90° reorientation in the vortex lattice of borocarbide superconductors

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We explain 90° reorientation in the vortex lattice of borocarbide superconductors on the basis of a phenomenological extension of the nonlocal London model that takes full account of the symmetry of the system. Microscopic mechanisms that could generate the correction terms are analyzed. We show that for any dispersion relation and longitudinal phonon-electron pairing mechanism the relevant quantity is strongly suppressed. Possible phenomenological interaction terms providing the effect are studied.

Abrikosov vortices in type II superconductors repel each other and therefore tend to form two dimensional lattices when thermal fluctuations or disorder are not strong enough to destroy lateral correlations. In isotropic s-wave materials the lattices are triangular, however in anisotropic materials or for “unconventional” d-wave or p-wave pairing interactions less symmetric vortex lattices (VL) can form, as recent experiment on high-$T_c$ cuprates,$^1$ SrRuO$_4$,$^2$ and borocarbides have showed. The high quality of samples in the last kind of superconductors allows detailed reconstruction of the phase diagram by means of small angle neutron scattering, scanning tunnelling microscopy or Bitter decoration technique. For $H \parallel c$ the presence of a whole series of structural transformations of VL was firmly established. At first, a high magnetic fields stable square lattice becomes rhombic, or “distorted triangular,” via a second order phase transition.$^{3,4}$

Then, at lower fields, a reorientation of VL by 45° relative to crystal axes occurs.$^{5,6}$ For $H \parallel a$ a continuous lock-in phase transition was predicted.$^5$ Above the critical field of this transition the apex angle of the elementary rhombic cell of VL does not depend on magnetic field, but below it such a dependence appears.

Theoretically the mixed state in nonmagnetic borocarbide superconductors RNi$_2$B$_2$C, $R = Y, Lu$ can be understood in the framework of the extended London model$^7$ (in regions of the phase diagram close to $H_{c2}(T)$ the extended Ginzburg-Landau model can be used.$^{4,8}$) So far this theory has always provided a qualitative and even quantitative description of phase transitions in VL and various other properties such as magnetization behavior,$^9$ dependence of nonlocal properties on the disorder,$^{10}$ etc. However, recently another “reorientation” phase transition has been clearly observed in neutron scattering experiment on LuNi$_2$B$_2$C, which cannot be explained by the theory despite considerable efforts. When a magnetic field of 0.3 T was applied along the $a$ axis of this tetragonal superconductor a sudden 90° reorientation of VL has been seen.$^{11}$ At this point rhombic (nearly hexagonal, apex angle $\approx 60°$) lattice, oriented in such a way that the crystallographic axes are its symmetry axes, gets rotated by 90°.

Both the initial and rotated lattices are found to coexist in the field range of width 0.1 T around the transition. Similar observations have been made in magnetic material ErNi$_2$B$_2$C.

In this paper we explain why the extended London model in its original form cannot generally explain even the existence of the 90° reorientation transition. The reason is that it possesses a “hidden” spurious fourfold symmetry preventing such a transition. Then we generalize the model to include the symmetry breaking effect and explain why the reorientation take place. Then we search for a microscopic origin of this effect. Using BCS type theory we find that anisotropy of the Fermi surface is ruled out due to the smallness of its contribution. It is the anisotropy of the pairing interaction that provides the required mechanism. We, therefore, suggest that there exist a correlation between the critical field of 90° reorientation in VL and the value of the anisotropy of the gap.

A convenient starting point of any generalized “London” model$^{7,12}$ is the linearized relation between the supercurrent $j_i$ and the vector potential $A_j$:

$$ (4 \pi/c) j_i(q) = - K_{ij}(q) A_j(q). \quad (1) $$

In the standard London model the kernel $K_{ij}(q)$ is approximated just by its $q = 0$ limit, inverse mass matrix, while in the extended London model the quadratic terms of the expansion of the kernel near $q = 0$ are also kept$^7$

$$ K_{ij}(q) = m_{ij}^{-1} + n_{ij,kl} q_k q_l. \quad (2) $$

The significance of the tensor $n_{ij,kl}$ is that it accounts properly for the symmetry of any crystal system while a rank two tensor $m_{ij}$ does not guarantee this. At the same time $n_{ij,kl}$ expresses nonlocal effects which are inherent to the electrodynamics of superconductors and below we call its component or their combination nonlocal parameters. From its definition, $n_{ij,kl} = \langle \frac{1}{2} (\partial^2/j \partial q \partial q_k) K_{ij}(q) \rangle_{q = 0}$ is a symmetric tensor with respect to both the first and the second pairs of indices. However, the way $n_{ij,kl}$ transforms when the first and the second pairs of indices are interchanged is not obvious because the “origin” of these indices are quite different. The first pair $(ij)$ comes, roughly speaking, from the variation of the free energy of the system “a superconductor in weakly inhomogeneous magnetic field” with respect to the vector
potential while the second pair \((kl)\) comes from the expansion in the vector \(q\). Below we show that in general no symmetry \(n_{kl,ij} = n_{kl,ij}\) is expected.

The original derivation of Eq. (2) from BCS theory in quasiclassical Eilenberger formulation produced a fully symmetric rank four tensor: \(n_{ij,kl} \sim (v_i, v_j, v_k, v_l)\) with \(v_i\) being components of the velocity of electrons at the Fermi surface. In this calculation independence of the gap function on the orientation was assumed. Let us consider the vortex lattice problem with this result. Specializing to tetragonal borocarbides, the number of independent components of the tensor \(n_{ij,kl}\) is four: \(n_{aaa\bar{a}}, n_{aabb}, n_{aacc}\) and \(n_{cccc}\). In the case of an external magnetic field oriented along \(a\) axis the free energy of VL, which is the relevant thermodynamic potential for a thin plate sample in perpendicular external field, reads

\[
F = (B^2/8\pi) \sum \left[ 1 + D \langle g_x, g_y \rangle \right]^{-1},
\]

\[
D = \lambda \left( m_a g_x^2 + m_c g_y^2 \right) + \lambda^4 \left( n_a m_a g_x^2 + m_c g_y^2 \right)^2 + d g_x^2 g_y^2.
\]

Here \(B\) is the magnetic induction and the summation runs over all vectors \(g\) of the reciprocal VL. The nonlocal parameters appearing in this equation have the form \(n = n_{aacc}\) and \(d = n_{cccc} m_c^2 + n_{aacc} m_a^2 - 6 n_{aacc} m_a m_c\). The free energy of Eq. (3) has been extensively studied first minimizing it on the class of rhombic lattices with symmetry axes coinciding with the crystallographic axes and more recently by us for arbitrary lattices with one flux per unit cell. Despite the fact that a great variety of vortex lattice transformation were identified, not a single 90° reorientation has ever been seen. The reason is quite simple: the free energy considered is actually effectively fourfold symmetric. After rescaling the reciprocal lattice vectors

\[
g_x \mapsto \tilde{g}_x = g_x / \sqrt{m_a}, \quad g_y \mapsto \tilde{g}_y = g_y / \sqrt{m_c}
\]

the sum in Eq. (3) becomes explicitly fourfold symmetric. Based on this observation one concludes that the energies of the lattices participating in the 90° reorientation are equal exactly. Therefore no phase transition between them is possible in the framework of the extended London model of Eq. (3) and further corrections are necessary to account for this transition.

There might be a slight possibility that the observed 90° reorientation presents the lock-in transition described in the beginning of this paper. For this to happen the rescaled square VL should looks almost hexagonal and, correspondingly, a particular value of the mass asymmetry \(m_a/m_c = [\cos(60°)/\cos(45°)]^2 = 1/2\) is required. This is very different from the figures quoted in literature: \(m_a/m_c = 0.91/1.22 = 0.74\). More importantly, according to this scenario one should see two degenerate lattices at small fields below the transition and only a single lattice at high fields above the transition which experimentally is clearly not the case.

To explain the 90° reorientation we proceed by correcting the model of Eq. (3). On general symmetry grounds for \(H||a\) one can expect more terms in the expression for \(D\) which describes vortex-vortex interactions. Given twofold symmetry of the present case we write down for \(D\) the expansion in Fourier series up to the fourth harmonic, perform rescaling defined by Eq. (4) and obtain

\[
D_{\text{eff}} = D_0(\tilde{g}) + D_4(\tilde{g}) \cos(4\varphi) + D_2(\tilde{g}) \cos(2\varphi),
\]

where \(\varphi\) is the polar angle in the rescaled \(b-c\) plane. The quantity \(D\) from Eq. (3) produces only fourfold invariant terms:

\[
D_0(\tilde{g}) = \lambda^2 g_x^2 + (n + d/8m_a m_c) \lambda^4 g_y^4,
\]

\[
D_4(\tilde{g}) = -(d/8m_a m_c) \lambda^4 g_y^4.
\]

The new term \(D_2(\tilde{g})\) expresses the effective fourfold symmetry breaking. Experimentally, it should be small as indicated by recent success in the qualitative understanding of the angle dependence of magnetization of LuNi\(_2\)B\(_2\)C.\(^9\) with a field lying in the \(a-b\) plane on the basis of the theory without \(D_2\) term. Accordingly, we can treat it perturbatively: \(F = F^{(0)} + F^{(\text{pert})}\) with

\[
F^{(0)} = (B^2/8\pi) \sum \left[ 1 + D_0 + D_4 \cos(4\varphi) \right]^{-1},
\]

\[
F^{(\text{pert})} = -(B^2/8\pi) \sum \frac{D_2 \cos(2\varphi)}{[1 + D_0 + D_4 \cos(4\varphi)]^2},
\]

where the summation is over \(\tilde{g}\) [see Eq. (4)]. The original degeneracy of the two VL rotated by \(90°\) with respect to each other is split now. To explain the \(90°\) reorientation the sign of the perturbation should change at certain field \(B_{\text{reo}}\). The magnetic field influences the sum via the constraint that the area of the unit cell carries one fluxon. Roughly speaking \(D_2(\tilde{g})\) should change sign when \(\tilde{g} = \sqrt{B_{\text{reo}}/4\lambda_0}\). The simplest way to implement this idea is to write for \(D_2(\tilde{g})\) the two lowest order terms in \(\tilde{g}\):

\[
D_2 = w_4 \tilde{g}_x^4 + w_8 \tilde{g}_y^8.
\]

A quadratic term is not present since we have already rescaled it out in the derivation of Eq. (5). In principle the coefficient \(w_6\) can be derived from BCS similarly to the \(n_{ij,kl}\) tensor within the framework of the original extended London model.\(^7\) Then it is proportional to the Fermi surface average of six components of the Fermi velocity. To obtain \(w_4\), however, the result \(n_{ij,kl} \sim (v_i, v_j, v_k, v_l)\) of Ref. 7 is not sufficient. Indeed, using the general expression for \(n_{ij,kl}\) and repeating the derivation of Eq. (3) from Eqs. (1) and (2) we see that

\[
w_4 = (n_{aaa\bar{c}} - n_{cc,\bar{a}})/2.
\]

In what follows we first demonstrate the presence of a first order phase transition in the model of Eq. (10) and then provide a microscopical derivation of \(w_4\). In order to be relevant for the 90° reorientation this coefficient should not be negligible. Otherwise a treatment of the reorientation of the vortex lattice in terms of the kernel \(K(q)\) expanded near \(q = 0\) [see Eq. (2)] appears not appropriate.

The critical magnetic field of the 90° reorientation \(B_{\text{reo}}\) depends only on the ratio \(r = \lambda^2 w_4/w_8\). We determined this dependence numerically using standard computational methods. At first, for a fixed \(B\) the equilibrium form of VL unit cell was obtained by minimization of Eq. (9). Then, the zero of the perturbation energy Eq. (9) was found. As usual during the numerical calculations the cutoff factor exp
\(-\xi_{g2}\) was introduced inside the above sums in order to properly account for the failure of the London approach in the vortex core. Figure 1 presents the result of calculations with nonlocal parameters \(d=0.05\) and \(n=0.015\) typical for LuNi\(_2\)B\(_2\)C. The critical magnetic field quickly drops as \(r\) becomes larger. Within the approximation of Eq. (10) the 90° reorientation cannot happen at very low magnetic fields. For LuNi\(_2\)B\(_2\)C with \(\lambda\approx710\) Å the field unit \(\Phi_0/(2\pi\lambda)^2\) is about 100 G. From the experimentally observed transition field \(B_{c2}=2.95\) kOe,\(^1\) we estimate the relative strength of the sixth and fourth order terms in \(D_2\) [see Eq. (10)] as \(r=0.036\).

Now let us discuss the possible microscopic origin of \(w_4\). We start from an effective many body Hamiltonian for electrons written in second quantized form

\[
H = \sum_x \left[ \psi^\dagger_{\alpha}(x) \left( \varepsilon(-i\mathbf{\nabla}) - \mu \right) \psi_{\alpha}(x) + V(\psi^\dagger_{\alpha}, \psi_{\alpha}) \right],
\]

where a summation over spin indices \(\alpha=\uparrow, \downarrow\) is assumed and \(V\) is a two body interaction. The dispersion \(\varepsilon(k)\) will be kept general because of the complicated band structure of borocarbides. We define it in coordinate space replacing \(k\rightarrow-k\) in Eq. (12) in order to couple the magnetic field by minimal substitution \(-i\mathbf{\nabla}\rightarrow i\mathbf{\nabla}\rightarrow A\). This procedure is not unique because the components of \(\mathbf{A}\) do not commute with each other. Therefore, \(\varepsilon(k)\) is presented by a Taylor expansion in symmetrized form.

The kernel \(K_{ij}(q)\) from Eq. (1) is obtained by treating the effect of a slowly varying magnetic field in the linear response approximation. The change in the Hamiltonian due to the presence of a magnetic field

\[
K_{ij}(x-y) = \left( \frac{\delta^2 H_1}{\delta A_i(x) \delta A_j(y)} - \frac{\delta H_1}{\delta A_i(x)} \frac{\delta H_1}{\delta A_j(y)} \right),
\]

where angular brackets denote the statistical average with the unperturbed density operator. Thus, we have to expand the functional \(H_1\) up to the terms quadratic in \(A\). Because our aim is to calculate \(w_4\) we need only the coefficients of this expansion for \(A_i\) and \(\partial A_i/\partial x\).

In its full generally the problem of Eq. (12) in a magnetic field is quite intractable and below we consider two particular cases in order to estimate quantitatively the magnitude of the different contributions to \(w_4\): (i) isotropic local interaction leading to pairing describing the major effect of longitudinal phonons (overpowering Coulomb attraction)

\[
V_1 = -\frac{g}{4} \int_x \psi^\dagger_{\alpha} \psi^\dagger_{-\alpha} \psi_{-\alpha} \psi_{\alpha}
\]

and an arbitrary dispersion relation \(\varepsilon(k)\); (ii) more complicated anisotropic model interactions with isotropic dispersion \(\varepsilon(k) = k^2/(2m)\).

In the case (i) the part of \(H_1\) dependent on \(A_2\) can be presented as follows:

\[
H_1 = -\frac{1}{2} \int_x \psi^\dagger_{\alpha} \left[ A_2 \varepsilon_{-\alpha}^z \delta A_2 \right] \psi_{\alpha} + \left( \frac{\partial^2}{\partial x^2} \right) \psi_{\alpha} + \left( \frac{\partial^2}{\partial y^2} \right) \psi_{\alpha}.
\]

At zero temperature \(R\) and thereby \(w_4\) vanishes exponentially. As temperature increases, \(w_4\) increases monotonically and reaches its maximal value at \(T=T_c\) where it smoothly joins the corresponding component of the \(q\)-dependent magnetic susceptibility tensor of the normal metal. For estimation we considered a simple dispersion relation \(\varepsilon(k) = (1/(2m))k^2 + (\alpha/4)k^4\) and assumed the deviations from a spherical Fermi surface to be small: \(\alpha = m^2/2\). Expanding in \(\alpha\) we obtain at \(T=T_c\) that

\[
w_4^{FS} = 2\alpha \Phi_0^2 \sqrt{\hbar^2/\mu/2m},
\]

where \(\Phi_0=2e/\hbar c\). This quantity is very small: comparing it with the components of \(n_{ij,kl}\) which produce contributions to Eq. (3) we see that \(w_4^{FS} \ll n_{x\perp x\perp} \sim (\Delta/\mu)^2\). It is not probable that such a tiny value of the asymmetry parameter \(w_4\) [see Eq. (11)] is responsible for the reorientation. What maybe more important is that temperature dependence of \(w_4\) given by Eq. (17) is not in accordance with the experiments which show only a slow dependence of the critical magnetic field of 90° reorientation on temperature.\(^1\)

Therefore, the origin of the 90° reorientation should be looked for elsewhere and we turn to the case (ii). In addition to the conventional local operator \(V_1\) defined in Eq. (15)
The function \( \varepsilon(q) \) originates from both the phonon propagator and the electron-phonon matrix element. However when the magnetic field is coupled via minimal substitution \( V_2 \) will not lead to any contribution to \( H_{\text{tr}}[\varepsilon, A] \). This follows from a basic property of the longitudinal phonon-electron interaction: the phonon couples to the electron density \( \rho(x) = \psi_{-a}^\dagger \psi_a \) which is a neutral operator and therefore \(-i \nabla\) should not be substituted by \( \mathbf{H} \) in Eq. (19). Only when derivatives act on a charged operator there is a possibility to generate \( w_4 \).

We therefore consider a phenomenological interaction

\[
V_3 = \frac{g}{4N} \psi_{-a}^\dagger [1 - \delta_0 \nabla^2] \psi_a [1 - \delta_0 \nabla^2] \psi_a^\dagger ,
\]

where \( N \) is the number of (real or auxiliary) ‘copies’ of the Fermi surface enumerated by \( a, b \). We calculated averages in Eq. (14) using the \( 1/N \) expansion\(^{13} \) rather than the BCS approximation. The reason to resort to the \( 1/N \) expansion is twofold. First, the BCS expression for \( w_4 \) contains diagrams up to three loops [see Fig. 2(c)] which are very complicated. Secondly, unlike BCS, this nonperturbative scheme is systematically improvable. The last property is important when questions of principle are concerned.

The corresponding perturbation Hamiltonian found by the minimal substitution reads

\[
H_1 = i \int_x \left[ \frac{\lambda}{2m} \partial_a \psi_a \partial_a \psi_{-a}^\dagger + \lambda \delta_0 \frac{4N}{N} S_a^\dagger U_{-1} - c \right],
\]

\[
S_{ab} = \psi_a^\dagger \partial_a \psi_b + (\partial_a \psi_a^\dagger \psi_b^\dagger),
\]

\[
U_{ab} = \psi_a^\dagger \psi_b^\dagger + \frac{\delta_0}{2} \left[ \psi_a^\dagger \partial_a^2 \psi_b^\dagger + (\partial_a^2 \psi_a^\dagger \psi_b^\dagger) \right].
\]

Here the terms proportional to \( A_\perp^2 \) are omitted since they are local and cannot contribute to the derivatives of \( K_{zz}(q) \) with respect to \( q_x \), required to obtain \( w_4 \). For simpler situations like the case (i) the leading order in \( 1/N \) expansion, with \( N \) set to 1, simply coincides with the BCS approximation. After observing that the order \( 1/N \) contributions, Fig. 2(a), all vanish due to \( k \leftrightarrow -k \) symmetry, we calculated the leading \( 1/N^2 \) contributions to the magnetic kernel, Fig. 2(b). At \( T = 0 \) to leading order in \( \delta_0 \) (further reducing number of integrals) the result reads

\[
w_4^{\text{int}} = -\frac{\delta}{N^2} \frac{8\pi}{105} \left( \frac{\mu}{\Delta} \right)^2 \Phi_0^2 \sqrt{h \tilde{\mu}/2m},
\]

where \( \delta = \delta_0 m \mu \) is the dimensionless gap anisotropy. Therefore, in the physical case of interest \( N = 1 \) we obtain

\[
w_4^{\text{int}} \sim -\delta \quad \text{(not necessary very small. This result is}
\]

\[
\text{to be compared with } w_4^{\text{FS}} \quad \text{originating from the Fermi surface}
\]

\[
\text{anisotropy which has a huge suppression factor } (\Delta/\mu)^2.
\]

The physical origin of an interaction of the type Eq. (20) is not clear at this stage. It might be a transverse phonon-electron coupling or some other force which first should be studied experimentally. We analyzed one possible candidate: the current-current interaction in metals. Although a relativistic effect, this coupling in normal metals has a long range at zero frequency.\(^{14} \) In superconductors it is cut off by the penetration depth. The current-current interaction is isotropic and gives a contribution to \( w_4 \) in the case of an anisotropic dispersion relation only. This contribution turns out to be small, of order \( a(e^2/hc)^2 (\nu_F/c)^2 \).

To conclude, we found that the extended London model is incapable of explaining the 90° reorientation in VL for \( H || a \) because it produces an effective fourfold symmetry of the free energy of VL. This symmetry becomes explicit after a rescaling transformation. We showed that in the general case one should include into the extended London model correction terms for which \( n_{ijkl} \equiv n_{klij} \) [see Eq. (2)]. As a result, the true twofold symmetry of the system in a magnetic field \( H || a \) is restored and the 90° reorientation can be explained naturally. We proved that for an arbitrary dispersion relation and conventional phonon pairing the correction terms vanish at \( T = 0 \) and are strongly suppressed at \( T = T_c \). Therefore, experimental observation of the reorientation points to the existence of a more intricate interaction. Note that inclusion of the correction terms will not change any conclusions of the extended London model for \( H || c \).

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