Quantum limit in a magnetic field for triplet superconductivity in a quasi-one-dimensional conductor

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We theoretically consider the upper critical magnetic field, perpendicular to a conducting axis, in a triplet quasi-one-dimensional superconductor. In particular, we demonstrate that, at high magnetic fields, the orbital effects against superconductivity in a magnetic field are reversible and, therefore, superconductivity can be restored. It is important that the above mentioned quantum limit can be achieved in a presumably triplet quasi-one-dimensional superconductor $Li_{0.9}Mo_6O_{17}$ [J.-F. Mercure *et al.*, Phys. Rev. Lett. **108**, 187003 (2012).] at laboratory available pulsed magnetic fields of the order of $H = 500$–700 T.

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High magnetic field properties of quasi-one-dimensional (Q1D) conductors and superconductors have been intensively studied since the discovery of the field-induced spin-density-wave (FISDW) cascade of phase transitions [1–4]. Note that the FISDW phenomenon, experimentally discovered in the $(TMTSF)_2X$ compounds [1,2], where $X = ClO_4$ and PF_6, was historically the first one which was successfully explained in terms of quasiclassical three-dimensional to two-dimensional (3D $\rightarrow$ 2D) crossover in high magnetic fields [3,5–7]. At present, it has been established that different kinds of quasiclassical dimensional crossovers in a magnetic field are responsible for such unusual phenomena in layered Q1D conductors as the field-induced charge-density-wave (FICDW) phase transitions [3,5,8,9], Danner-Kang-Chaikin oscillations [3,10], Lebed magic angles [3,11,12], and Lee-Naughton-Lebed oscillations [3,13–16]. Note that a characteristic property of the quasiclassical dimensional crossovers is that the typical "sizes" of electron trajectories in a magnetic field are much lager than the interplane or interchain distances in layered Q1D conductors.

On the other hand, a different type of dimensional crossover in a magnetic field—the so-called quantum dimensional crossover [3]—was suggested in Ref. [17] to describe the magnetic properties of a superconducting phase. More specifically, it was shown [17–22] that, at high enough magnetic fields, the typical "sizes" of electron trajectories become of the order of interplane distances and superconductivity can be restored as a pure 2D phase. Note that the above mentioned conclusion is valid only for some triplet superconducting phases which are not sensitive to the Pauli paramagnetic effects in a magnetic field. Due to this reason, Q1D superconductors $(TMTSF)_2X$ were considered for many years to be the best candidates for this reentrant superconductivity (RS) phenomenon, since triplet superconducting pairing was suggested [23,24] to exist in these materials. Recently, it has been shown [22,25,26] that a d-wave singlet superconducting phase is more likely to exist in the $(TMTSF)_2ClO_4$, therefore, the RS phenomenon experimentally reveals itself in this compound only as a hidden RS phase [22]. As for the superconductor $(TMTSF)_2PF_6$, the existing experimental data about the nature of the superconducting pairing in this compound are still controversial [3]. In this difficult situation, it is important that a strong candidate for triplet superconducting pairing—the Q1D superconductor $Li_{0.9}Mo_6O_{17}$—has been recently proposed [27–29]. In particular, it has been shown in Refs. [28,29] that a quantitative description by a triplet scenario of superconductivity, with a magnetic field applied along the conducting axis, can account for the experimental field that exceeds the so-called Clogston-Chandrasekhar paramagnetic limit [30] by five times [27].

The goal of our paper is to show theoretically that the triplet superconductivity scenario can be tested in the $Li_{0.9}Mo_6O_{17}$ superconductor in ultrahigh magnetic fields of the order of $H \simeq 500$–700 T, where triplet superconductivity is shown to be restored with a transition temperature $T_c^* \simeq 0.75T_c \simeq 1.4$–1.7 K. Note that the suggested effect is different from the RS phenomenon [17–22] since we consider a magnetic field, which has a nonzero out-off conducting plane component. Therefore, at high magnetic fields, the 3D $\rightarrow$ 2D crossover [3,17] does not happen. Instead, a quantum 3D $\rightarrow$ 1D crossover happens. We call such a crossover the Q1D $\rightarrow$ 1D quantum limit (QL) [31]. (Note that below we apply the Fermi-liquid approach to the Q1D transition-metal oxide $Li_{0.9}Mo_6O_{17}$. The validity of the Fermi-liquid picture as well as the Q1D nature of the electron spectrum in this conductor have been firmly established in Refs. [27–29].)

First, let us demonstrate the suggested QL superconductivity phenomenon using qualitative arguments. Below, we consider the electron spectrum of a Q1D conductor in a tight-binding approximation,

$$\epsilon(\mathbf{p}) = -2t_x \cos(p_x a_x) - 2t_y \cos(p_y a_y) - 2t_z \cos(p_z a_z), \quad (1)$$

where $t_x \gg t_y > t_z$ are overlap integrals of the electron wave functions along the **x**, **y**, and **z** crystallographic axes, respectively. Since $t_x \gg t_y, t_z$, the electron spectrum (1) corresponds to two slightly deformed pieces of the Fermi surface (FS) and can be linearized near $p_x \simeq \pm p_F$,

$$\epsilon(\mathbf{p}) = \pm v_F (p_x \mp p_F) - 2t_y \cos(p_y a_y) - 2t_z \cos(p_z a_z), \quad (2)$$

(see Fig. 1) where p_F and v_F are the Fermi momentum and Fermi velocity, respectively. In a magnetic field, perpendicular

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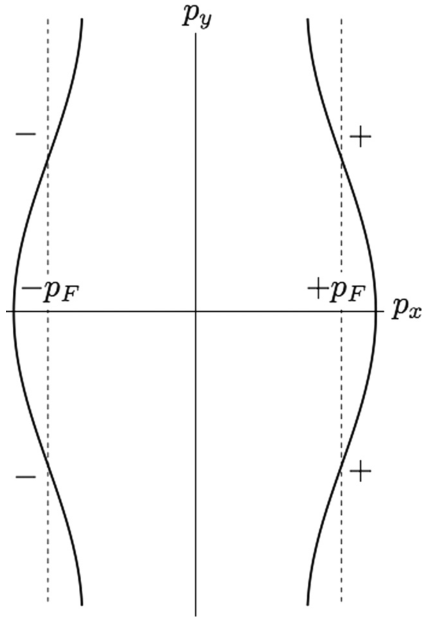

FIG. 1. The Q1D Fermi surface consists of two slightly corrugated sheets extending in the z direction. The triplet superconducting order parameter changes its sign on the two sheets of the Q1D Fermi surface.

to the conducting axis,

$$\mathbf{H} = (0, \cos\alpha, \sin\alpha)H, \quad \mathbf{A} = (0, -\sin\alpha, \cos\alpha)Hx, \quad (3)$$

(see Fig. 2) it is possible to write quasiclassical equations of electron motion,

$$\frac{d\mathbf{p}}{dt} = \left(\frac{e}{c}\right)[\mathbf{v}(\mathbf{p}) \times \mathbf{H}], \quad (4)$$

in the following way:

$$\frac{d(p_z a_z)}{dt} = \omega_z(\alpha)t, \quad \frac{d(p_y a_y)}{dt} = -\omega_y(\alpha)t, \quad (5)$$

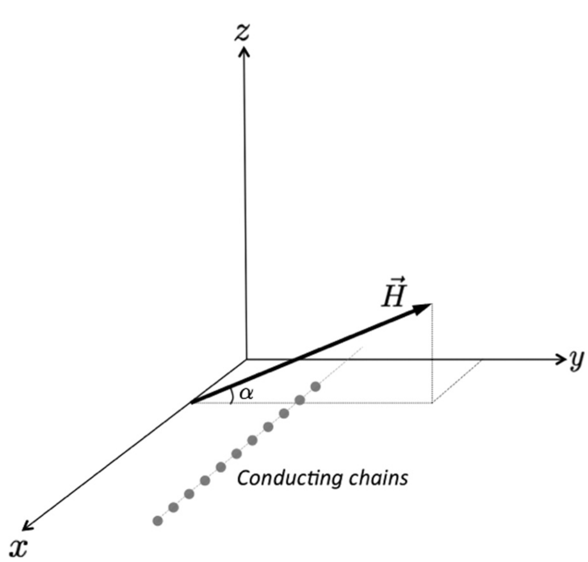

FIG. 2. The magnetic field makes an angle α with respect to the y axis, perpendicular to the conducting chains.

where

$$\omega_y(\alpha) = ev_F a_y H \sin\alpha/c, \quad \omega_z(\alpha) = ev_F a_z H \cos\alpha/c. \quad (6)$$

Since the electron velocity components can be expressed as functions of time,

$$\begin{aligned} v_y(p_y) &= \partial\epsilon(\mathbf{p})/\partial p_y = -2t_y a_y \sin[\omega_y(\alpha)t], \\ v_z(p_z) &= \partial\epsilon(\mathbf{p})/\partial p_z = 2t_z a_z \sin[\omega_z(\alpha)t], \end{aligned} \quad (7)$$

their trajectories in a real space are described by the following equations:

$$\begin{aligned} y &= l_y(\alpha)a_y \cos[\omega_y(\alpha)t], \quad l_y(\alpha) = 2t_y/\omega_y(\alpha), \\ z &= -l_z(\alpha)a_z \cos[\omega_z(\alpha)t], \quad l_z(\alpha) = 2t_z/\omega_z(\alpha). \end{aligned} \quad (8)$$

As directly follows from Eq. (8), electron motion in a real space in the magnetic field (3) is free along the conducting axes and is periodic and restricted perpendicular to the axes. If the magnetic field is strong enough,

$$H \gg H^* = \max\left\{\frac{2t_y c}{ev_F a_y \sin\alpha}, \frac{2t_z c}{ev_F a_z \cos\alpha}\right\}, \quad (9)$$

then electron motion in the perpendicular directions becomes localized on the conducting axes. This fact is directly seen from Eqs. (8) and (9) since the characteristic "sizes" of the electron trajectories $l_y(\alpha)a_y$ and $l_z(\alpha)a_z$ become less than the corresponding interchain distances a_y and a_z. In this case, electron motion is "one dimensionalized" and, as we show below, the Cooper instability restores the superconducting phase. [Note that the above suggested localization of the Q1D electrons (2) on conducting chains is completely different from another possible phenomenon—electron localization in unreasonable high magnetic fields, which correspond to a flux quantum per unit cell.]

Below, we study the QL superconductivity phenomenon by means of quantitative quantum mechanical methods appropriate for the problem under consideration. In a particular, in the magnetic field (3), we use the Peierls substitution method [5], based on the Fermi-liquid description of Q1D electrons (2):

$$\begin{aligned} &p_x \mp p_F \to \mp i(d/dx), \quad p_y a_y \to p_y a_y - \omega_y(\alpha)/v_F, \\ &p_z a_z \to p_z a_z + \omega_z(\alpha)/v_F. \end{aligned} \quad (10)$$

As a result, the Schrödinger-like equation for electron wave functions in the mixed (p_y, p_z, x) representation can be written as

$$\left\{\mp i v_F \frac{d}{dx} - 2t_y \cos\left[p_y a_y - \frac{\omega_y(\alpha)}{v_F}x\right] - 2t_z \cos\left[p_z a_z + \frac{\omega_z(\alpha)}{v_F}x\right]\right\}\psi_\epsilon^\pm(p_y, p_z, x) = \delta\epsilon\,\psi_\epsilon^\pm(p_y, p_z, x), \quad (11)$$

where the electron energy is counted from the Fermi energy, $\delta\epsilon = \epsilon - \epsilon_F$, $\epsilon_F = p_F v_F$. Note that in Eq. (11) we disregard electron spin since below we consider such a triplet superconducting phase where the Pauli paramagnetic effects do not reveal themselves. It is important that Eq. (11) can be solved analytically:

$$\psi_\epsilon^\pm(p_y,p_z,x) = \exp\left(\frac{\pm i\delta\epsilon x}{v_F}\right)\exp\left\{\pm 2il_y(\alpha)\left(\sin\left[p_y a_y - \frac{\omega_y(\alpha)}{v_F}x\right] - \sin[p_y a_y]\right)\right\}\exp\left\{\mp 2il_z(\alpha)\left(\sin\left[p_z a_z - \frac{\omega_z(\alpha)}{v_F}x\right] - \sin[p_z a_z]\right)\right\}. \quad (12)$$

Since electron wave functions are known (12), we can define the finite temperature Green's functions by means of the standard procedure [32]:

$$g^\pm_{i\omega_n}(p_y,p_z;x,x_1) = \int_{-\infty}^{+\infty} d(\delta\epsilon)[\psi^\pm_\epsilon(p_y,p_z;x)]^* \times\psi^\pm_\epsilon(p_y,p_z;x_1)/(i\omega_n - \delta\epsilon), \quad (13)$$

where ω_n is the so-called Matsubara frequency.

In this paper, we consider the following gapless triplet superconducting order parameter in $Li_{0.9}Mo_6O_{17}$, which, as shown in Refs. [28,29], well satisfies the experimental data [27]:

$$\hat{\Delta}(p_x,x) = \hat{I}\,\mathrm{sgn}(p_x)\Delta(x), \quad (14)$$

where $\hat{I}$ is a unit matrix in spin space, and $\mathrm{sgn}(p_x)$ changes the sign of the triplet superconducting order parameter on two slightly corrugated sheets of the Q1D FS (2) (see Fig. 1).

We use the Gor'kov equations for unconventional superconductivity [33,34] to obtain the so-called gap equation for the superconducting order parameter $\Delta(x)$. As a result, we derive the following equation:

$$\Delta(x) = \frac{g}{2}\int_{|x-x_1|>d}\frac{2\pi T dx_1}{v_F\sinh\left[\frac{2\pi T|x-x_1|}{v_F}\right]}\Delta(x_1) \times J_0\left\{4l_y(\alpha)\sin\left[\frac{\omega_y(\alpha)(x-x_1)}{2v_F}\right]\sin\left[\frac{\omega_y(\alpha)(x+x_1)}{2v_F}\right]\right\} \times J_0\left\{4l_z(\alpha)\sin\left[\frac{\omega_z(\alpha)(x-x_1)}{2v_F}\right]\sin\left[\frac{\omega_z(\alpha)(x+x_1)}{2v_F}\right]\right\}, \quad (15)$$

where g is the electron coupling constant and d is the cutoff distance.

Note that the QL superconductivity phenomenon is directly seen from Eq. (15). Indeed, at high enough magnetic fields (9), the parameters $l_y(\alpha)$ and $l_z(\alpha)$ become less than 1. Under this condition, arguments of the Bessel functions in Eq. (15) go to zero and the superconducting transition temperature goes to its value in the absence of magnetic field T_c:

$$\lim_{H\to\infty} T_c^*(H) \to T_c. \quad (16)$$

It is also important that Eq. (15) predicts that superconductivity in a triplet Q1D superconductor without impurities can survive at any magnetic field, including magnetic fields lower than that in Eq. (9). Nevertheless, we point out that for magnetic fields less than (9), the superconducting transition temperatures are very low and an account of a small amount of impurities would presumably kill the superconducting phase.

For experimental applications of our results, it is important to calculate how quickly superconductivity tends to $T_c(0)$ in Eq. (16). For this purpose, we expand each Bessel function in Eq. (15) to second order with respect to the small parameters $l_y(\alpha), l_z(\alpha) \ll 1$:

$$J_0\{\cdots\}J_0\{\cdots\} \simeq 1 - 4l_y^2(\alpha)\sin^2\left[\frac{\omega_y(\alpha)(x-x_1)}{2v_F}\right]\sin\left[\frac{\omega_y(\alpha)(x+x_1)}{2v_F}\right] - 4l_z^2(\alpha)\sin^2\left[\frac{\omega_z(\alpha)(x-x_1)}{2v_F}\right]\sin\left[\frac{\omega_z(\alpha)(x+x_1)}{2v_F}\right]. \quad (17)$$

In the second approximation with respect to the small parameters $l_y(\alpha)$ and $l_z(\alpha)$, it is possible to use in the integral gap equations (15) and (17) the following trial function:

$$\Delta(x) = \Delta(y) = \text{const}. \quad (18)$$

In this approximation, we can also average Eqs. (15) and (17) over the variable $x + x_1$ and, after using the following formula,

$$\frac{1}{g} = \int_d^{+\infty}\frac{2\pi T_c dz}{\sinh\left(\frac{2\pi T_c z}{v_F}\right)}, \quad (19)$$

we obtain

$$T_c^*(H)=T_c\left\{1 - l_y^2(\alpha)\ln\left[\frac{\gamma\omega_y(\alpha)}{\pi T_c}\right] - l_z^2(\alpha)\ln\left[\frac{\gamma\omega_z(\alpha)}{\pi T_c}\right]\right\}, \quad (20)$$

where γ is the Euler constant. From Eq. (20) it is directly seen that, at high enough magnetic fields (9), Eq. (16) is valid.

For experimental applications of our results it is important to estimate the value of $T_c^*(H)$ in Eq. (20) for the presumably triplet [27–29] Q1D superconductor $Li_{0.9}Mo_6O_{17}$ in the experimental range of magnetic fields. Using known values of the parameters a_y, a_z, v_F, t_y, and t_z (see Table I in Ref. [28]), it is possible to find that

$$\begin{aligned}
&\omega_y(H = 1\ \mathrm{T}, \alpha = \pi/2) = 0.76\ \mathrm{K},\\
&\omega_z(H = 1\ \mathrm{T}, \alpha = 0) = 0.57\ \mathrm{K},\\
&l_y(H = 1\ \mathrm{T}, \alpha = \pi/2) = 116,\\
&l_z(H = 1\ \mathrm{T}, \alpha = 0) = 49.
\end{aligned} \quad (21)$$

Our next step is to input these parameters into Eq. (20) and to plot $T_c^*(\alpha)$ as a function of α at given H. (We recall that the superconducting transition temperature in the absence of a magnetic field is equal to $T_c = 2.2$ K.) In Fig. 3, we plot the angular dependence of the QL superconducting phase transition temperature for two values of a magnetic field, $H =$ 500 and 700 T. As seen from Fig. 3, the maximum values of $T_c^*(H)$ correspond to an angle $\alpha^* \simeq 58^\circ$ in both cases, with the highest $T_c^*(H = 700\ \mathrm{T}) \simeq 1.7$ K. Note that region of validity of Eq. (20) corresponds to the condition $|T_c^*(H) - T_c| \ll T_c$, therefore, we conclude that Fig. 3 correctly represents the calculated transition temperatures near its maxima for both values of the magnetic field. It is important that magnetic fields of the order of $H = 500$–700 T are currently experimentally

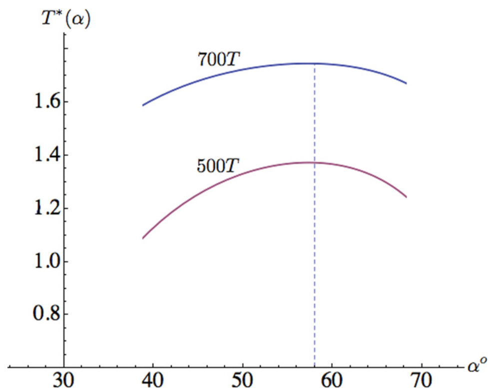

FIG. 3. (Color online) The QL superconducting transition temperature dependence of the angle α for magnetic fields of 500 and 700 T. Both maxima occur at an angle of $\alpha \approx 58^\circ$. The maximum temperature at 700 T is approximately 1.7 K.

available as destructive pulsed magnetic fields. Note that there exist several serious difficulties to investigate the low temperature superconducting phases in a pulsed magnetic field. One of them is that the characteristic time of the pulse has to be longer than the superconducting relaxation time. Another obvious difficulty is that it is necessary to maintain low temperature in a sample during the pulse. All these and other related problems have been successfully solved in experimental work [35], where the superconducting phase in an optimally doped yttrium barium copper oxide (YBCO) sample is studied in magnetic fields up to $H = 400$ T and temperatures down to $T = 1.6$ K by a contactless radio frequency transmission technique.

In the paper, we have demonstrated that superconductivity can be restored in a triplet Q1D superconductor in a magnetic field, perpendicular to its conducting axis, as the quantum limit (QL) superconducting phase. It happens if a magnetic field is high enough [see Eq. (9)] to localize electrons on conducting chains of a Q1D conductor. Note that such "one dimensionalization" of a Q1D electron spectrum promotes also the FISDW instability [5–7] and non-Fermi-liquid properties [3]. Therefore, we suggest that superconducting instability is a leading one and that electron wave function delocalizations between adjacent chains are high enough for the Fermi-liquid picture to survive. Note that the FICDW instability [8,9] is not expected in high magnetic fields since the Pauli paramagnetic effects significantly decrease the FICDW transition temperature [36]. We suggest to carry out the corresponding experiment on the presumably triplet superconductor $Li_{0.9}Mo_6O_{17}$ in feasibly available pulsed magnetic fields of the order of $H = 500$–700 T and temperatures less than $T_c^* \simeq 1.4$–1.7 K. We have also determined the most convenient geometry of the experiment which, as shown, corresponds to an inclination angle of $\alpha = 58^\circ$ [see Eq. (3) and Fig. 2]. It is important that the QL superconductivity phenomenon is not very sensitive to possible deviations in geometry from the most convenient one, as seen from Eq. (20) and Fig. 3. If the result of the suggested experiment is positive, it will confirm the triplet superconductivity scenario [27–29] in the above mentioned compound and establish the survival of superconductivity in ultrahigh magnetic fields.

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