Nodeless versus nodal scenarios of possible triplet superconductivity in the quasi-one-dimensional layered conductor $Li_{0.9}Mo_6O_{17}$

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We consider the problem of the orbital upper critical magnetic field, parallel to the most conducting axis of a quasi-one-dimensional layered superconductor. It is shown that superconductivity can be destroyed through orbital effects at fields much higher than the so-called Clogston-Chandrasekhar paramagnetic limiting field H_p, provided that superconducting pairing of electrons are of a triplet nature. We demonstrate that the superconducting state of the quasi-one-dimensional layered conductor $Li_{0.9}Mo_6O_{17}$ is well described by the suggested theory. To this end, we consider two competing scenarios: (1) a superconducting order parameter without zeros on the Fermi surface, and (2) one with zeros on the Fermi surface—both are shown to lead to destruction of superconductivity at a magnetic field H_{c2}^x, five times higher than H_p. With recent experimental measurements on the $Li_{0.9}Mo_6O_{17}$ favoring the nodeless order parameter, we present a strong argument supporting triplet pairing in this compound.

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I. INTRODUCTION

Detailed studies of the upper critical magnetic fields that lead to the destruction of superconductivity in type-II superconductors can provide essential information as to the nature of superconductivity in a given compound. Theoretical analysis of the upper critical magnetic fields along different directions in superconducting crystals is crucial in highly anisotropic, quasi-one-, and quasi-two-dimensional (Q1D and Q2D) materials, where such fields depend on the orientation, and can reveal fundamental properties, such as the pairing symmetry of the superconducting state. In a magnetic field, destruction of superconductivity that results from the breaking of the Cooper pairs can manifest itself through two distinct mechanisms, as the field couples to both electron's charge and spin. In the first case, the magnetic field alters the orbital wave functions of electrons, leading to the orbital pair-breaking effect. Superconductors can experience this Meissner effect irrespective of their pairing nature. The second mechanism that leads to destruction of superconductivity in a magnetic field is due to Pauli spin splitting, as pairing of electrons in spin-singlet states (spins anti-aligned, total spin $s = 0$) becomes energetically unfavorable. In this case, the difference in Pauli energy levels $\Delta E = 2\mu_B H_p$ is of the order of the superconducting energy gap Δ, where μ_B is the Bohr magneton, and H_p is the so-called Clogston-Chandrasekhar paramagnetic limiting field.[1] A detailed analysis shows that $H_p = \frac{\Delta}{2\sqrt{2}\mu_B} \approx 1.83 T_c$ (T/K), based on the BCS result[2] of $\Delta = 3.53 k_B T_c$. In the case of the recently examined[3] Q1D compound $Li_{0.9}Mo_6O_{17}$, with $T_c = 2.2$ K, this result gives $H_p \approx 4$ T. We also note that a paramagnetic limiting field of $H_p \approx 3.1$ T in this compound has been extracted experimentally[3] from the Pauli susceptibility and the specific heat jump at T_c. This value is five times smaller than the measured upper critical field $H_{c2}^x \approx 15$ T, parallel to the most conducting axis.

Survival of superconductivity for the upper critical magnetic fields greatly exceeding H_p, suggests the possibility of spin-triplet pairing (where the total spin of a Cooper pair, $s = 1$)—a rather rare and intriguing phenomenon in unconventional superconductivity. In contrast to singlet pairing, Cooper pairs in triplet superconductors can be insensitive to Pauli splitting, the orbital pair-breaking effect being the prevalent mechanism that destroys superconductivity. In this regard, highly anisotropic, Q1D layered conductors have attracted considerable attention from theorists and experimentalists alike. Important candidates for unconventional superconductivity include the organic superconductors[4,5] that have been experimentally investigated since 1980. Initial experiments performed on the Q1D superconductors $(TMTSF)_2X$ ($X = PF_6$ and ClO_4), called the Bechgaard salts, alluded to their unconventional nature.[6–9] Interest in these compounds was further intensified due to the possible existence of such peculiar phenomena as reentrant superconductivity,[10–13] as well as the Larkin-Ovchinnikov-Fulde-Ferrel (LOFF) phase,[14–17] and hidden reentrant superconductivity.[18] Currently the leading candidate for triplet superconductivity is the heavy-fermion compound[19] UPt_3, while strong evidence in favor of triplet pairing[20,21] has been found in Sr_2RuO_4, as theoretical studies of the latter have been motivated by similarities to triplet pairing in superfluid ^{3}He. As for the members from the family $(TMTSF)_2X$, NMR measurements of the Knight shift provide evidence for d-wave-like pairing[22,23] for $X = ClO_4$, while the pairing nature of $X = PF_6$, although initially hypothesized to be spin triplet, has not yet been unequivocally settled.[13,24] Investigation of the superconducting state in Q1D conductors poses considerable general interest as more new compounds with unconventional pairing symmetry (the possibility of triplet pairing, other exotic phases) are being experimentally investigated.

In our paper we study two scenarios of triplet electron pairing in the Q1D layered superconductor $Li_{0.9}Mo_6O_{17}$. Using Gor'kov's equations for unconventional superconductivity,[25–27] we obtain the so-called gap equations for superconducting order parameters with and without zeros on the Q1D Fermi surface. We show quite generally that in the absence of paramagnetic limiting the orbital pair-breaking effects lead to destruction of superconductivity in a Q1D layered conductor at fields much higher than the Clogston-Chandrasekhar limit $H_{c2}^x \gg H_p$, with **H** aligned along the most conducting ($\hat{x}$) crystallographic axis, provided that the

interplane distance is less than the corresponding coherence length ξ_z. This is in contrast to the common belief[3] stipulating that the orbital destructive effects are minimized for fields parallel to the most conducting axis, and thus are not able to destroy the superconducting phase. We define the band and superconducting parameters of $Li_{0.9}Mo_6O_{17}$ and show that, indeed, the coherence length of Cooper pairs perpendicular to the planes ξ_z is greater than the interplane separation. Thus, the conducting layers in $Li_{0.9}Mo_6O_{17}$ are well coupled, leading to a 3D anisotropic description of superconductivity. We compare our results with the experimental data,[3] and demonstrate that the Q1D superconductor $Li_{0.9}Mo_6O_{17}$ is better described by the nodeless triplet order parameter, in contrast to the nodal case. The temperature dependence of the upper critical field $H^x_{c2}(T)$ obtained in this paper is in excellent quantitative and qualitative agreement with the experiment. Note that the case of nodeless triplet superconductivity was considered before in brief in our Rapid Communication.[28]

This paper is organized as follows: In Sec. II the Hamiltonian of electrons with Q1D anisotropic energy spectrum in a magnetic field is introduced and the wave functions are calculated. In Sec. III the Green's functions of the Q1D electrons in a magnetic field are obtained and the rest of the section is devoted to the general formalism of obtaining the so-called gap equation for a triplet superconducting order parameter in a magnetic field. Section IV is devoted to the analysis and analytical simplification of the integral gap equations and their numerical solutions for the nodeless and nodal triplet superconducting order parameters. In Sec. V the upper critical magnetic field as a function of temperature $H_{c_2}(T)$ is extracted for both kinds of order parameters, and compared to the recently measured experimental values for the Q1D conductor $Li_{0.9}Mo_6O_{17}$, concluding with subsequent arguments in favor of triplet pairing described by the nodeless case. In Sec. VI we summarize and discuss the obtained results.

II. WAVE FUNCTIONS OF ELECTRONS WITH Q1D ANISOTROPIC ELECTRON SPECTRUM IN A MAGNETIC FIELD

We begin by considering the tight binding model for a Q1D electron spectrum of a layered conductor:

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

where we set $\hbar \equiv 1$. In the equation above, a_i are the lattice constants, and t_i are the transfer integrals for electron wave functions along the crystallographic axes. In the highly anisotropic Q1D layered conductor under consideration, $t_x \gg t_y \gg t_z$, a fact that will allow us to linearize the dispersion relation. Our initial step is to define the appropriate Hamiltonian, and solve a Schrödinger-like equation to obtain the exact wave functions. To this end, we consider a magnetic field parallel to the conducting chains (along $\hat{\mathbf{x}}$) of a Q1D layered conductor $\mathbf{H} = H\hat{\mathbf{x}}$. The vector potential corresponding to this magnetic field can be chosen to be $\mathbf{A} = Hy\,\hat{\mathbf{z}}$. Consider a Q1D Fermi surface (FS)—two open, slightly corrugated sheets centered at at $p_x = \pm p_F$, extending along $\hat{\mathbf{p}}_z$ depicted in Fig. 1. On the surface of constraint (i.e., the FS) the following linearized relation holds (the $\pm$ correspond to the left/right sides of the FS):

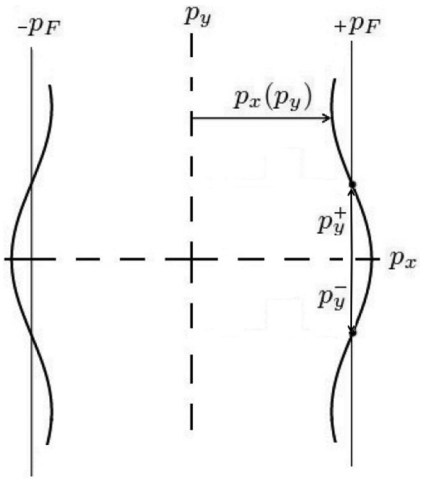

FIG. 1. Fermi surface for a Q1D layered conductor. Throughout the text, the $\pm$ in expressions refer to the right (+) and left (−) sheets of the Fermi surface.

$$p_x(p_y) = \pm p_F \pm \frac{2t_y}{v_F}\cos(p_y a_y), \tag{2}$$

where $v_F = 2t_x a_x \sin(p_F a_x)$ is the Fermi velocity of electrons along the most conducting $\hat{\mathbf{x}}$ axis. Equation (2) implicitly defined p_y as a function of p_x on the Q1D Fermi surface. Let $p_y^{\pm}$ stand for the two values (upper and lower) of p_y for which $p_x(p_y^{\pm}) = p_F$. We further define

$$v_y(p_x) = \partial\epsilon(\mathbf{p})/\partial p_y = 2t_y a_y \sin[p_y(p_x)a_y].$$

The energy dispersion relation can be linearized near the left and right sheets of the FS. Measured with respect to the Fermi energy $\epsilon = E - E_F$, the linearized dispersion relation takes the form

$$\epsilon^{\pm}(\mathbf{p}) = \pm v_y(p_y)[p_y - p_y^{\pm}(p_x)] - 2t_z\cos(p_z a_z). \tag{3}$$

To obtain the Hamiltonian in a magnetic field $\mathbf{H} = H\hat{\mathbf{x}}$, the Pierels substitution method is used:

$$p_y - p_y^{\pm}(p_x) \to -i\frac{\partial}{\partial y} \quad \text{and} \quad p_z \to p_z - \frac{e}{c}A_z, \tag{4}$$

where $A_z = Hy$ is the z component of the vector potential.

Using the substitution in Eq. (4) for the dispersion relation in Eq. (3), as well as including the spin-dependent interaction, the following Hamiltonian is obtained:

$$\hat{\epsilon}^{(\pm)} = \mp i v_y(p_y^{\pm})\frac{\partial}{\partial y} - 2t_z\cos\left(p_z a_z - \frac{\omega_z}{v_F}y\right) - 2\mu_B s H, \tag{5}$$

where $\omega_z = eHa_z v_F/c$, μ_B is the Bohr magneton, and s is the projection of the spin along the direction of the magnetic field $\hat{x}$. The simultaneous orbital eigenfunctions of energy and momentum component p_x, with eigenvalues ϵ can be represented in the factored form

$$\Psi^{\pm}_{\epsilon,p_x}(x,y,p_z) = e^{\pm ip_x x}\, e^{\pm ip_y^{\pm}(p_x)y}\, \psi^{\pm}_{\epsilon}(y,p_z). \tag{6}$$

The wave functions $\psi_\epsilon^\pm(y,p_z)$ are obtained from a Schrödinger-like equation $\hat{\epsilon}^{(\pm)}\,\psi_\epsilon^\pm(y,p_z)=\epsilon\,\psi_\epsilon^\pm(y,p_z)$:

$$\mp i v_y(p_y^\pm)\frac{\partial\psi_\epsilon^\pm(y,p_z)}{\partial y} = \left[\epsilon + 2t_z\cos\left(p_z a_z - \frac{\omega_z}{v_F}y\right) + 2\mu_B s H\right]\psi_\epsilon^\pm(y,p_z). \tag{7}$$

The equation above admits exact solutions of the form

$$\psi_\epsilon^\pm(y,p_z) = \exp\left[\pm i\frac{2t_z}{v_y(p_y^\pm)}\int_0^y \cos\left(p_z a_z - \frac{\omega_z}{v_F}y'\right)dy'\right] \times \exp\left(\pm i\frac{\epsilon\, y}{v_y(p_y^\pm)}\right)\exp\left[\pm\frac{2i\mu_B s H y}{v_y(p_y^\pm)}\right]. \tag{8}$$

Thus, the complete, normalized solutions for the wave functions are

$$\begin{aligned}\Psi_{p_x}^\pm(\epsilon;x,y,p_z) &= \frac{e^{\pm ip_x x}e^{\pm ip_y^\pm y}}{\sqrt{2\pi|v_y(p_y^\pm)|}}\exp\left[\pm i\frac{\epsilon\, y}{v_y(p_y^\pm)}\right] \\ &\times\exp\left[\pm i\frac{2t_z}{v_y(p_y^\pm)}\int_0^y\cos\left(p_z a_z-\frac{\omega_z}{v_F}y'\right)dy'\right] \\ &\times\exp\left[\pm\frac{2i\mu_B s H y}{v_y(p_y^\pm)}\right].\end{aligned} \tag{9}$$

III. GREEN'S FUNCTIONS IN A MAGNETIC FIELD AND TRIPLET SUPERCONDUCTING PAIRING

Having obtained the wave functions, we can calculate the Green's functions. From the standard expression for the finite temperature Green's function, we have

$$G_{i\omega_n}^\pm(\mathbf{r},\mathbf{r}') = \sum_\epsilon \frac{\Psi_\epsilon^*(\mathbf{r}')\Psi_\epsilon(\mathbf{r})}{i\omega_n-\epsilon}, \tag{10}$$

where $\omega_n = 2\pi T(n+1/2)$ are the so-called Matsubara frequencies. For convenience, we define the phase entering one of the exponential factors in Eq. (9) as

$$\phi^\pm(y,p_z) = \frac{2t_z}{v_y(p_y^\pm)}\int_0^y\cos\left(p_z a_z-\frac{\omega_z}{v_F}y'\right)dy'. \tag{11}$$

Substituting the wave functions from Eq. (9) into Eq. (10), and converting the summation into integration over the energy variable, we obtain the following expressions for the Green's functions:

$$\begin{aligned}G_{i\omega_n}^\pm(x,x';y,y';p_z) &= e^{\pm ip_x(x-x')}e^{\pm ip_y^\pm(p_x)(y-y')} \\ &\times\exp\left[\pm\frac{2i\mu_B s H(y-y')}{v_y(p_y^\pm)}\right]\hat{g}_{i\omega_n}^\pm(y,y';p_z),\end{aligned} \tag{12}$$

where the factor

$$\hat{g}_{i\omega_n}^\pm(y,y';p_z) = e^{\pm i[\phi^\pm(y,p_z)-\phi^\pm(y',p_z)]}g_{i\omega_n}^\pm(y,y'), \tag{13}$$

and the factor

$$g_{i\omega_n}^\pm(y,y') = \frac{1}{2\pi v_y(p_y^\pm)}\int_{-\infty}^{\infty}\frac{\exp\left[\pm i\frac{\epsilon(y-y')}{v_y(p_y^\pm)}\right]}{i\omega_n-\epsilon}d\epsilon. \tag{14}$$

In order to evaluate the integral in Eq. (14), a closed contour in upper (lower) complex plane is used when $\omega_n>0(\omega_n<0)$, which results in the following expressions for $g_{i\omega_n}^\pm(y,y')$:

$$g_{i\omega_n}^+(y,y') = \begin{cases}\frac{-i\cdot\mathrm{sgn}(\omega_n)}{v_y(p_y^+)}\exp\left[\frac{-\omega_n(y-y')}{v_y(p_y^+)}\right] & :\omega_n(y-y')>0\\ 0 & :\omega_n(y-y')<0\end{cases}$$

$$g_{i\omega_n}^-(y,y') = \begin{cases}\frac{-i\cdot\mathrm{sgn}(\omega_n)}{v_y(p_y^-)}\exp\left[\frac{\omega_n(y-y')}{v_y(p_y^-)}\right] & :\omega_n(y-y')<0\\ 0 & :\omega_n(y-y')>0.\end{cases}$$

Therefore, the expression for the Green's functions becomes, explicitly:

$$\begin{aligned}G_{i\omega_n}^\pm(x,x';y,y';p_z) &= \frac{-i\cdot\mathrm{sgn}(\omega_n)}{v_y(p_y^\pm)}e^{\pm ip_x(x-x')}e^{\pm ip_y^\pm(p_x)(y-y')} \\ &\times\exp\left[\pm i\frac{2t_z}{v_y(p_y^\pm)}\int_{y'}^y\cos\left(p_z a_z-\frac{\omega_z}{v_F}y''\right)dy''\right] \\ &\times\exp\left[\frac{\mp\omega_n(y-y')}{v_y(p_y^\pm)}\right]\exp\left[\pm\frac{2i\mu_B s H(y-y')}{v_y(p_y^\pm)}\right].\end{aligned} \tag{15}$$

In the above expression, the $+$ $(-)$ signs in the spin factor $e^{\pm 2i\mu_B s H(y-y')/v_y(p_y^\pm)}$ correspond to electron in the up $(\uparrow)$ or down $(\downarrow)$ state, respectively.

The derivation of the general expression for the superconducting order parameter in the case of triplet pairing for a Q1D layered conductor involves the use of Gor'kov's equation for unconventional superconductivity. To this end, let us consider the general expression[25] for a multicomponent superconducting order parameter:

$$\begin{aligned}\Delta_{\alpha\beta}(\mathbf{k},\mathbf{q}) = -T\sum_n\sum_{k'k''q'}V_{\beta\alpha,\lambda\mu}(\mathbf{k},\mathbf{k}')\Delta_{\lambda\mu}(\mathbf{k}'',\mathbf{q}') \\ \times G_\lambda\left(\mathbf{k}'+\frac{\mathbf{q}}{2},\mathbf{k}''+\frac{\mathbf{q}}{2};\omega_n\right) \\ \times G_\mu\left(-\mathbf{k}'+\frac{\mathbf{q}}{2},-\mathbf{k}''+\frac{\mathbf{q}}{2};-\omega_n\right).\end{aligned} \tag{16}$$

In the above expression, $G(\mathbf{k}',\mathbf{k}'')$ are the Fourier transformed Green's functions, the Greek subscripts represent spin indexes (that can take on two values represented by $\uparrow$ or $\downarrow$), and a summation with respect to the repeated index is implied. The spin dependent interaction $V_{\beta\alpha,\lambda\mu}(\mathbf{k},\mathbf{k}')$ can be factorized in the absence of spin-orbit coupling as $V_{\beta\alpha,\lambda\mu}(\mathbf{k},\mathbf{k}') = V(\mathbf{k},\mathbf{k}')\Gamma_{\alpha\beta,\lambda\mu}$. In the case of triplet superconducting pairing, the factors above have the following properties: $V(\mathbf{k},\mathbf{k}') = -V(-\mathbf{k},\mathbf{k}') = -V(\mathbf{k},-\mathbf{k}')$, i.e., it is antisymmetric, whereas the factors $\Gamma_{\alpha\beta,\lambda\mu}$ are symmetric under cyclic interchange of the spin indexes, with nonzero values in the case of triplet pairing being $\Gamma_{\uparrow\uparrow,\uparrow\uparrow} = \Gamma_{\downarrow\downarrow,\downarrow\downarrow} = 1$.

We consider a triplet superconducting order parameter $\Delta_t(\mathbf{k},\mathbf{q})$ that is a linear combination

$$\Delta_t(\mathbf{k},\mathbf{q}) = \Delta_{\uparrow\uparrow}(\mathbf{k},\mathbf{q}) + \Delta_{\downarrow\downarrow}(\mathbf{k},\mathbf{q}). \tag{17}$$

Using the form of the interaction above and performing the summation over the spin indexes in Eq. (16), we obtain the following expression for $\Delta_{\uparrow\uparrow}$ and $\Delta_{\downarrow\downarrow}$:

$$\Delta_{\uparrow\uparrow}(\mathbf{k},\mathbf{q}) = -T\sum_{n}\sum_{k'k''q'}\frac{V(\mathbf{k},\mathbf{k}')}{2}[\Delta_{\uparrow\uparrow}(\mathbf{k}'',\mathbf{q}')\Omega_{\uparrow\uparrow}(\mathbf{k}',\mathbf{k}'',\mathbf{q}) + \Delta_{\downarrow\downarrow}(\mathbf{k}'',\mathbf{q}')\Omega_{\downarrow\downarrow}(\mathbf{k}',\mathbf{k}'',\mathbf{q})], \quad (18)$$

where

$$\Omega_{\alpha\beta}(\mathbf{k}',\mathbf{k}'',\mathbf{q}) = \delta_{\alpha\beta}\, G_{\alpha}\left(\mathbf{k}'+\frac{\mathbf{q}}{2},\mathbf{k}''+\frac{\mathbf{q}}{2};\omega_n\right) \times G_{\beta}\left(-\mathbf{k}'+\frac{\mathbf{q}}{2},-\mathbf{k}''+\frac{\mathbf{q}}{2};-\omega_n\right). \quad (19)$$

In the expression above, $\alpha,\beta = \uparrow$ or $\downarrow$. An expression similar to Eq. (18) is obtained for $\Delta_{\downarrow\downarrow}(\mathbf{k},\mathbf{q})$. Adding the two quantities in Eq. (17), we obtain the general gap equation for the triplet superconducting order parameter:

$$\Delta_t(\mathbf{k},\mathbf{q}) = -T\sum_{n}\sum_{k'k''q'} V(\mathbf{k},\mathbf{k}')\Delta_t(\mathbf{k}'',\mathbf{q}') \times [\Omega_{\uparrow\uparrow}(\mathbf{k}',\mathbf{k}'',\mathbf{q}) + \Omega_{\downarrow\downarrow}(\mathbf{k}',\mathbf{k}'',\mathbf{q})]. \quad (20)$$

IV. THE TRIPLET SUPERCONDUCTING ORDER PARAMETER: NODELESS VERSUS NODAL CASES

We consider two scenarios of triplet pairing in which superconductivity is insensitive to Pauli paramagnetic effects. The simplest such triplet superconducting order parameter takes the form

$$\hat{\Delta}(p_x,y) = \hat{I}\,\mathrm{sgn}(p_x)\Delta(y), \quad (21)$$

where $\hat{I}$ is a unit matrix in spin space, and the function $\mathrm{sgn}(p_x) = \pm 1$ changes the sign of the order parameter on the two sheets of the Q1D FS. The gap equation for $\Delta(y)$ that determines the upper critical field $H_{c2}^{x}(T)$ at which superconductivity is destroyed is obtained by means of the general Eq. (20). We will first consider the case when the order parameter does *not* have zeros on the Q1D Fermi surface [i.e., the order parameter (21)]. It is possible to show that Eq. (20) for such a nodeless order parameter that includes orbital destructive effects is reduced to the following integral equation:

$$\Delta(y) = g\left\langle \int_{|y-y'|>\frac{|v_y(p_y)|}{\Omega}} \frac{2\pi T dy'}{v_y(p_y)\sinh\left[\frac{2\pi T|y-y'|}{v_y(p_y)}\right]}\Delta(y') \times J_0\left\{\frac{8t_z v_F}{\omega_z v_y(p_y)}\sin\left[\frac{\omega_z(y-y')}{2v_F}\right] \times \sin\left[\frac{\omega_z(y+y')}{2v_F}\right]\right\}\right\rangle_{p_y}, \quad (22)$$

where $\langle\cdots\rangle_{p_y}$ indicates averaging over momentum p_y, introduced when the magnetic field is parallel to the conducting axis. Here g is a dimensionless electron coupling constant, Ω is the cutoff energy, and $\omega_z = eHa_z v_F/c$.

Equation (22) is very general. Its solution defines a triplet superconducting order parameter that includes the possibility of reentrant superconductivity[10] (in layered Q1D and Q2D compounds) at very high magnetic fields and/or very low temperatures, where the quantum nature of electron motion in a magnetic field becomes important. Below, in analyzing the integral in Eq. (22), we will work in the regime of relatively high temperatures and relatively low magnetic fields, defined respectively by the following conditions:

$$T \geqslant T^*(H) \approx \frac{\omega_z(H)v_y^0}{2\pi^2 v_F}, \quad (23)$$

$$\omega_z(H) \ll \frac{8t_z v_F}{v_y^0}, \quad (24)$$

where $v_y^0 = 2t_y a_y$. This is equivalent to neglecting quantum effects resulting from Bragg reflection of electrons moving along open FS, and amounts to replacing the first sine in the above expression with its argument. It will be demonstrated that the conditions in Eqs. (23) and (24) are well satisfied for $Li_{0.9}Mo_6O_{17}$. These conditions render following simplification to the arguments of the Bessel functions appearing inside the integrals:

$$\Delta(y) = g\left\langle \int_{|y-y'|>\frac{|v_y(p_y)|}{\Omega}} \frac{2\pi T dy'}{v_y(p_y)\sinh\left[\frac{2\pi T|y-y'|}{v_y(p_y)}\right]}\Delta(y') \times J_0\left\{\frac{4t_z(y-y')}{v_y(p_y)}\sin\left[\frac{\omega_z(y+y')}{2v_F}\right]\right\}\right\rangle_{p_y}, \quad (25)$$

where $v_y(p_y) = v_y^0\sin(p_y a_y)$. This equation for $\Delta(y)$ incorporates the description provided by the so-called Lawrence-Doniah (LD) model,[29,30] where the coherence length perpendicular to the conducting plane satisfies $\xi_z < a_z/\sqrt{2}$. However, in the compound $Li_{0.9}Mo_6O_{17}$, the coherence length $\xi_z > a_z$, as will be shown below. Therefore, the LD model does not apply, and the description of 3D anisotropic superconductivity results. This fact further simplifies Eq. (25):

$$\Delta(y) = g\left\langle \int_{|y-y'|>\frac{|v_y(p_y)|}{\Omega}} \frac{2\pi T dy'}{v_y(p_y)\sinh\left[\frac{2\pi T|y-y'|}{v_y(p_y)}\right]}\Delta(y') \times J_0\left[\frac{2t_z\omega_z(y^2-y'^2)}{v_y(p_y)v_F}\right]\right\rangle_{p_y}. \quad (26)$$

In order to recast Eq. (26) into a form appropriate for numerical analysis, we employ the following change of variables:

$$y'-y = \frac{v_y(p_y)}{v_y^0}z, \quad \tilde{\omega}_z = \frac{v_y^0}{v_F}\omega_z,$$

with $\frac{v_y(p_y)}{v_y^0} = \sin\alpha$, after which, Eq. (26) can be expressed as

$$\Delta(y) = g\left\langle \int_{d}^{\infty} \frac{2\pi T dz}{\sqrt{2t_z\tilde{\omega}_z}\sinh\left[\frac{2\pi T}{\sqrt{2t_z\tilde{\omega}_z}}z\right]}\Delta(y+z\sin\alpha) \times J_0[z(2y+z\sin\alpha)]\right\rangle_{\alpha}, \quad (27)$$

where cutoff distance $d = \sqrt{2t_z\tilde{\omega}_z}/\Omega$, and the averaging is now over the angular variable $0 < \alpha < 2\pi$.

In the case where the triplet superconducting order parameter has zeros on the FS, we take

$$\hat{\Delta}(\alpha,y) = \hat{I}\,\mathrm{sgn}(p_x)\sqrt{2}\,\sin(\alpha)\,\Delta(y).$$

With analogous change of variables, the simplified integral equation corresponding to the nodal case is

$$\Delta(y) = g\left\langle \int_d^\infty \frac{2\pi T\, dz}{\sqrt{2t_z\tilde{\omega}_z}\sinh\left[\frac{2\pi T}{\sqrt{2t_z\tilde{\omega}_z}}z\right]} 2\sin^2\alpha \times \Delta(y + z\sin\alpha) J_0\left[z(2y + z\sin\alpha)\right] \right\rangle_\alpha . \quad (28)$$

V. CALCULATED UPPER CRITICAL MAGNETIC FIELDS AND THEIR COMPARISON WITH THE EXPERIMENT

The band and superconducting parameters for the Q1D electron spectrum of $Li_{0.9}Mo_6O_{17}$ can be determined from the GL slopes of the measured upper critical fields $H^i_{c2}(T)$ near T_c. The ratios of linearly extrapolated zero-temperature upper critical fields along different axes are related to the ratios of the corresponding coherence lengths through the Ginzburg-Landau relation

$$\frac{H^i_{c2}}{H^j_{c2}} = \frac{\xi_i}{\xi_j}.$$

Supplemented with the GL expression for the upper critical field

$$H^i_{c2} = \frac{\Phi_0}{2\pi\xi_j\xi_k},$$

where $\Phi_0 = hc/2e$ is the magnetic flux quantum, the coherence lengths ξ_i can be determined. In the vicinity of the superconducting transition temperature $|T - T_c|/T_c \ll 1$, the anisotropic 3D Ginzburg-Landau expressions for the upper critical magnetic field along different axes can be derived for both nodeless and nodal order parameters.

It is possible to show that for the *nodeless* order parameter, Eq. (27) gives

$$H^x_{c2}(T) = \frac{4\pi^2 c T_c^2}{7\zeta(3) e t_y t_z a_y a_z}\left(\frac{T_c - T}{T_c}\right), \quad (29)$$

while the GL upper critical fields for directions perpendicular to the most conducting axis are given by[31]

$$H^y_{c2}(T) = \frac{4\sqrt{2}\pi^2 c T_c^2}{7\zeta(3) e v_F t_z a_z}\left(\frac{T_c - T}{T_c}\right), \quad (30)$$

$$H^z_{c2}(T) = \frac{4\sqrt{2}\pi^2 c T_c^2}{7\zeta(3) e v_F t_y a_y}\left(\frac{T_c - T}{T_c}\right), \quad (31)$$

where $\zeta(3)$ is the value of the Riemann ζ function. The GL coherence lengths for the nodeless case are

$$\xi_x = \frac{\sqrt{7\zeta(3)}v_F}{4\pi T_c}, \quad \xi_y = \frac{\sqrt{7\zeta(3)}t_y a_y}{2\sqrt{2}\pi T_c}, \quad \xi_z = \frac{\sqrt{7\zeta(3)}t_z a_z}{2\sqrt{2}\pi T_c}.$$

For the *nodal* order parameter Eq. (28), the expression for H^y_{c2} remains identical to the nodeless case, while the expressions for H^x_{c2} and H^z_{c2} are changed according to

$$H^x_{c2}(T) = \frac{4\sqrt{2}\pi^2 c T_c^2}{7\zeta(3)\sqrt{3} e t_y t_z a_y a_z}\left(\frac{T_c - T}{T_c}\right), \quad (32)$$

$$H^z_{c2}(T) = \frac{8\pi^2 c T_c^2}{7\zeta(3)\sqrt{3} e v_F t_y a_y}\left(\frac{T_c - T}{T_c}\right), \quad (33)$$

TABLE I. Electron spectrum and superconducting parameters calculated in the case of nodeless order parameter.

$Li_{0.9}Mo_6O_{17}$	$\hat{x}$	$\hat{y}$	$\hat{z}$
a_i (Å)	5.53	12.73	9.51
ξ_i (Å)	426	77	20
t_i (K)	370	41	14
v_i (cm/s) $\times 10^6$	$v_F = 5.3$	1.4	0.25

with the change only in the ξ_y coherence length:

$$\xi_y = \frac{\sqrt{3\cdot 7\zeta(3)}t_y a_y}{4\pi T_c}.$$

The band and superconducting parameters for the nodeless case are summarized in Table I.

A numerical solution of Eqs. (27) and (28) is implemented by iteration, using a method of successive approximations both near $T = 0$, and for arbitrary (but small enough) values of T. The solution for $\Delta(y)$ at $T = 0.1$ K for both nodeless and nodal cases is shown in Fig. 2. Note the qualitative difference compared with the isotropic 3D superconductor: $\Delta(y)$ exhibits decaying oscillations as a function of y. The period of these oscillations is of the order of the coherence length ξ_x. Furthermore, the temperature dependence of Δ can be shown to be quadratic for small T. The solid lines in Figs. 3 and 4 correspond to the numerical solution to $H^x_{c2}(T)$ for nodeless and nodal cases, respectively. The experimental data for $Li_{0.9}Mo_6O_{17}$ taken from Ref. 3 is overplotted as squares, while the Ginzburg-Landau linear dependence (valid near T_c) is plotted as a dashed line.

We can check the validity of approximations made in arriving at the integral in Eq. (26) by using the values from the table above, and the conditions in Eqs. (23) and (24). The results are

$$T \geqslant T^* \approx 0.06\,\text{K} \quad \text{and} \quad H \ll 300\,\text{T}.$$

These conditions are well satisfied in the experiments of Ref. 3. Furthermore, as the coherence length $\xi_z \approx 20$ Å $> a_z/\sqrt{2} = 6.7$ Å, i.e., is it much greater than the interlayer spacing, the layered are well coupled, and the so called Lawrence-Doniah model does not apply in this context. Thus,

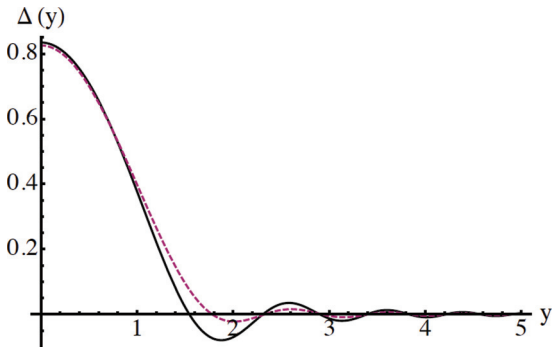

FIG. 2. (Color online) Spatial dependencies of the nodal (solid curve) and nodeless (dashed curve) triplet superconducting order parameters calculated at $T = 0.1$ K.

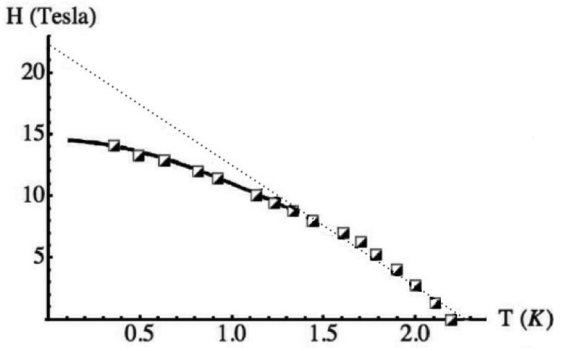

FIG. 3. Calculated temperature dependence of the upper critical magnetic field $H^x_{c2}(T)$ for the case of the nodeless order parameter is represented by a solid line; squares represent recently measured experimental values as reported in Ref. 3; and the dashed line is the Ginzburg-Landau linear dependence valid for $|T - T_c| \ll T_c$.

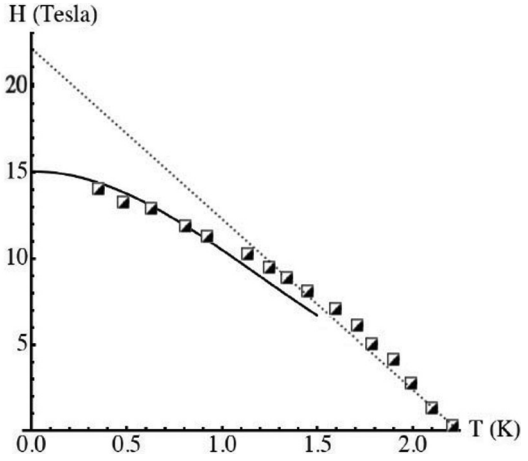

FIG. 4. Calculated temperature dependence of the upper critical magnetic field $H^x_{c2}(T)$ corresponding to the nodal order parameter. Notations are the same as in Fig. 3.

our problem is that of anisotropic 3D superconductivity. As shown previously by us[28] for a magnetic field parallel to the most conducting axis of a Q1D layered conductor, orbital effects are capable of destroying superconductivity in the absence of paramagnetic effects. Although both nodeless and nodal triplet order parameters (Fig. 2) reproduce qualitatively similar results for the phase diagram of $H^x_{c2}(T)$, the nodeless case is in a better quantitative agreement with the data from Ref. 3.

As an additional concluding remark, we discuss another possible explanation of a very high upper critical magnetic field, parallel to conducting axis in a Q1D superconductor. As shown in Ref. 32, in a pure 1D singlet superconductor Pauli spin-splitting effects in a magnetic field do not destroy superconductivity at $T = 0$ in arbitrarily high magnetic fields due to formation of the LOFF phase[14,15] in a form of the soliton superstructure. Nevertheless, in Ref. 11 it was shown that in a real singlet Q1D superconductor with electron spectrum (1), there exists paramagnetically limiting magnetic field for the LOFF phase even in the case where the orbital effects against superconductivity are negligible. The field that paramagnetically limits singlet superconductivity in a Q1D superconductor is evaluated[33] as

$$H_p^{\mathrm{LOFF}} = 0.6\,\sqrt{t_x/t_y}\;H_p\;. \tag{34}$$

Substituting the corresponding parameters for the $Li_{0.9}Mo_6O_{17}$ superconductor (see Table I), we obtain $H_p^{\mathrm{LOFF}} \simeq$ 6 T. As shown in Ref. 16, the orbital effects against superconductivity decrease this paramagnetically limiting field. Therefore, we conclude that the possible appearance of the LOFF phase in the framework of a singlet scenario of superconductivity is very unlikely to be responsible for the very large experimental upper critical field $H^x_{c2} \approx 15$ T in the $Li_{0.9}Mo_6O_{17}$ superconductor.

VI. SUMMARY

In this paper we have explored two competing scenarios within the framework of triplet superconducting pairing in a Q1D layered conductor. We have demonstrated how in a parallel magnetic field superconductivity can be destroyed through orbital effects, and have calculated $H^x c_2(T)$ when the triplet order parameters have and do not have nodes on the FS. Our findings show that the nodeless order parameter leads to the temperature dependence of upper critical field that is in a better quantitative agreement with the experimental data in Ref. 3. In particular, such a nodeless triplet order parameter is consistent with the large value of the experimentally observed specific heat jump at the superconducting transition in zero field. Note that all our calculations have been done within a validity of the so-called Fermi-liquid picture. In this context it is important that the quadratic dependence of low temperature magnetoresistance is reported in Ref. 3, which we consider as a main argument in favor of the Fermi liquid description. In more details, we state that the low temperature regime ($T < T_c \approx 2.2$ K) at which our calculation are performed avoids the Luttinger liquid behavior that is expected to emerge in Q1D conductors at higher temperatures,[33–35] as was observed in $Li_{0.9}Mo_6O_{17}$.

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