Physica B 460 (2015) 231–235

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Quantum limit and reentrant superconducting phases in the Q1D conductor $Li_{0.9}Mo_6O_{17}$

O. Sepper [a], A.G. Lebed [a,b,*]

[a] Department of Physics, University of Arizona, 1118 E. 4-th Street, Tucson, AZ 85721, USA
[b] L.D. Landau Institute for Theoretical Physics, 2 Kosygina Street, 117334 Moscow, Russia

ARTICLE INFO

Available online 24 November 2014

PACS:
74.20.Rp
74.70.Kn
74.25.Op

Keywords:
High magnetic field
Triplet superconductor
Unconventional superconductor

ABSTRACT

We solve the theoretical problem of restoration of superconductivity in a triplet quasi-one-dimensional, layered superconductor in an ultra-high magnetic field. With the field perpendicular to the conducting chains as well as having a component normal to the layers, we suggest a new quantum limit superconducting phase and derive an analytical expression for the transition temperature as a function of magnetic field, $T^*(\mathbf{H})$. Using our theoretical results along with the known band and superconducting parameters of the presumably triplet superconductor $Li_{0.9}Mo_6O_{17}$, we determine the orientation of $\mathbf{H}$ that maximizes $T^*(\mathbf{H})$ for a given value of the field. Subsequently, we show that reentrant superconductivity in this compound is attainable with currently available non-destructive pulsed magnetic fields of order $H \simeq 100$ T, when such fields are perpendicular to conducting chains and parallel to the layers. For its possible experimental discovery, we give a detailed specification on how small angular inclinations of the magnetic field from its best experimental geometry decrease the superconducting transition temperature of the reentrant phase.

1. Introduction

Theoretical studies of quasi-one-dimensional (Q1D) layered conductors under high magnetic fields have led to the description of a range of phenomena that result from a quasi-classical 3D → 2D field induced dimensional crossover [1–4] characterized by electron trajectories that extend through length scales much larger than the inter-plane distances in these layered compounds. These phenomena include the field induced spin- [1,5–7] and charge- [1,2,8,9] density-wave transitions, Danner–Kang–Chaikin oscillations [1,10], Lebed magic angles [1,11,12], and Lee–Naughton–Lebed oscillations [1,13–15]. In contrast, a quantum 3D → 2D dimensional crossover [1,16] occurs when a magnetic field localizes electrons on Q2D layers, with typical sizes of electron orbits comparable or less than the inter-plane distance. Thus, superconductivity is restored [16] on the layers through suppression of orbital destructive effects. This can happen if the Pauli paramagnetic spin-splitting is absent – as would be the case for superconductors with equal spin-triplet pairing. In this regard, a strong possibility of triplet pairing has been recently proposed [17–19] in the Q1D layered transition metal oxide – $Li_{0.9}Mo_6O_{17}$, where experimental measurements of upper critical magnetic field, H^x_{c2}, parallel to the most conducting axis yielded values 5 times the so-called Clogston–Chandrasekhar limit [20]. A quantitative theoretical analysis [18,19] has shown that, indeed, a triplet pairing scenario can account for such H_{c2} values through pure orbital destructive effects, so long as the out-of-plane superconducting coherence length exceeds the inter-plane distance.

In what follows, we solve a fully quantum mechanical problem of a Q1D layered conductor in an ultra-high magnetic field perpendicular to conducting chains. First, we examine the case when the field has a component normal to the x–y plane (i.e. subtends an angle α with respect to the layers), resulting in localization of electrons along the conducting chains. We show that this leads to restoration of superconductivity as a quantum limit phase through a 3D → 1D dimensional crossover [21], where the characteristic sizes of electron orbits becoming comparable to both inter-plane and inter-chain length scales. We demonstrate that it corresponds to experimentally available destructive pulsed magnetic fields of the order of $H \simeq 500 - 700$ T. Subsequently, we suggest experimental discovery of the reentrant superconducting phase in $Li_{0.9}Mo_6O_{17}$ using the currently available pulsed (non-destructive) magnetic fields of order $H \simeq 100$ T. Our calculations show that such fields, parallel to the layers and perpendicular to the conducting chains lead to the appearance of the reentrant superconductivity phenomenon below a reentrant transition temperature of $T^*(H = 100T) \simeq T_c/2 \simeq 1$ K in the superconductor

* Corresponding author at: Department of Physics, University of Arizona, 1118 E. 4-th Street, Tucson, AZ 85721, USA. fax: +1 520 621 4721.
E-mail address: lebed@physics.arizona.edu (A.G. Lebed).

http://dx.doi.org/10.1016/j.physb.2014.11.078
0921-4526/

$Li_{0.9}Mo_6O_{17}$. We calculate the angular dependence of $T^*(\alpha, H)$ for small angles to account for inclination of the same magnetic field from the optimal geometry of the corresponding experiment. The latter will allow to conduct the experiments with necessary accuracy.

2. Quasi-classical electron orbits in high magnetic fields

In this section we qualitatively consider electron trajectories in a high magnetic field to show how confinement in the y and z directions leads to the 3D → 1D dimensional crossover. To this end, let the magnetic field be perpendicular to the conducting chains, and subtend an angle α in the y–z plane, as shown in Fig. 1. The magnetic field and the vector potential corresponding to this configuration are

$$\mathbf{H} = (0, \cos\alpha, \sin\alpha)H, \quad \mathbf{A} = (0, \sin\alpha, -\cos\alpha)Hx. \tag{1}$$

We use the tight-binding approximation to describe electron motion in the Q1D conductor, for which the anisotropic dispersion relation is

$$\epsilon(\mathbf{p}) = -2t_x\cos(p_x a_x) - 2t_y\cos(p_y a_y) - 2t_z\cos(p_z a_z), \tag{2}$$

where t_i are the electron hopping integrals along different crystallographic directions, and a_i are the crystal lattice constants. The quasi-classical electron orbits in a magnetic field are governed by the Lorentz force,

$$\frac{d\mathbf{p}}{dt} = \left(\frac{e}{c}\right)\mathbf{v}\times\mathbf{H}, \tag{3}$$

where electrons moving on Q1D Fermi surface have the Fermi velocity $v_x \approx v_F = const.$ and

$$v_i = \frac{\partial\epsilon(\mathbf{p})}{\partial p_i} = 2t_i a_i\sin(p_i a_i), \quad i = y, z. \tag{4}$$

By substituting the component of the magnetic field, Eqs. (3) and (4) can be integrated with respect to time to find the form of quasi-classical orbits:

$$y(t) = \frac{2t_y}{\omega_y(\alpha)}a_y\cos\left[\omega_y(\alpha)t\right], \quad z(t) = \frac{2t_z}{\omega_z(\alpha)}a_z\cos\left[\omega_z(\alpha)t\right], \tag{5}$$

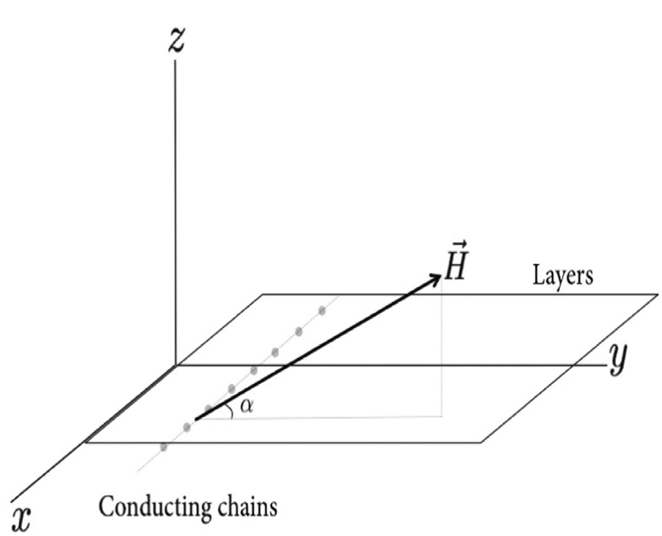

Fig. 1. The magnetic field makes an angle α with respect to the y-axis, perpendicular to the conducting chains.

where the angle dependent oscillation frequencies are

$$\omega_y(\alpha) = \frac{ev_F a_y H}{c}\sin\alpha, \quad \omega_z(\alpha) = \frac{ev_F a_z H}{c}\cos\alpha. \tag{6}$$

These results directly demonstrate that for high enough magnetic field the amplitudes of the quasi-classical periodic electron orbits (inversely proportional to H) become smaller than the inter-chain and inter-plane distances – effectively localizing electrons on the conducting chains. This occurs for a magnetic field

$$H > H^* = \max\left\{\frac{2t_y c}{ev_F\sin\alpha}, \frac{2t_z c}{ev_F\cos\alpha}\right\}. \tag{7}$$

This is the qualitative basis for the quantum limit superconductivity phenomenon. In the next section we present a quantitative solution to this problem and show that $2t_i/\omega_i$ are important quantum parameters.

3. Electron wave functions and the spin-triplet superconducting order parameter

In this section we derive an integral gap equation to describe the restoration of superconductivity in ultra-high magnetic field. We use Gor'kov's equation for non-uniform superconductivity under the assumption of equal spin-triplet pairing and derive an analytical solution under the conditions that give rise to the quantum limit superconducting phase. To this end, consider the Q1D Fermi surface consisting of two slightly warped sheets, shown in Fig. 2. The anisotropic electron spectrum with $t_z << t_y << t_x$ in Eq. (2) can be linearized on the right (+) and left (−) sheets of the Fermi surface:

$$\epsilon^{\pm}(\mathbf{p}) = \pm v_F(p_x - p_F) - 2t_y\cos(p_y a_y) - 2t_z\cos(p_z a_z). \tag{8}$$

The Hamiltonian is obtained from Eq. (8) by the method of Peierls' substitution: $p_x \to -i\partial_x$, $p_y \to p_y - (e/c)A_y$, $p_z \to p_z - (e/c)A_z$:

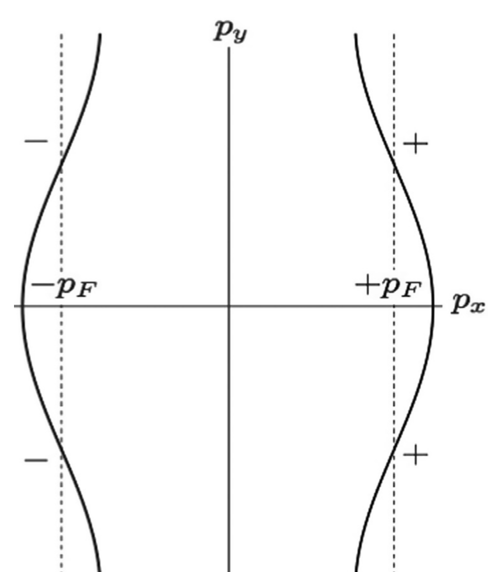

Fig. 2. Q1D Fermi surface consists of two slightly warped sheets centered at $p_x = \pm p_F$ and extending in the z direction. The triplet order parameter changes its sign on the right (+) and left (−) sheets.