

# Theoretical Study on Vortex Lattices in Tetragonal Superconductors

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## Abstract

Vortex lattices of four-fold symmetric superconductors are studied numerically on the basis of the quasiclassical theory. The four-fold symmetric anisotropy of the Fermi velocity or the superconducting gap function causes the vortex lattice transformation. The transformation as observed in LuNi<sub>2</sub>B<sub>2</sub>C could be understood with the four-fold symmetric anisotropy. We show the temperature and field phase diagram for four-fold symmetric superconductors and the spatial structures of the pair potential and zero energy states in the case of the stable square vortex lattice at the low field.

*Key words:* vortex lattice; quasiclassical theory; four-fold symmetric anisotropy; borocarbide superconductors

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Recently, Eskildsen *et al.* discovered vortex lattice transformation for applied field  $\mathbf{H} \parallel [001]$  in LuNi<sub>2</sub>B<sub>2</sub>C[1]. As increasing  $H$ , the rhombic vortex lattice changes into the square vortex lattice, and this backs to rhombic vortex lattice again in a higher field. The boundary between a rhombic lattice and square lattice bends away approaching  $H_{c2}$  and never crosses upper critical field  $H_{c2}$  line. Since the phase diagram of vortex lattice is not known in all temperature and field region in borocarbide superconductors, we investigate the stable vortex lattice configuration from basic electronic properties. The angle resolved thermal conductivity measurement suggests that the gap function has a four-fold symmetric anisotropy and minimum gap is located along (100) and (010)-directions[2]. The band calculation and angular correlation of electron-positron annihilation radiation measurements tell us that the Fermi velocity is larger in (100) than in (010), or angle resolved density of states on the Fermi surface is larger in (110) than in (100)[3]. It seems reasonable that the superconducting gap and angle-resolved density of states on the Fermi surface have in the same direction (110).

Based on earlier theoretical studies with a four-fold symmetric superconductors, it is expected that the vor-

tex lattice can transform from triangular to square as the magnetic field increases[4,5]. In addition, the orientation of the vortex lattice can take two possible directions under the condition mentioned for borocarbide superconductors. The [100]-direction square ( $\square_g$ ) vortex lattice is stabilized by the gap anisotropy, while the [110]-direction square ( $\square_v$ ) is stabilized by the Fermi velocity anisotropy. These competing effect about vortex lattice is nontrivial problem. To understand this problem, we study vortex properties on the basis of the quasiclassical theory.

We consider two-dimensional case in a real space. With polar angle  $\theta$  relative to [100] axis, Eilenberger equations are

$$(2\omega + \mathbf{v}_F(\theta) \cdot \mathbf{\Pi}) f(\omega, \mathbf{r}, \theta) = 2\Delta(\mathbf{r}, \theta)g(\omega, \mathbf{r}, \theta), \quad (1)$$

$$(2\omega - \mathbf{v}_F(\theta) \cdot \mathbf{\Pi}^*) f^\dagger(\omega, \mathbf{r}, \theta) = 2\Delta^*(\mathbf{r}, \theta)g(\omega, \mathbf{r}, \theta) \quad (2)$$

where  $\mathbf{\Pi} = \nabla + (2\pi i/\Phi_0)\mathbf{A}$ ,  $\mathbf{A}$  is vector-potential and  $\Phi_0$  is flux quantum.  $\omega = \pi T(2n + 1)$  with integer  $n$  is Matsubara frequency. Normalization condition  $g^2 + f f^\dagger = 1$ . Pair potential and Fermi velocity are set as  $\Delta(\mathbf{r}, \theta) = \Psi(\mathbf{r})\phi(\theta)$ ,  $\mathbf{v}_F(\theta) = \overline{\mathbf{v}_F}\mathbf{v}(\theta)$ . These angle-dependence are written as

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$$\phi(\theta) = \sqrt{\frac{1 - \alpha \cos 4\theta}{1 + \frac{\alpha}{\beta}(1 - \sqrt{1 - \beta^2})}}, \quad (3)$$

$$v(\theta) = \frac{1 + \beta \cos 4\theta}{\sqrt{1 - \beta^2}}. \quad (4)$$

We assume the Fermi surface is cylindrical, gap function and Fermi velocity have four-fold symmetric anisotropy. Concerning borocarbide superconductors, the anisotropic parameter  $\alpha$  and  $\beta$  are set as positive sign. Self-consistent conditions for the pair potential  $\Psi(\mathbf{r})$  and vector potential  $\mathbf{A}$  are

$$\Psi(\mathbf{r}) \ln \frac{T_c}{T} = 2\pi T \sum_{\omega>0} \left[ \frac{\Psi(\mathbf{r})}{\omega} - \left\langle \frac{\phi(\theta)f}{v(\theta)} \right\rangle \right], \quad (5)$$

$$\nabla \times \nabla \times \mathbf{A} = -\frac{16\pi^3}{\Phi_0} N_0 T v_F \sum_{\omega>0} \text{Im} \langle \mathbf{g} \mathbf{u} \rangle. \quad (6)$$

Here,  $\langle \dots \rangle = 1/2\pi \int \dots d\theta$ ,  $\mathbf{u} = (\cos(\theta), \sin(\theta))$ .  $N_0$  is the density of states at the Fermi energy. Once we have the self-consistent solution, the local density of states and free energy density are calculated by

$$N(\mathbf{r}, E) = N_0 \left\langle \frac{1}{v(\theta)} \text{Re} g(\omega \rightarrow -iE + \eta, \theta, \mathbf{r}) \right\rangle, \quad (7)$$

$$F = \frac{\overline{H^2(\mathbf{r})}}{8\pi} - \pi T N_0 \sum_{\omega>0} \left\langle \frac{1-g}{1+g} \frac{\phi(\theta)(\Psi^* f + \Psi f^\dagger)}{v(\theta)} \right\rangle \quad (8)$$

Here,  $\overline{a} = (B/\Phi_0) \int_{\text{cell}} a \, d\mathbf{r}$ .

Since the numerical calculation is time consuming, we examine four kinds vortex lattices. Two kinds of square vortex lattices are the nearest neighbor vortex located along [100] or along [110]. Two kinds of triangular vortex lattices are laid on [100] or on [110]. The phase diagram of the vortex lattice is obtained by comparing free energy density of each case (see details in Ref. 6).

The phase diagram of the vortex lattice for  $\alpha = 0.3$  and  $\beta = 0.3$  is shown in Fig. 1. Although the anisotropic parameters are estimated small, it is enough for observed reentrant vortex lattice transformation to appear. It is remarkable that square vortex lattice appears again in a higher field, and the low-field stable square and high-field stable square orientation are different. This result shows that the effect of the gap anisotropy becomes dominant for constructing square vortex lattice as increasing  $H$ . The spatial structures of the pair potential and zero-energy density of states are displayed in Fig. 2. This vortex lattice is stable in a lower field, and corresponds to observed square lattice[1]. The zero energy quasiparticles spread in [100], which is consistent result expected by the gap anisotropy.

In summary, due to the two anisotropy effects realized in borocarbides, we obtain the rich vortex phase di-

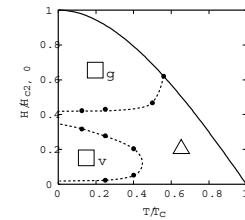


Fig. 1. The temperature and field phase diagram of the vortex lattice for  $\alpha = 0.3$  and  $\beta = 0.3$ .  $\square$  ( $\triangle$ ) is a square (triangular) lattice.  $H_{c2,0}$  is upper critical field at zero temperature. The orientation “v” (“g”) is that the nearest neighbor vortex is located along [110]-direction ([100]-direction).

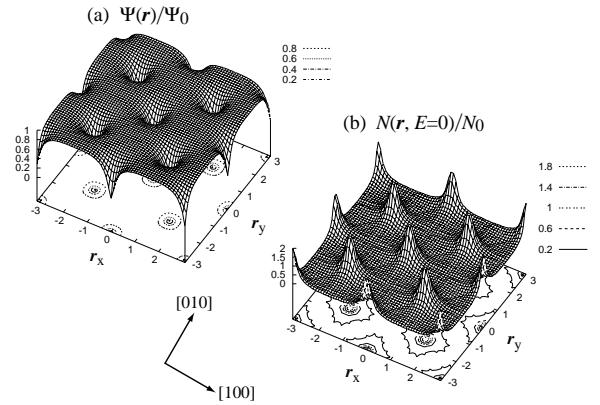


Fig. 2. (a) The spatial structure of the pair potential. (b) The zero-energy local density of states.  $T = 0.25T_c$ ,  $H = 0.15H_{c2,0}$ . In this  $(T, H)$ ,  $\square$  is stable (see Fig. 1). Here,  $\Psi_0$  is for zero temperature and zero field. In (b), the peak at the vortex center  $(N(\mathbf{r}, E = 0)/N_0 \sim 20)$  is truncated.

agram. The observed transformation of the vortex lattice appears in reasonable field and temperature, which is accessible experimentally. The two anisotropies in the gap function and the Fermi velocity prefer different orientation of the square vortex lattice. The observed lattice transformation in borocarbide superconductors could be understood by this competing effect. This physics on the vortex lattice transformation is not limited in borocarbides. High- $T_c$  cuprates and 2H-NbSe<sub>2</sub> are also in the same situation. We will study it for future.

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