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Superconductivity of Quasi-One- and Quasi-Two-Dimensional Tight-Binding Electrons in a Magnetic Field

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The upper critical field $H_{c2}(T)$ of tight-binding electrons in a three-dimensional lattice is investigated. The electrons form Cooper pairs between eigenstates with the same energy in a strong magnetic field. The transition lines in the quasi-one-dimensional case are shown to deviate from the previously obtained results when the hopping matrix elements along the magnetic field are neglected. In the absence of Pauli pair breaking the transition temperature $T_c(H)$ of the quasi-two-dimensional electrons is found to increase in an oscillatory manner as the magnetic field becomes large and to reach $T_c(0)$ in the strong field, as in the quasi-one-dimensional case.

KEYWORDS: field-induced superconductivity, organic conductors, quasi-two-dimension, quasi-one-dimension

In the semiclassical approximation, the upper critical field $H_{c2}(T)$ of isotropic superconductors is derived from the Ginzburg-Landau-Abrikosov-Gor'kov (GLAG) theory.[1,2] Lawrence and Doniach[3] have applied the GLAG theory to layered superconductors. Klemm *et al.*[4,5] and Bulaevskii and Guseinov[6] have shown that $H_{c2}(T)$ displays upward curvature when the magnetic field is applied parallel to the layer. When the coherence length $\xi(T)$ of the order parameter becomes smaller than the distance between layers, $H_{c2}(T)$ is infinite. However, these results are based on a semiclassical approximation, in which only the phase of the wave function of electrons is changed by the magnetic field.

It has been shown that the quantum effect of electrons in the BCS theory leads to reentrance into the superconducting state in a strong magnetic field.[7-15] The reentrance due to Landau quantization has attracted theoretical interest.[8,9] In that case, Cooper pairs are formed between electrons at the lowest Landau level in a strong magnetic field. However, when only the lowest Landau level is filled in the three-dimensional case, the system can be treated as a 1D system, i.e., energy depends only on the momentum parallel to the magnetic field, and it has been shown that the system is unstable due to the density wave state rather than the superconductivity.[16,17]

Recently, superconductivity in a strong magnetic field has been observed in the organic superconductor $(TMTSF)_2PF_6$.[18,19] A similar result has also been observed in $(TMTSF)_2ClO_4$.[19-21] Organic superconductors $(TMTSF)_2X$ are well described by quarter-filled tight-binding electrons (actually holes) with $t_a \sim 3000$ K, $t_b/t_a \sim 0.1$ and $t_c/t_a \sim 0.003$. Since the magnetic field of 10T corresponds to $\phi/\phi_0 \sim 1/1000$ in $(TMTSF)_2X$, where ϕ is flux per unit area and ϕ_0 is the flux quantum, the effect of Landau level quantization is negligible. However, when the magnetic field is applied perpendicular to the $a-b$ plane, a field-induced spin density wave (FISDW) is stabilized. The existence of FISDWs shows that the quantum effect is important in quasi-one-dimensional (Q1D) systems and the semiclassical approximation of the magnetic field is not appropriate in these systems.

Lebed[7] has predicted that the Q1D superconductors should exhibit superconductivity in a strong magnetic field. The superconductivity observed in $(TMTSF)_2PF_6$ and $(TMTSF)_2ClO_4$ is thought to be the realization of Q1D superconductivity in a strong magnetic field. The mechanism of the reentrance of Q1D superconductivity is similar to that of the generation of FISDW. In the presence of the magnetic field, the dimensionality of the system is reduced. When the magnetic field is applied in the c direction in the system with hopping matrix elements $t_a \gg t_b \gg t_c$, the effect of t_b, which makes the nesting of the Fermi surface imperfect with the imperfectness parameter of the order of t_b^2/t_a, disappears and a spin-density-wave is induced. When the magnetic field is applied in the b direction, the nesting of the Fermi surface stays imperfect but the orbital frustration is removed if we take account of the eigenstates in the magnetic field. In the Q1D case, the magnetic field necessary for the reentrance of the superconductivity is much smaller than that in the case of Landau level quantization. Dupuis *et al.*[10-12] have extensively studied the mean field transition line $T_c(H)$ of Q1D superconductors and demonstrated the cascade transitions to the superconducting states. We have studied the anisotropic superconductivity with line nodes of the energy gap,[13,14] which is thought to be realized in organic superconductors $(TMTSF)_2X$. In those studies,[7,10-14] however, only warping of the Fermi surface in the k_z direction normal to H has been considered, and that in the k_y direction has been neglected.

As t_b increases, a quasi-one-dimensional system becomes a quasi-two-dimensional system. Quasi-two-dimensional (Q2D) electrons, for example, β-(BEDT-

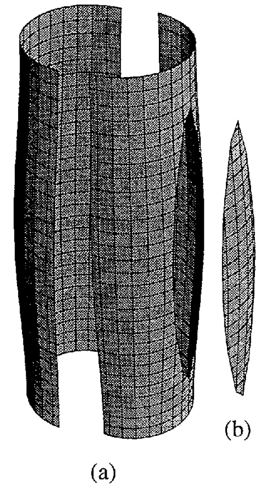

Fig. 1. The Fermi surface of a quasi-two-dimensional conductor. In the presence of a magnetic field along k_y, the electrons move in open orbit (a) and closed orbit (b).

TTF)$_2$I$_3$ ($t_a \sim 3000$ K, $t_b/t_a \sim 0.5$ and $t_c/t_a \sim 0.02$) have a two-dimensional cylindrical Fermi surface with weak warping along the k_z direction. When the magnetic field H is applied in the b direction, the electrons move either in open orbit reaching the zone boundary or in closed orbit, as is schematically shown in Fig. 1. The former gives a similar effect to that observed in Q1D superconductors. It has been proposed by Lebed[7] and Dupuis *et al.*[11] that the Q2D superconductors will evolve from the GLAG region to the reentrant phase. Recently, Lebed and Yamaji[15] calculated the mean field transition temperature of a Q2D superconductor and demonstrated the reentrant behavior. They used the parabolic band in the conducting plane, i.e., the lattice structure is neglected in the plane.

In this paper, we calculate the mean field transition temperature numerically by taking account of the eigenstates of three-dimensional tight-binding electrons in a magnetic field. In this formation, we can treat both Q1D and Q2D systems by changing t_b/t_a.

We start from the tight-binding Hamiltonian (we take $\hbar = k_B = c_0 = 1$, where c_0 is the velocity of light),

$$\mathcal{H}_0 = -t_a \sum_{(i,j)_a,\sigma} e^{i\theta_{ij}} c^\dagger_{i,\sigma} c_{j,\sigma} - t_b \sum_{(i,j)_b,\sigma} e^{i\theta_{ij}} c^\dagger_{i,\sigma} c_{j,\sigma} - t_c \sum_{(i,j)_c,\sigma} e^{i\theta_{ij}} c^\dagger_{i,\sigma} c_{j,\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} - \sum_{i,\sigma} \sigma \mu_B H c^\dagger_{i,\sigma} c_{i,\sigma}, \quad (1)$$

where $c^\dagger_{i,\sigma}$ and $c_{i,\sigma}$ are creation and annihilation operators, μ is the chemical potential and $\sigma\mu_B H$ is the Zeeman energy for $\uparrow$ ($\downarrow$) spin ($\sigma = +(-)$) and

$$\theta_{ij} = \frac{2\pi}{\phi_0} \int_i^j \boldsymbol{A} dl. \quad (2)$$

In the above, $\boldsymbol{A}$ is the vector potential. We consider the anisotropic system with the hopping matrix elements $t_a \geq t_b \gg t_c$. We neglect the field dependence of μ, since the energy gap due to the magnetic field is very small in the anisotropic system with $\phi/\phi_0 \ll 1$, except at the bottom and the top of the band.

In this paper, the magnetic field H is applied in the b direction. We use the vector potential $\boldsymbol{A} = (0, 0, -Hx)$ and the noninteracting Hamiltonian is written as

$$\mathcal{H}_0 = \sum_{\sigma,\boldsymbol{k}} C^\dagger_\sigma \begin{pmatrix} \ddots & & & & V^* \\ & M_{-1} & V & 0 & \\ & V^* & M_0 & V & \\ & 0 & V^* & M_1 & \\ V & & & & \ddots \end{pmatrix} C_\sigma, \quad (3)$$

where

$$M_n = -2t_a \cos[a(k_x + nG)] - 2t_b \cos(bk_y) - \mu - \sigma\mu_B H, \quad (4)$$

$$V = -t_c e^{ick_z}, \quad (5)$$

$$C^\dagger_\sigma = (\cdots, c^\dagger_\sigma(\boldsymbol{k} - \boldsymbol{G}), c^\dagger_\sigma(\boldsymbol{k}), c^\dagger_\sigma(\boldsymbol{k} + \boldsymbol{G}), \cdots), \quad (6)$$

$$\boldsymbol{G} = (G, 0, 0) = \left(\frac{2\pi}{a}\frac{\phi}{\phi_0}, 0, 0\right). \quad (7)$$

The creation operators of electrons can be written in terms of those of the eigenstates ($\Psi^\dagger_\sigma(n, \boldsymbol{k})$) of eq. (3) as

$$c^\dagger_\sigma(\boldsymbol{k} + m\boldsymbol{G}) = e^{imck_z} \sum_n \phi^*_{k_x,k_z}(m, n) \Psi^\dagger_\sigma(n, \boldsymbol{k}), \quad (8)$$

where m and n are integers.

Using eq. (8), the real-space one-particle Green's function is given by

$$G_\sigma(\boldsymbol{r}, \boldsymbol{r}', i\omega_l) = -\int_0^\beta d\tau e^{i\omega_l \tau} \left\langle T_\tau C_{\boldsymbol{r},\sigma}(\tau) C^\dagger_{\boldsymbol{r}',\sigma}(0) \right\rangle = \sum_{\boldsymbol{k},n} \sum_{m,m'} \frac{\phi_{k_x,k_z}(m, n) \phi^*_{k_x,k_z}(m', n)}{i\omega_l - \varepsilon_{n,\boldsymbol{k},\sigma}} \times e^{i(m'-m)ck_z} e^{i(\boldsymbol{r}'-\boldsymbol{r})\cdot\boldsymbol{k} + i(m'\boldsymbol{r}' - m\boldsymbol{r})\cdot\boldsymbol{G}}, \quad (9)$$

where $\omega_l = (2l+1)\pi T$ is the Matsubara frequency and l is an integer. In this paper, we neglect the Zeeman energy for simplicity. The coefficients $\phi_{k_x,k_z}(m, n)$ and eigenvalues

$$\varepsilon_{n,\boldsymbol{k}} = \epsilon(n, k_x, k_z) - 2t_b \cos(bk_y) - \mu \quad (10)$$

can be calculated by diagonalizing the matrix in eq. (3) numerically, where $\epsilon(n, k_x, k_z)$ is the eigenvalue of eq. (3) for $-2t_b \cos(bk_y) - \mu = 0$. If $\phi/\phi_0 = p/q$, where p and q are mutually prime integers, the matrix size of eq. (3) is $q \times q$ and the magnetic Brillouin zone is given by $-\pi/(qa) < k_x < \pi/(qa)$.

Since we are interested in the instability of superconductivity in the quarter-filled tight-binding electrons at a temperature much smaller than the band width, the eigenstates near the top of the band are not important in the anisotropic hopping case ($t_c \ll t_a$). Thus, we calculate only $3/4 \sim 1/2$ of the states from the bottom of the band in eq. (3) by neglecting V and V^* for $c(\boldsymbol{k}+n\boldsymbol{G})$ with $|k_x + nG| \geq (3/4)\pi/a$ or $|k_x + nG| \geq (1/2)\pi/a$. We have checked that the result is unaltered by this approximation. In this approximation, we can take the matrix size as $\sim [\pi/G] \times [\pi/G]$ and $-G/2 < k_x < G/2$. The eigenvalues and coefficients do not depend on k_z in this approximation, therefore we can use $\epsilon(n,k_x,k_z) = \epsilon(n,k_x)$ and $\phi_{k_x,k_z}(m,n) = \phi_{k_x}(m,n)$ ($\phi_{k_x}(m,n)$ can be taken as real).

In the mean field approximation, the linearized gap equation for s-wave pairing in coordinate representation is obtained as

$$\Delta(r) = \lambda \int \mathrm{d}\boldsymbol{r}' K(\boldsymbol{r},\boldsymbol{r}')\Delta(\boldsymbol{r}'), \tag{11}$$

where

$$K(\boldsymbol{r},\boldsymbol{r}') \equiv T \sum_{\omega_l} G(\boldsymbol{r},\boldsymbol{r}',\mathrm{i}\omega_l)G(\boldsymbol{r},\boldsymbol{r}',-\mathrm{i}\omega_l), \tag{12}$$

and λ is the coupling constant. We write

$$\Delta(x) = \sum_{q_x;N} \mathrm{e}^{\mathrm{i}(q_x+NG)x}\Delta_N(q_x), \tag{13}$$

where q_x is taken as $-G/2 < q_x \le G/2$. For even N, using eqs. (9) and (13), the linearized gap equation is written as a matrix equation

$$\Delta_{2j}(q_x) = \lambda \sum_{j'} \Pi_{2j,2j'}\Delta_{2j'}(q_x), \tag{14}$$

where

$$\Pi_{2j,2j'}(q_x) = \sum_{k_x;k_y}\sum_{n,n'}\sum_{m} \phi_{k_x}(m-j,n)\phi_{k_x}(m-j',n) \times\phi_{-k_x}(-m-j,n')\phi_{-k_x}(-m-j',n') \times\frac{1-f(\varepsilon_{n,k_x,k_y})-f(\varepsilon_{n',-k_x-q_x,-k_y})}{2(\varepsilon_{n,k_x,k_y}+\varepsilon_{n',-k_x-q_x,-k_y})}, \tag{15}$$

where $f(\varepsilon)$ is the Fermi distribution function.

For odd N, we get

$$\Delta_{2j+1}(q_x) = \lambda \sum_{j'} \Pi_{2j+1,2j'+1}\Delta_{2j'+1}(q_x), \tag{16}$$

where

$$\Pi_{2j+1,2j'+1}(q_x) = \sum_{k_x,k_y}\sum_{n,n'}\sum_{m} \phi_{k_x}(m-j,n)\phi_{k_x}(m-j',n)\phi_{-k_x}(-m-j-1,n')\phi_{-k_x}(-m-j'-1,n') \times\frac{1-f(\varepsilon_{n,k_x,k_y})-f(\varepsilon_{n',-k_x-q_x,-k_y})}{2(\varepsilon_{n,k_x,k_y}+\varepsilon_{n',-k_x-q_x,-k_y})}. \tag{17}$$

The transition line is given by $1-g\lambda = 0$ for eqs. (14) and (16), where g is the maximum eigenvalue of matrix Π for even or odd N. In this paper, we calculate the field dependence of the effective coupling constant g at low temperature instead of calculating the transition temperature. In the BCS theory, Cooper pairs are formed by electrons with wave numbers $\boldsymbol{k}$ and $-\boldsymbol{k}$, and the energy of these states is different in the presence of a magnetic field, which causes orbital frustration. From eqs. (14) and (16), however, we can take the states $(n,\boldsymbol{k})$ and $(n',-\boldsymbol{k})$ which have the same energy $\varepsilon_{n,k_x,k_y} = \varepsilon_{n',-k_x,-k_y}$. Therefore the superconductivity is not destroyed by orbital frustration in a strong magnetic field. This is similar to the mechanism of FISDW generation.[22] In a weak magnetic field the coefficient $\phi_{k_x}(m,n)$ becomes small and the present results reproduce the GLAG results.

For the Q1D superconductors with open Fermi surfaces, the energy dispersion in k_x was taken to be linear and the Fermi velocity and the density of states were taken to be constant in the previous calculations.[7;10-14] As a first approximation, we take

$$M_n \approx \mathrm{sgn}(n)v_\mathrm{F}(k_y)(|k_x+nG|-k_\mathrm{F}), \tag{18}$$

where $v_F(k_y) = 2t_a a\sin ak_\mathrm{F}(k_y)$ and $k_F(k_y)$ are the Fermi velocity and Fermi wave number depending on k_y, respectively. We may diagonalize the matrix for $k_x+nG \sim k_\mathrm{F}(k_y)$ and $k_x+nG \sim -k_\mathrm{F}(k_y)$ independently, as in the previous calculations. Then the eigenstates are given with the coefficients

$$\phi_{k_x}(m,n) \cong J_{m-n}\left(\frac{2t_c}{v_\mathrm{F}(k_y)G}\right) \quad \text{for } n,m>0 \tag{19}$$

and

$$\phi_{k_x}(m,n) \cong J_{-m+n}\left(\frac{2t_c}{v_\mathrm{F}(k_y)G}\right) \quad \text{for } n,m<0, \tag{20}$$

where J is the Bessel function. Note that in this approximation $\phi_{k_x}(m,n)$ does not depend on k_x, rather it depends on k_y through $v_\mathrm{F}(k_y)$. In Fig. 2, we plot the effective coupling constant g/g_0 obtained by this linearized dispersion as solid, dashed, and dot-dashed lines as a function of $aG/(2\pi)$, where g_0 is the effective coupling constant for $t_c = 0$, which corresponds to that in the absence of magnetic field. In a strong magnetic field, the effective coupling constant of the even part is increased and that of the odd part is decreased for each t_b/t_a. In the case of $t_b = 0$, we get the same result as has been previously reported.[10-12] As can be seen in Fig. 2, for larger t_b/t_a the oscillation becomes small.

Next, we calculate the effective coupling constant g/g_0 by numerically diagonalizing the lower 3/4 or 1/2 of the matrix in eq. (3) without using the approximation eq. (18) and plot the results as circles, triangles and diamonds in Fig. 2. For $t_b/t_a = 0.1$ the results are almost the same as those obtained by the approximation with the k_y-dependent Fermi velocity (eq. (18)) as expected, but the deviation is large for larger t_b/t_a.

We also study the quasi-two-dimensional superconductor with $t_b/t_a = 0.5$ and 1.0. In Fig. 3 we plot the effective coupling constant as a function of $aG/(2\pi)$. As is seen in Fig. 3, the effective coupling constant reaches that for $t_c = 0$ as magnetic field is increased.

The reason why g/g_0 is small for $t_b/t_a = 0.3$ is as follows. In Fig. 4, we plot the effective coupling constant as a function of t_b/t_a. In the case of $t_c = 0$, there is a logarithmic divergence at about $t_b/t_a \sim 0.3$, which is the van Hove singularity for the quarter-filled band. Therefore, the effective coupling constant normalized by

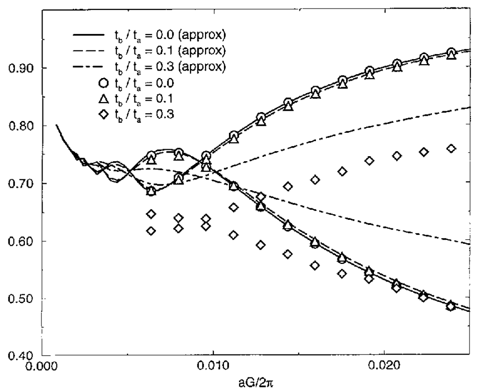

Fig. 2. Effective coupling constant as a function of $aG/(2\pi)$ in the case of $t_c/t_a = 0.02$ and $T/t_a = 0.001$. In a strong magnetic field, the effective coupling constant obtained by diagonalizing the even part of matrix H reaches that observed in the absence of magnetic field. The coupling constant for the odd part is zero in a strong magnetic field. Results plotted as solid, dashed and dot-dashed lines are obtained in the approximation of linearized energy dispersion. Data represented by circles, triangles and diamonds are obtained without that approximation.

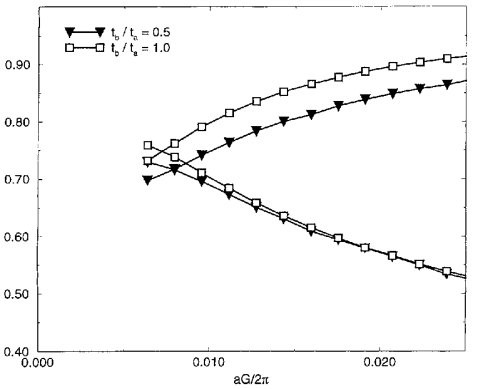

Fig. 3. Effective coupling constant as a function of $aG/(2\pi)$ in the case of $t_c/t_a = 0.02$ and $T/t_a = 0.001$.

that for $t_c = 0$ is small for $t_b/t_a \sim 0.3$.

In this paper we have neglected the Zeeman term for simplicity. However, we can calculate the transition line with the Zeeman term in this expression. The Zeeman term does not play any important role in the equal-spin-pairing case of the spin triplet. If the Zeeman energy is taken into account, the transition temperature of a spin singlet is reduced due to the effect of Pauli pair breaking, except for the Q1D case ($t_b = 0$). The superconductivity of Q1D systems is not completely destroyed,[7, 10-14] since half of the density of states is available to make Cooper pairs for the Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) state,[23, 24] as in the pure 1D case.[25-27]

In conclusion, we have shown the transition lines of quasi-one-dimensional and quasi-two-dimensional superconductors in a tight-binding model. The Green function in Q1D systems is described by the Bessel function if we apply the approximation that the energy dispersion in

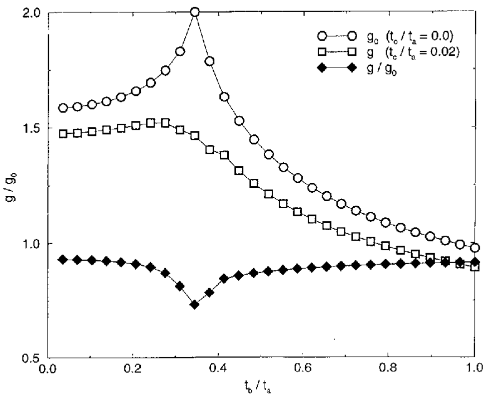

Fig. 4. Effective coupling constant as a function of t_b/t_a at $aG/(2\pi)$=0.025 and $T/t_a = 0.001$.

the k_x direction is taken to be linear. In this paper, we have shown that the Green function of tight-binding electrons can be numerically calculated without using the linearization of the energy dispersion. In a strong magnetic field, Cooper pairs are formed in eigenstates with equal energy. We have obtained the transition line $T_c(H)$ for both Q1D and Q2D cases. As H becomes large, $T_c(H)$ increases in an oscillatory manner in both cases.

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