Vortex lines in the high-$T_c$ superconductivity in presence of lattice distortions.

Teresa Lenkowska-Czerwińska
Laboratory for Physics of Structured Media, IFTR Polish Academy of Sciences
Świętokrzyska 21, 00-049 Warsaw, Poland

We investigate the superconducting states of the high-$T_c$ superconductors which we argue to be commensurately locked by the tilted rigid octahedral distortion. The method is based on the analysis of the kinematics of the rigid-octahedra lattice model. The distortion modes cause the competing superconducting state of the $s$ and $d$ type symmetry. The vortex structure of the competing orders is analysed on the ground of the Ginzburg-Landau model.

PACS: 03.75, 03.75, 05.70

1. Introduction

Many low temperature properties of high-$T_c$ superconductivity appear to be well described in the framework of the conventional BCS theory. Controversies have arisen around the underdoped materials where the instabilities to the various coexisting spin and charge density wave states appear. In this regime there are no well-defined quasiparticles and no Fermi surface in the normal state [1].

There are several indications that the structural phase diagram in a $La_{2-x}M_xCuO_4$ crystal ($M =$ Sr, Ca, Ba, $\delta$-doping) involves a lower-symmetry structure at low temperatures [2]. A tetragonal to orthorhombic distortion can be viewed as a result of superlattice formation due to rigid octahedral tiltings. According to the suggestions given in the paper by Jorgensen et al. [3], static displacement with octahedral tilting can be written as a superposition of two modes with equal amplitudes, and wave vectors in directions $[110]$ and $[-110]$. The tilting-mode distortion manifests itself by opening up an energy gap at the Fermi surface and leads to a structural phase transition from tetragonal $I4/mmm (D_{4h}^{17})$ to orthorhombic $Cmca (D_{2h}^{18})$ phase. The structural transition takes place within a background of superconducting order, and there is a second order phase transitions between the phase with coexisting the ordinary superconducting phase and lattice distortion. It is interesting to know how the structural and superconducting phase transitions in the materials under consideration depend on the microscopic quantities represented by the vector of the rigid rotation of the octahedra.

Many experiments and also various theoretical models suggested that the ground state of the underdoped superconductors $La_{2-x}M_xCuO_4$ exhibits a unidirectional density wave which consists of a coupled spin- (SDW) and charge-density wave (CDW), called stripes [9]. The stripe order appears as spatial modulation of the superconducting (SC) order parameters. On the other hand, the charge neutrality criterion suggest a strong coupling between charge modulated state and lattice.

2. Tilting Modes in the Rigid-Octahedra Lattice Model

We analyze a one layer of coupled rigid octahedra $CuO_6$ in the coordinate frame with origin in the copper central atom and axes $(x,y)$ directed along the diagonals of the quadratic lattice in the base layer. The $z$-axis is directed perpendicularly to the plane along the $c$-tetragonal direction.

The kinematic equations for the displacements of the oxygen atoms, $\vec{u}(r)$ in the $CuO_2$ plane, are given by Eq.(1) where $\vec{\varphi}$ means the octahedral ro-
tation vector, \( \vec{d}_1, \vec{d}_2 \) are local vectors in the direction \((x, y)\) and \( ||\vec{d}_1|| = ||\vec{d}_2|| = a, ||\vec{d}_3|| = c/2 \), \( a \) is the lattice constant. Because of the connection of the neighboring octahedrals in a plane, the continuity equation is added

\[
\vec{u}(\vec{r} \pm \frac{a}{2}\vec{e}_x) = \vec{u}(\vec{r}) + \frac{1}{2}\vec{d}_1 \times \vec{\phi}(\vec{r}),
\]

\[
\vec{u}(\vec{r} \pm \frac{a}{2}\vec{e}_y) = \vec{u}(\vec{r}) + \frac{1}{2}\vec{d}_2 \times \vec{\phi}(\vec{r}),
\]

\[
\vec{u}(\vec{r} \pm ae) = \vec{u}(\vec{r}) - \frac{1}{2}\vec{d}_2 \times \vec{\phi}(\vec{r} \pm ae).
\]

We define the differential \( D(\vec{r}) \) and arithmetic mean values \( S(\vec{r}) \) lattice operators

\[
D_{1,2}\vec{u}^{\text{def}} = \vec{u}(\vec{r} + \frac{a}{2}\vec{e}_{x,y}) - \vec{u}(\vec{r} - \frac{a}{2}\vec{e}_{x,y}),
\]

\[
S_{1,2}\vec{u}^{\text{def}} = \frac{1}{2} \left( \vec{u}(\vec{r} + \frac{a}{2}\vec{e}_{x,y}) + \vec{u}(\vec{r} - \frac{a}{2}\vec{e}_{x,y}) \right).\]

Then we can write equations (1) in the form \((i, j = 1, 2)\)

\[
D_2S_1\varphi_3 = 0, \quad D_1S_2\varphi_3 = 0,
\]

\[
D_2S_1\varphi_2 + D_1S_2\varphi_1 = 0,\]

\[
d_i \times D_j S_i \vec{\phi} = \vec{d}_j \times D_i S_j \vec{\phi}.
\]

We are looking for the solution of (2) in the form of sign-alternating distortion modes with reciprocal lattice vectors (wave vectors) in-plane \( \vec{k} = (\frac{\pi}{a}, \frac{\pi}{a}, 0) \) for the plane alternating, and \( \vec{k} = (\frac{\pi}{a}, 0, 0) \) and \( \vec{k} = (0, \frac{\pi}{a}, 0) \) for the chain-alternating modes. Because the apex oxygen atoms above and below the CuO\(_2\) plane are not directly bound, we postulate the \( z \)-dependence of the mode functions. We can obtain the three dimensional lattice model as a two-layer structure, one above the another, at the distance \( \frac{c}{2} \), where the upper layer has an additional shift in the plane direction above \( \vec{t}_1 = (\frac{\pi}{a}, \frac{\pi}{a}, 0) \) (because of a body centered lattice). Next we consider the two kinds of zero modes: homogeneous - the same for all layers, and space-alternating - changing sign under elementary translation \( \vec{t}_3 = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}) \). We obtain two kinds of modes : the plane-alternating \( \varphi_i (i = 1, 2, 3) \), and chain-

alternating \( (\tilde{\varphi}_1, \tilde{\varphi}_2) \)

\[
\varphi_i = q_i^+ \epsilon_+ (\vec{r}) + q_i^- \epsilon_- (\vec{r}),
\]

\[
\tilde{\varphi}_1 = \bar{q}_1^+ \epsilon_+ (y, z) + \bar{q}_1^- \epsilon_- (y, z),
\]

\[
\tilde{\varphi}_2 = \bar{q}_2^+ \epsilon_+ (x, z) + \bar{q}_2^- \epsilon_- (x, z).
\]

The sign-alternating functions \( \epsilon_\pm \) are even functions of the arguments, and change the sign under elementary lattice translation \( t_1 (a, 0, 0), t_2 (0, a, 0), t_3 (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}) \): \( \epsilon_\pm (\vec{r} \pm t_{1,2}) = -\epsilon_\pm (\vec{r}) \), \( \epsilon_\pm (\vec{r} \pm t_3) = \pm \epsilon_\pm (\vec{r}) \).

The amplitudes \( q_i^\pm, \bar{q}_i^\pm \) of the functions \( \varphi_i, \tilde{\varphi}_{1,2} \) \((i=1,2,3)\) are the micro-order parameters. The macro-order parameters are constructed from the microparameters as translationally invariant polynomials of the degrees \( n \leq 4 \). Macroparameters change under the action of the point group elements. In dealing with the symmetry class \( D_{4h} \), for the generating elements of the group we choose the rotations \( C_1^4 \), inversion \( I \) and reflection \( \sigma_d \). Finally, the translational and rotational invariant polynomials for \( D_{4h} \) - the macro-order parameters are found [4]. The distortion instability can change the lattice symmetry due to coupling between the distortion and lattice deformation [5]. These allow one to construct the appropriate thermodynamic potential for describing the second order structural phase transitions in the superconducting materials of the La214 class. Some invariants could lead to phase transitions in low symmetry phase - orthorhombic \( D_{2h} \) and monoclinic \( C_2 \), and to the phase transitions without the symmetry change [4].

### 3. Symmetries of the Cooper Pair Function

In a superconducting material La\(_{2-\delta}\)Sr\(_\delta\)CuO\(_4\) two different superconducting phases, in orthorhombic and tetragonal material structures have been distinguished [7]. The temperature of the both structural and superconducting phase transitions depends on the doping. The critical temperature for superconducting phase transition, \( T_s \), has a maximum very near the intersection point of the structural and superconducting phase lines in the \((\delta, T)\) plane (optimal doping). In the neighborhood of this point, the
structural and superconducting order parameters are strongly correlated and the order parameter of the lattice distortion allows a rich variety of phases and phase transitions in the presence of the background superconducting order.

The finite distortion produces a confining potential for the charge carriers and we thereby establish a direct relation between the symmetry of the structural and superconducting order parameters. Thus, about the superconducting state under consideration we assume: (i) The singlet superconducting state which means, that the resulting spin of the electron pairs (Cooper pairs) equal zero. Therefore, the symmetry group \( G \) under consideration contains the space group \( G = D_{17h} \), time inversion \( K \) and gauge \( U(1) \) groups, \( G = G \times K \times U(1) \). (ii) The wave function of the Cooper pairs in the form \( \Psi(r_1, r_2) = e^{-c_0(r_1)c_1(r_2)} \psi(r_1) \psi(r_2) \), where \( r_1 \) stands for the center of mass of the two electrons located in the lattice points \( (r_1, r_2) \). The function \( \psi(r) \) changes under elementary lattice translations. The function \( \psi(r_1 - r_2) \) depends on the rotational symmetry of the Cooper pair. (iii) The symmetries of the superconducting and distortions order parameters are conformable. We therefore postulate: \( \psi(r) = \varepsilon^\pm(r) \) for the plane alternating modes, and \( \psi(r) = \{\varepsilon^\pm(y, z), \varepsilon^\pm(x, z)\} \) for the chain alternating modes.

The superconducting order parameter (or Cooper pair wave function) involve relative and a centre of mass pieces, and the latter is what enters the standard Ginzburg-Landau theory. The general form of Landau free energy has been discussed in the paper [4].

4. Vortices in the inhomogeneous superconducting states

Now we focus our attention on the state which are chain-alternating in the \((x, y)\) copper-oxide plane, and uniform in the space direction \( z \) (\( k = k_x + k_y \))

\[
\begin{align*}
\psi_x(k) &= \varepsilon_+(x) \eta_x, & \psi_y(k) &= \varepsilon_+(y) \eta_y, \\
\varepsilon_+(x) &= e^{ik_x x}, & \varepsilon_+(y) &= e^{ik_y y}.
\end{align*}
\]

In the absence of the external magnetic field, the complex functions \( \eta_{x,y} \) are space independent.

We define the order parameters for two nondegenerate states \(^2\)

\[
\begin{align*}
\psi_s(k_+) &= \psi_x(k) + \psi_y(k), \\
\psi_d(k_-) &= \psi_x(k) - \psi_y(k).
\end{align*}
\]

After little algebra we can see that \( \psi_s \) has the full \( s \)-type rotational symmetry while \( \psi_d \) (the lower-energy mode) is \( d_{2- \gamma} \) - type (change the sign in the diagonal direction). In the external magnetic field directed perpendicularly to the superconducting plane, the amplitudes \( \psi_s \) and \( \psi_d \) become the space-dependent order parameters while the functions \( \zeta \) remain field independent.

Thus under conditions \( k_z = -k_- \) the simplest free energy density allowed by the symmetry results from the coupling between the distortion-dependent local order parameters

\[
F = \alpha_s |\psi_s|^2 + \alpha_d |\psi_d|^2 + \beta_s |\psi_s|^4 + \beta_d |\psi_d|^4 + \beta_m (\psi_s^2 \psi_d^2 + \psi_d^2 \psi_s^2) + \gamma_s |D\psi_s|^2 + \gamma_d |D\psi_d|^2 + \gamma |(D_x \psi_s)^* (D_x \psi_d) - (D_y \psi_s)^* (D_y \psi_d)| + \frac{\hbar^2}{8\pi}.
\]

Here \( D = -i \nabla - e^A/\hbar c \), \( \alpha_s(d) = a_\delta (T - T_{c(d)}), a_\delta \) depends on the doping, \( \delta \) and \( A \) means the vector potential of the external field. Following the standard procedure [5] we derive the system of nonlinear, coupled equations for the order parameters by varying the free energy with respect to the field \( \psi_d^* \) and \( \psi_s^* \)

\[
\begin{align*}
(\gamma_d D^2) \psi_d + \gamma (D_x^2 - D_y^2) \psi_s + 2\beta_d |\psi_d|^2 \psi_d \\
2\beta_m \psi_d^2 \psi_d^2 + \alpha_s \psi_d = 0,
\end{align*}
\]

\[
\begin{align*}
(\gamma_s D^2) \psi_s + \gamma (D_x^2 - D_y^2) \psi_d + 2\beta_d |\psi_s|^2 \psi_s \\
2\beta_m \psi_s^2 \psi_s^2 + \alpha_s \psi_s = 0.
\end{align*}
\]

Like in [3] the asymptotic solutions of the equations (inside and outside of the vortex core) can be found for the isolated vortex line in the strongly II-type materials. They allow us to conclude that near the structural phase transitions caused by distortion modes the \( d \)-wave superconducting vortices arise close to \( T_d \) where \( ^2The \ degeneration \ is \ removed \ by \ the \ lattice \ distortion.\)
The competing orders of the s-wave reach a maximum inside the core of vortices and decay algebraically outside the core region (where the d-wave component reach the maximum bulk value). As a result, in the presence of a vortex line, the four s-wave vortices appear outside the vortex core due to the collinear distortion modes [10].

4. Conclusion

It has been shown on the ground of kinematics lattice model [4] that the chain-alternating superconducting states may appear in the lattice under the tilt-mode distortions. From the point of view of the rigid octahedral lattice as a micropolar Cosserat model [6] the structural microscopic order parameters for the tilting, sign-alternated modes for one CuO$_2$ base layer has been defined. The macroscopic properties are determined by the quantities invariant under any microscopic translation. Therefore, the macro-order parameters were constructed from the translation invariants of the microparameters. The macro-order parameters, which are zero above the critical temperature $T_c$ of the second order phase transition and nonzero below $T_c$, allowed us to distinguish among the various symmetries of the crystalline states. We thereby establish a direct relation between the distortion modulations and the superconducting state. The appropriate symmetries of the superconducting order parameters have been discussed. We therefore conclude that the superconducting states are closely related to the distortion modulation of the rigid CuO$_6$ octahedra.

The finite distortion produces a confining potential for charge carries and causes the distribution of the charge (CDW) and Cooper pair (SC) density in the CuO$_2$ plane to be inhomogeneous. From the symmetry considerations we conclude that the phase modulations of s and d-wave Cooper pairs arise in the presence of the isolated vortex line.

I am grateful to Prof. Dominik Rogula for many valuable discussions and useful suggestions.

The Scientific Research Committee (Poland) under grant No. 5 T0 7A 040 22 supported this work.

REFERENCES

1. L.P. Pryadko, S. Kivelson, D.W. Hone, Phys. rev. Lett, 80 (1998) 5651.
2. J. G. Bednorz and K. A. M¨uller, Rev. Mod. Phys. 60 (1988) 585.
3. J. D. Jorgensen, H.-B. Schüttler, D. G. Hinks, D. W. Capone, II, K. Zhang, M. B. Brodsky, and D. J. Scalapino, Phys. Rev. Lett., 58 (1987) 1024.
4. T. Lenkowska-Czerwińska, J. Tech. Phys., 40, (1999) 3.
5. D. Rogula, and T. Lenkowska-Czerwińska, J. Tech. Phys., 42 (2001) 269.
6. Czesław Rymarz, Mechanics of Continua (in Polish), PWN Warszawa, 1993.
7. B. Keimer, N. Belk, R. J. Birgeneau, A. Casanho, C. Y. Chen, M. Greven, M. A. Kastner, A. Aharony, Y. Endoh, R. W. Erwin, and G. Shirane, Phys. Rev. B 46, (1992)14034-14053.
8. Y. Ren, J. H. Xu, and C. S. Ting, Phys. Rev. Lett. 74 (1995) 3680.
9. C. Panagopoulos, J. R. Cooper, T. Xiang, Y. S. Wang, and C. W. Chu, Phys. Rev. B 61, R3808-R3810 (2000); Y. S. Lee, R. J. Birgeneau, M. A. Kastner, Y. Endoh, S. Wakimoto, K. Yamada, R. W. Erwin, S.-H. Lee, and G. Shirane, Phys. Rev. B 60, 3643-3654 (1999); J. Orenstein and A. Millis, Science 288 (2000) 468.
10. M. Franz, C. Kallin, P. I. Soininen, A. J. Berlinsky, and A. L. Fetter, Phys. Rev. B 53, (1996) 5795-5814.