ appears to approach $\lambda_1'(\eta')$ asymptotically. Since η' is proportional to the magnetic field H, one immediate implication of this phase diagram is that, for a given sample, by increasing H one should encounter two phase transitions. This prediction can be tested directly by a number of experimental techniques.

We would like to briefly describe here another, rather exotic possibility. The one-field approach allows one to consider the negative η case. This cannot be obtained from the two field formulation in which η is always positive if we only assume one critical temperature [8,9]. However, the possibility of negative η cannot be ruled out theoretically. In the one component theory with exact fourfold symmetry, the negative η is equivalent to the d_{xy} pairing, while in the BCS theory, it could happen if the Fermi surface is elongated along the $y = \pm x$ direction. When η' is negative, the minus sign replaces φ in the $\exp(4i\varphi)$ factor in Eq. (3) by $\varphi \pm 45°$, and then both F_{4d} and F_{xy} will prefer the diagonal direction. As a result there will be no competition and we will always get rectangular body centered lattices along [110] or [1$\bar{1}$0].

In conclusion, we have investigated the effects of explicit fourfold symmetry breaking on the Abrikosov lattice structure with the one-field formulation. The complete phase diagram was constructed. We found a quite rich phase diagram with three different phases separated by two phase transition lines. The vortex lattice observed in Keimer *et al.*'s experiment [6] can be accommodated in the new phase diagram. It turns out that the vortex lattices are no longer centered rectangular, but rather general oblique ones. Other experiments fit quite well into the D_{4h} symmetric phase in which the triangular to square phase transition takes place.

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