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Ginzburg-Landau slopes of the anisotropic upper critical magnetic field and band parameters in the superconductor $(TMTSF)_2ClO_4$

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We theoretically determine the Ginzburg–Landau slopes of the anisotropic upper critical magnetic field in a quasi-one-dimensional superconductor and correct the previous works on this issue. By using the experimentally measured values of the Ginzburg–Landau slopes in the superconductor $(TMTSF)ClO_4$, we determine band parameters of its electron spectrum. Our main result is that the so-called quantum dimensional crossover has to happen in this material in magnetic fields, $H = 3{-}8$ T, which are much lower than the previously assumed. We discuss how this fact influences metallic and superconducting properties of the $(TMTSF)_2ClO_4$.

Since a discovery of the field-induced spin-density-wave (FISDW) phase diagrams [1,2], high magnetic field properties of organic superconductors $(TMTSF)_2X$ ($X = ClO_4$, PF_6, AsF_6, etc.) have been intensively studied [3,4]. Phase transitions from metallic to the FISDW phases, exhibiting three-dimensional quantum Hall effect, were successfully explained [5–11] in terms of the simplest quasi-classical $3D \to 2D$ dimensional crossover [3]. More complicated $3D \to 1D \to 2D$ quasi-classical dimensional crossovers in a magnetic field successfully explain such phenomena in a metallic phase as the Lebed Magic Angles (LMA) [12,13] and the Lee–Naughton–Lebed (LNL) oscillations [14,15]. The characteristic feature of the quasi-classical dimensional crossovers is that a typical size of electron orbits in a magnetic field is much larger than inter-chain and inter-plane distances in these layered quasi-one-dimensional (Q1D) conductors.

Other dimensional crossovers – the quantum ones [3] – were suggested in [16–18] to demonstrate the Reentrant superconductivity phenomenon [16], where high magnetic fields can improve superconducting pairing. Under condition of the quantum dimensional crossover, a typical size of electron trajectories in a magnetic field becomes of the order or even less than interlayer distance in $(TMTSF)_2X$ conductors [16,19]. Note that the quantum dimensional crossovers have been supposed to happen in magnetic fields of the order of 10–20 T, parallel to conducting layers of $(TMTSF)_2X$ materials.

The main goal of our Letter is to determine carefully band parameters of Q1D electron spectrum of the conductor $(TMTSF)_2ClO_4$ [20],

$$\epsilon(\mathbf{p}) = -2t_a \cos(p_x a/2) - 2t_b \cos(p_y b) - 2t_c \cos(p_z c^*), \tag{1}$$

where $t_a \gg t_b \gg t_c$ correspond to electron hoping integrals along $\mathbf{a}$-, $\mathbf{b}$-, and $\mathbf{c}^*$-axes, respectively. Using the determined band parameters, we show that the quantum dimensional crossover in the conductor $(TMTSF)_2ClO_4$ happens at much lower magnetic fields, $H \simeq 3{-}8$ T. We discuss how this fact influence its magnetic properties in metallic and superconducting phases and discuss the related experimental data. Below, we simplify electron spectrum (1) near two slightly corrugated sheets of Q1D Fermi surface (FS) as

$$\delta\epsilon^{\pm}(\mathbf{p}) = \pm v_F(p_x \mp p_F) - 2t_b \cos(p_y b) - 2t_c \cos(p_z c^*), \tag{2}$$

where $+(-)$ stands for right (left) sheet of Q1D FS, $v_F = t_a a/\sqrt{2}$, $\hbar \equiv 1$.

Let us consider electron motion in a magnetic field, perpendicular to conducting chains and parallel to conducting layers,

$$\mathbf{H} = (0, H, 0), \quad \mathbf{A} = (0, 0, -Hx). \tag{3}$$

In accordance with [16], electron spectrum (2) is "two-dimensionalized" in a magnetic field (3). More specifically, electrons are characterized by free unrestricted motion within conducting $(\mathbf{a}, \mathbf{b})$ plane, whereas their motion along $\mathbf{z}$-axis is periodic and restricted [16]:

$$z(t, H) = l_\perp(H)\ c^* \cos(\omega_c t), \quad l_\perp(H) = 2t_c/\omega_c, \tag{4}$$

where $\omega_c = e v_F H c^*/c$. By using quantum mechanical methods, it is possible to show [21,19,16] that the quantum $3D \to 2D$ dimensional crossover happens if a size of the quasi-classical orbit (4) is approximately in the range between c^* and $c^*/2$,

$$l_\perp(H) \simeq 0.5{-}1.0. \tag{5}$$

Classically, this corresponds to situation, where either electron orbits from two neighboring conducting layers do not intersect each other or do not intersect neighboring layers, respectively.

Here, we express a value of the dimensionless parameter $l_\perp(H)$ in terms of ratio of electron hoping integrals along **z**- and **x**-axes. It is possible to show that

$$l_\perp(H) = \frac{2\sqrt{2}}{\pi}\frac{\phi_0}{ac^* H}\frac{t_c}{t_a} \simeq \frac{2\cdot 10^3}{H(T)}\frac{t_c}{t_a}, \tag{6}$$

where $H(T)$ is a magnetic field, measured in Teslas. Let us first use values of the parameters of the electron spectrum (1) of $(\mathrm{TMTSF})_2\mathrm{ClO}_4$, accepted in literature [22], $t_a = 1200\,\mathrm{K}$ and $t_c = 7\,\mathrm{K}$. In this case, as it follows from Eqs. (5), (6), the quantum $3D \to 2D$ dimensional crossover happens approximately at $H \geq H^* \simeq 12{-}23\,\mathrm{T}$. In this Letter we show that in reality $t_c \simeq 2{-}2.3\,\mathrm{K}$ and $t_a \simeq 1340{-}1130\,\mathrm{K}$, which result in the quantum dimensional crossover at $H \geq H^* \simeq 3{-}8\,\mathrm{T}$.

Below, we derive the Ginzburg-Landau (GL) slope for the upper critical magnetic field, parallel to **b**-axis of a singlet s-wave Q1D superconductor with the electron spectrum (2). For this purpose, we rewrite the so-called gap equation of [16, 23] in the following way:

$$\Delta(x) = \frac{g}{2}\int\limits_{|z|>d} \frac{2\pi T dz}{v_\mathrm{F}\sinh\left(\frac{2\pi T|z|}{v_\mathrm{F}}\right)} \times \\ \times J_0\left[\frac{2t_c\omega_c}{v_\mathrm{F}^2}z(z+2x)\right]\Delta(x+z), \tag{7}$$

where g is an effective electron coupling constant, d is a cut-off distance. (Note that in Eq. (7) we disregard quantum effects of an electron motion in a magnetic field in the extended Brillouin zone and, thus, replace the functions $\sin(\omega_c z/2v_\mathrm{F})$ and $\sin[\omega_c(z+2x)/2v_\mathrm{F}]$ by their arguments. Here and everywhere below, we also disregards the Pauli paramagnetic destructive effects against superconductivity.)

The next step of derivation of the GL slop is to take into account that in the GL region, $(T_c - T)/T_c \ll 1$, $v_\mathrm{F}/2\pi T_c \ll v_\mathrm{F}/\sqrt{t_c\omega_c}$, where T_c is the superconducting transition temperature in the absence of a magnetic field. Therefore, we can expend the integral equation (7) with respect to a small parameter, $|z| \sim v_\mathrm{F}/2\pi T_c$. As a result of such expansion procedure, we obtain the following differential equation:

$$\left[-\frac{d^2\Delta(x)}{dx^2} + x^2\frac{8t_c^2\omega_c^2}{v_F^4}\Delta(x)\right]\int_0^\infty \frac{\pi T_c z^2 dz}{v_F\sinh\left(\frac{2\pi T_c z}{v_F}\right)} + \\ + \left[\frac{1}{g} - \int_d^\infty \frac{2\pi T dz}{v_F\sinh\left(\frac{2\pi T z}{v_\mathrm{F}}\right)}\right]\Delta(x) = 0. \tag{8}$$

If we take into account that

$$\frac{1}{g} = \int_d^\infty \frac{2\pi T_c dz}{v_\mathrm{F}\sinh\left(\frac{2\pi T_c z}{v_F}\right)} = 0, \tag{9}$$

then we can rewrite Eq. (8) in the following way:

$$-\xi_x^2\frac{d^2\Delta(x)}{dx^2} + \left(\frac{2\pi H}{\phi_0}\right)^2\xi_z^2 x^2\Delta(x) - \tau\Delta(x) = 0, \\ \xi_x^2 = \frac{7\zeta(3)v_\mathrm{F}^2}{16\pi^2 T_c^2},\ \xi_z^2 = \frac{7\zeta(3)t_c^2(c*)^2}{8\pi^2T_c^2},\ \tau = \frac{T_c - T}{T_c}, \tag{10}$$

where $\phi_0 = \pi\hbar c/e$ is the flux quantum, ξ_x and ξ_z are the coherence lengths along **a**- and **c***-axes, correspondingly. Note that above we use the following relationship:

$$\int_0^\infty \frac{z^2 dz}{\sinh(z)} = \frac{7\zeta(3)}{2}, \tag{11}$$

where $\zeta(n)$ is the Reimann zeta function [24].

To find the GL slope of the upper critical field along **b**-axis, we need to determine the lowest energy level of the Schrodinger-like GL equation (10). After standard calculations, we obtain

$$H_{c2}^b = \frac{\phi_0}{2\pi\xi_x\xi_z}\left(\frac{T_c - T}{T_c}\right) = \frac{8\pi^2 c\hbar T_c^2}{7\zeta(3)et_a t_c ac^*}\left(\frac{T_c - T}{T_c}\right). \tag{12}$$

It is important that the GL slope of the upper critical field along **c**-axis for a singlet s-wave Q1D-superconductor with electron spectrum (2) can be obtained from Eq. (12) by using the following substitutions:

$$\xi_z \to \xi_y,\ t_c \to t_b,\ c^* \to b. \tag{13}$$

As a result,

$$H_{c2}^c = \frac{\phi_0}{2\pi\xi_x\xi_y}\left(\frac{T_c - T}{T_c}\right) = \frac{8\pi^2 c\hbar T_c^2}{7\zeta(3)et_a t_b ab}\left(\frac{T_c - T}{T_c}\right). \tag{14}$$

Let us rewrite Eq. (13) of [25], determining the upper critical field along **a**-axis of a singlet d-wave Q1D-superconductor, for s-wave case,

$$\Delta(y) = \frac{g}{2}\left\langle \int\limits_{|z|>d} \frac{2\pi T dz}{v_\mathrm{F}\sinh\left(\frac{2\pi T|z|}{v_\mathrm{F}}\right)}\Delta\left[y + \frac{v_y(p_y)}{v_F}z\right] \times \\ \times J_0\left\{\frac{2t_c\omega_c}{v_\mathrm{F}^2}z\left[2y + \frac{v_y(p_y)z}{v_\mathrm{F}}\right]\right\}\right\rangle_{p_y}, \tag{15}$$

where $v_y(p_y) = 2t_b b \sin(p_y b)$, $\langle ... \rangle_{p_y}$ stands for averaging procedure over momentum component p_y. By using the same method, as for determination of the GL slope for $\mathbf{H} \parallel \mathbf{b}$, we obtain the following GL slope for the upper critical along $\mathbf{a}$-axis:

$$H^a_{c2} = \frac{\phi_0}{2\pi \xi_y \xi_z}\left(\frac{T_c - T}{T_c}\right) = \frac{4\pi^2 c\hbar T_c^2}{7\zeta(3) e t_b t_c b c^*}\left(\frac{T_c - T}{T_c}\right). \tag{16}$$

We stress that Eqs. (12), (14), (16) define the GL slopes of the upper critical fields in a singlet s-wave Q1D-superconductor with the electron spectrum (1), (2) for all principal directions of a magnetic field. These equations correct the previous results of [26] and contain additional common factor 2/3 comparable to the corresponding equations of [26]. As it follows from general theory [27], for a singlet d-wave like Q1D-superconductor (1), (2) with order parameter,

$$\Delta(\mathbf{p}) = \sqrt{2}\Delta \cos(p_y b), \tag{17}$$

we have to redefine the corresponding coherence lengths in the following way:

$$\tilde{\xi_x} = \xi_x, \quad \tilde{\xi_y} = \xi_y/\sqrt{2}, \quad \tilde{\xi_z} = \xi_z. \tag{18}$$

In terms of the redefined coherence lengths the GL slopes of the anisotropic upper critical field for d-wave like superconducting order parameter (17) can be expressed as

$$H^a_{c2} = \frac{\phi_0}{2\pi \tilde{\xi_y} \tilde{\xi_z}}\left(\frac{T_c - T}{T_c}\right) = \frac{4\sqrt{2}\pi^2 c\hbar T_c^2}{7\zeta(3) e t_b t_c b c^*}\left(\frac{T_c - T}{T_c}\right), \tag{19}$$

$$H^b_{c2} = \frac{\phi_0}{2\pi \tilde{\xi_x} \tilde{\xi_z}}\left(\frac{T_c - T}{T_c}\right) = \frac{8\pi^2 c\hbar T_c^2}{7\zeta(3) e t_a t_c a c^*}\left(\frac{T_c - T}{T_c}\right), \tag{20}$$

$$H^c_{c2} = \frac{\phi_0}{2\pi \tilde{\xi_x} \tilde{\xi_y}}\left(\frac{T_c - T}{T_c}\right) = \frac{8\sqrt{2}\pi^2 c\hbar T_c^2}{7\zeta(3) e t_a t_b a b}\left(\frac{T_c - T}{T_c}\right). \tag{21}$$

It is important that the GL slopes of the upper critical magnetic fields along $\mathbf{b}$- and $\mathbf{c}^*$-axes have been recently carefully experimentally measured in the superconductor $(\mathrm{TMTSF})_2\mathrm{ClO}_4$ [28, 29]. As to the GL slope for $\mathbf{H} \parallel \mathbf{a}$, it is still experimentally ill defined. The latter fact is due to rather strong paramagnetic destructive effect against superconductivity, which do not allow to define carefully the orbital upper critical field along $\mathbf{a}$-axis. Therefore, to determine the band parameters of Q1D electron spectrum (1), we need one more piece of information. It is provided by theoretical fitting [15] of the LNL angular oscillations in a metallic phase of the $(\mathrm{TMTSF})_2\mathrm{ClO}_4$ in a magnetic field. As a result, we use the following set of experimental data [28, 29, 15],

$$\left(\frac{dH^b_{c2}}{dT}\right)_{T_c} = 3.65\ \frac{T}{K}, \quad \left(\frac{dH^c_{c2}}{dT}\right)_{T_c} = 0.138\ \frac{T}{K}, \quad t_a/t_b = 10, \tag{22}$$

to determine all 3 band parameters in Q1D electron spectrum (1).

Band parameters of Q1D electron spectrum (1) and critical magnetic field for the quantum $3D \to 2D$ dimensional crossover, H^*, determined for $t_a/t_b = 10$ [15] by means of Eqs. (5), (6), (12), (14), (20), (21)

Superconductivity type	$t_a(K)$	$t_b(K)$	$t_c(K)$	$H^*(T)$
d-wave nodal	1340	134	2.0	3-6
d-wave nodeless	1127	112.7	2.34	4-8

The results of our calculations by means of Eqs. (12), (14), (20), (21) are summarized in Table, where we consider two scenarios of superconductivity in $(\mathrm{TMTSF})_2\mathrm{ClO}_4$: d-wave nodal [21, 25, 30–32] and d-wave nodeless [33, 34] ones. Although we think that the d-wave nodal scenario is much more probable one [30], we present also the results of our calculations for d-wave nodeless scenario, since we cannot completely exclude it at this point. (We note that the d-wave nodeless scenario is mathematically equivalent to the considered above s-wave one.) In table, we also present calculations of the critical magnetic field, corresponding to the quantum $3D \to 2D$ dimensional crossover by means of Eqs. (5), (6). As it follows from table, the quantum dimensional crossover happens at magnetic fields, $H \geq H^* \simeq 3{-}8$ T, which are much lower than that previously accepted.

Let us discuss possible experimental consequences of low value of the critical field, responsible for $3D \to 2D$ dimensional crossover, $H^* \simeq 3{-}8$ T. In this case, as shown in [21, 34], superconductivity can survive in a form the hidden Reentrant superconducting phase in a magnetic field, which is higher than both the quasi-classical upper critical field [35, 36] and Clogston paramagnetic limit [37]. In particular, in $(\mathrm{TMTSF})_2\mathrm{ClO}_4$ compound, the hidden Reentrant superconductivity, as shown [21], can exist up to $H = 6$ T. The expected quantum dimensional crossover has to change dramatically also metallic properties of $(\mathrm{TMTSF})_2\mathrm{ClO}_4$ conductor at $H \geq H^* \simeq 3{-}8$ T, if a magnetic field is applied parallel to its conducting plane and perpendicular to its conducting chains. Note that there already exist some preliminary experimental data in favor of this conclusion. Indeed, in [38], magnetoresistance of $(TMTSF)_2ClO_4$ conductor is studied in the above mentioned geometry. In particular, it is found that, at $H \geq 3$ T, the magnetoresistance does not follow the expected in quasi-classical theory [39] H^2-dependence. There exist also another evidence of importance of the quantum $3D \to 2D$ dimensional crossover for metallic properties of $(TMTSF)_2ClO_4$. It is a failure of the quasi-classical theory [39] to explain the LMA-minimum, experimentally observed at $\mathbf{H} \parallel \mathbf{b}$ (see, for example, Fig. 2 in [39]).

As it follows from the above discussion, it is important to create a quantum theory of magnetoresistance in a metallic phase under the quantum $3D \to 2D$ dimensional crossover condition (5). We anticipate that this theory will be very challenging and cannot be obtained by generalizing of the existing methods. We also pay attention that $(TMTSF)_2ClO_4$ conductor is very clean, where an inverse impurity scattering time is estimated as $\hbar/\tau \sim 0.1$ K (see [26]) and, thus, $\hbar/\tau \ll t_c \simeq 2{-}2.5$ K. Therefore, in this case, for estimation of a magnetic field, corresponding to $3D \to 2D$ dimensional crossover (4), (5), (6), we can use the physical picture of a coherent electron motion between the conducting planes, in contrast to the so-called weak-coherent regime [40].

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