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Quantum Interference Oscillation in DHvA Effect in the Two- and Three-dimensional Systems

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We study the behavior of the dHvA oscillation from the two-dimension to the three-dimension by changing the interlayer hopping t_z. We show that the oscillation of the chemical potential is gradually suppressed as t_z increases. It results from the broadening of the width of the Landau level. In the quasi-two-dimensional magnetic breakdown system such as κ-(BEDT-TTF)$_2$Cu(NCS)$_2$, the quantum interference oscillation such as β-α oscillation is suppressed, while the amplitude of the β+α oscillation has a maximum as a function of t_z. This interesting dependence on the dimensionality can be observed in quasi-two-dimensional metals under the uniaxial pressure.

KEYWORDS: dHvA oscillation, magnetic breakdown, quasi-two-dimensional system, κ-(BEDT-TTF)$_2$Cu(NCS)$_2$, Sr_2RuO_4, chemical potential oscillation

§1. Introduction

In the metal, the magnetization (M) periodically oscillates as a function of the inverse of the magnetic field (H), which is known as the de Haas-van Alphen (dHvA) oscillation.[1)] The experiment of the dHvA oscillation has been conventionally examined by the Lifshitz-Kosevich (LK) formula.[2)] When we neglect the impurity scattering in the spinless case and at $T = 0$, the LK formula is written as

$$M^{\rm LK} \propto -\sum_i \sum_{p=1}^{\infty} a_i(p,H) \sin\left(2\pi p\left(\frac{f_i}{H}+\frac{1}{2}\right)\right), \quad (1.1)$$

where $f_i = A_i(c\hbar/2\pi e)$ and A_i is the area of the extremal closed Fermi surface for each orbit (i). As the three-dimensionality and the value of p increase, $a_i(p,H)$ becomes small. This LK formula is derived from the oscillatory part of $M(\mu,H) = -\partial\Omega(\mu,H)/\partial H$, where $\Omega(\mu,H)$ is the thermodynamic potential obtained under the condition of the fixed chemical potential (μ). However, indeed, M should be calculated as $M(N,H) = -\partial F(N,H)/\partial H$ by using of the Helmholtz free energy, $F(N,H)$, obtained under the condition of the fixed electron number (N). In the three-dimensional system, as the width of the Landau level broadens (see Fig. 1(a)), the oscillation of μ as a function of H becomes very small, so that the LK formula treating μ independent of H is justified.

However, in the *two-dimensional system*, the LK formula is not appropriate because μ oscillates as a function of H due to the pinning of μ at the very sharp Landau level (see Fig. 1(b)). Thus, the calculation under the condition of the fixed N is needed. In fact, in the one-band system, Shoenberg[1)] has showed that the oscillatory part of $M(N,H)$ for the fixed N is given by

$$M_N^{\rm 2D} \propto \sum_{p=1}^{\infty} \frac{1}{p} \sin\left(2\pi p \frac{f}{H}\right), \quad (1.2)$$

where the spin and the impurity scattering are neglected at $T = 0$. This $M_N^{\rm 2D}$ is not in agreement with the LK formula ($M^{\rm LK}$) in which the three-dimensionality is reduced.

In the two-dimensional magnetic breakdown system,[3–5)] it has been shown that the β-α oscillation (so-called the quantum interference oscillation) exists in $M(N,H)$ under the condition of the fixed N.[6–20)] Experimentally, the β-α oscillation was confirmed in the quasi-two-dimensional oraganic conductors[21)] such as κ-(BEDT-TTF)$_2$Cu(NCS)$_2$[22,23)] and α-(BEDT-TTF)$_2$KHg(SCN)$_4$[24)] with the magnetic breakdown Fermi surface. The conventional FS theory based on the LK formula could not explain the β-α oscillation.

Next, we consider the quasi-two-dimensional system with the weak k_z-dispersion given as $-t_z \cos ck_z$.[25)] We introduce $2t_z/\hbar\omega$ as a parameter which determines the dimensionality under the magnetic field applied to k_z-axis. Then, two limits can be understood as follows;
(1) When $2t_z/\hbar\omega \gtrsim 1.0$, the oscillation of μ is very small

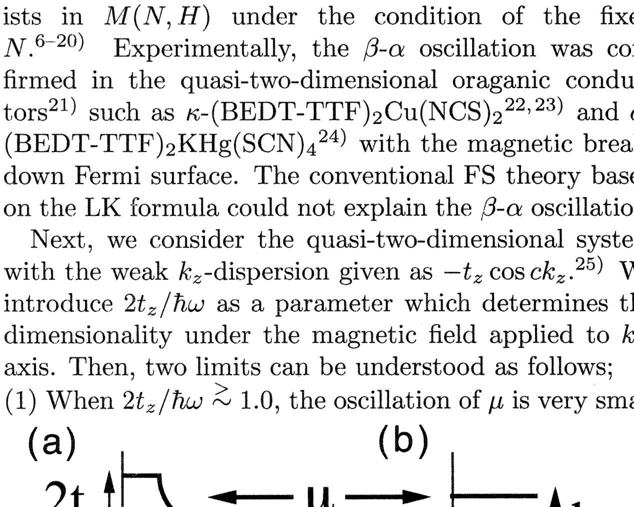

Fig. 1. Schematic density of the states in the magnetic field

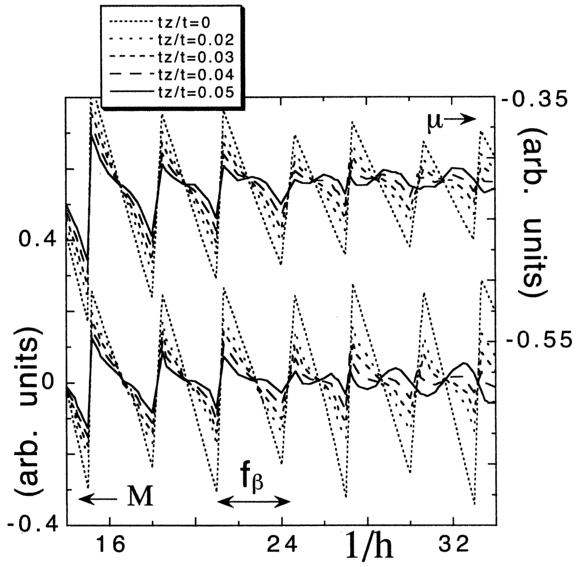

Fig. 2. $\mu(N,h)$ (upper figure) and $M(N,h)$ (lower figure) as a function of $1/h$ in the one-band model.

since the density of states becomes nearly the continuum. We regard this case as the *effective three-dimensional system*, where the LK formula is valid.

(2) For $2t_z/\hbar\omega \simeq 0$, we can neglect the three-dimensionality. Thus, the theory for two-dimensional system[1,6–20] is appropriate.

However, the theoretical and experimental studies of the dHvA oscillation from the two- to the *effective three-dimensional system* (that is, in $0 \leq 2t_z/\hbar\omega \lesssim 1$) have never been done.[26,27] This study is very important to understand the experiments of the dHvA oscillation of the actual quasi-two-dimensional materials such as κ-(BEDT-TTF)$_2$Cu(NCS)$_2$[28,29] and Sr_2RuO_4.

In this paper, by the numerical calculations under the condition that N is fixed, we show μ and M in the dimensional crossover region, where the oscillation of μ is gradually suppressed and M is smoothly changed (see Fig. 2). In the magnetic breakdown system, we find the anomalous enhancement of the amplitude of the $\beta+\alpha$ oscillation as a function of t_z (see Fig. 5).

§2. Formulation

We use a tight binding model. In the x-y plane, the nearest neighbor transfer integrals (t_x and t_y) with the lattice spacing (a and b) and an on-site potential (V) are considered. For $V = 0$, a closed Fermi surface exists, and we call it as β orbit and define its area as f_β in the unit of $4\pi^2/ab$ (see Fig. 3 (a)). For small V, there exit a small closed Fermi surface (called as α orbit) and the quasi-one-dimensional open Fermi surface, where the large β orbit is possible due to the magnetic breakdown (see Fig. 3 (b)). From this model, we can study both the one-band system ($V = 0$) and the magnetic breakdown system ($V \neq 0$). In the z-axis, we consider the weak interlayer hopping (t_z) with the lattice spacing (c).

For simplicity, we take $t_x = t_y = t$ and ignore the spin of the electrons to avoid additional complications. The magnetic field is applied in the z-direction.

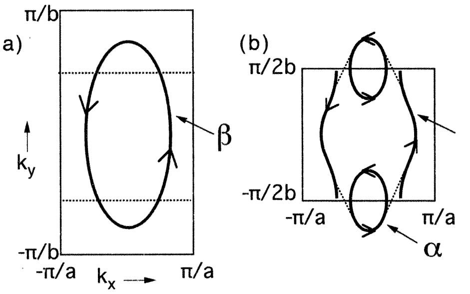

Fig. 3. (a) The Fermi surface at $k_z = 0$ for the one-band model ($V = 0$). (b) for magnetic breakdown model ($V \neq 0$).

The Hamiltonian is written as

$$\hat{\mathcal{H}}(h) = \hat{\mathcal{K}}(h) + \hat{\mathcal{V}}. \tag{2.1}$$

Without magnetic field in k-space representation,

$$\hat{\mathcal{K}}(0) = \sum_{\mathbf{k}} \hat{C}^\dagger(\mathbf{k})\mathcal{E}(\mathbf{k})\hat{C}(\mathbf{k}), \tag{2.2}$$

$$\hat{\mathcal{V}} = V\sum_{\mathbf{k}} \left\{\hat{C}^\dagger(k_x, k_y+g)\hat{C}(\mathbf{k}) + \text{h.c.}\right\}, \tag{2.3}$$

$$\mathcal{E}(\mathbf{k}) = -t\left(\cos ak_x + \cos bk_y\right) - t_z \cos ck_z, \tag{2.4}$$

where $g = \pi/b$.

The electron filling (N/N_s) is set to about 1/3 and 7/18 for $V = 0$ and $V \neq 0$, where N_s is the total site number. In this case, $f_\beta \simeq 1/3$ for $V = 0$, and $f_\alpha \simeq 1/18$, $f_\beta \simeq 7/18$ and $f_{\beta\pm\alpha} = f_\beta \pm f_\alpha$ for $V \neq 0$.

We introduce the magnetic field by the Peierls substitution $\mathbf{k} \to \mathbf{k} + e\mathbf{A}/\hbar$ in $\mathcal{E}(\mathbf{k})$, taking the Landau gauge $\mathbf{A}$=(Hy, 0, 0). The resultant kinetic energy operator is

$$\hat{\mathcal{K}}(h) = -\frac{t}{2}\sum_{\mathbf{k}} \left\{\exp(iak_x)\hat{C}^\dagger(k_x, k_y-\delta)\hat{C}(\mathbf{k}) + \text{h.c.}\right\}$$
$$+ \sum_{\mathbf{k}} \left(-t\cos(bk_y) - t_z\cos ck_z\right)\hat{C}^\dagger(\mathbf{k})\hat{C}(\mathbf{k}), \tag{2.5}$$

where $\delta = \frac{eaH}{\hbar c} = \frac{\phi}{\phi_0}\frac{2\pi}{b} = h\frac{2\pi}{b}$, $\phi = abH$ is the flux passing through a unit cell, $\phi_0 = 2\pi\hbar/e$ is the unit flux quantum, and $h = \phi/\phi_0$ is the number of the flux quantum per unit cell. Since the total band width is about $4t$, $\hbar\omega \simeq 4th = 4h$, and $2t_z/\hbar\omega \simeq t_z/2h$. When $t_z/t = 0.05$, $2t_z/\hbar\omega \simeq 1$ at $h \simeq 1/40$. We describe the magnetic field as h, hereafter. In this study, h is changed from 1/60 to 1/8, which corresponds to $20 \lesssim n \lesssim 3$, where n is the number of the highest occupied Landau level.

From the eigenvalue ($E_i(h)$) obtained by diagonalizing $\hat{\mathcal{H}}(h)$, the chemical potential is given by

$$\mu(N,h) = E_N(h). \tag{2.6}$$

The free energy, $F(N,h)$, at $T = 0$ is given by

$$F(N,h) = \frac{1}{N_s}\sum_{i=1}^{N} E_i(h). \tag{2.7}$$

The magnetization is obtained from

$$M(N,h) = -\partial F(N,h)/\partial h. \tag{2.8}$$

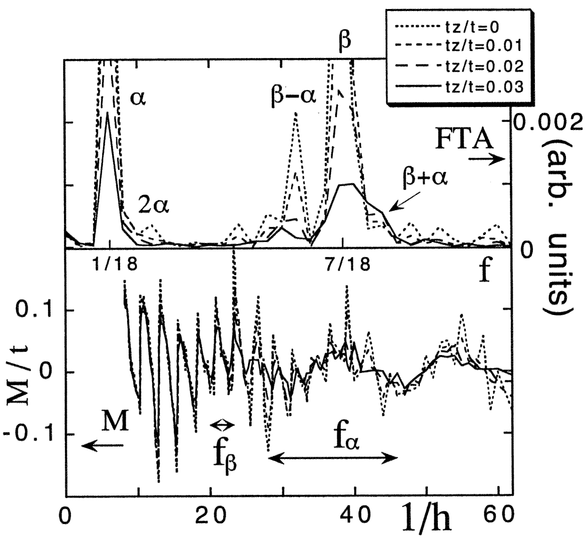

Fig. 4. $M(N, h)$ (lower figure) and its FTA (upper figure). The region of the Fourier transform is $12 \leq 1/h \leq 62$.

§3. Results and Discussions

3.1 One-band Model

In Fig. 2, we show $\mu(N, h)$ and $M(N, h)$ under the condition of the fixed N as a function of $1/h$ by changing t_z continuously. The period of the oscillation of $\mu(N, h)$ and $M(N, h)$ is 1/3, which is consistent with the period of f_β. The *effective three-dimensionality* due to the larger t_z and/or the lower h results in the smooth damping of the oscillation of $\mu(N, h)$ and the smooth decreasing of the amplitude of the oscillation of $M(N, h)$. When the three-dimensionality becomes large (see the case of $t_z/t = 0.05$ in Fig. 2), the oscillation of $\mu(N, h)$ is very small at the low field ($1/h \gtrsim 30$), i.e. $2t_z/\hbar\omega \gtrsim 1.0$.

3.2 magnetic breakdown Model

In the magnetic breakdown system ($V/t = 0.1$), $M(N, h)$ and its Fourier transform amplitudes (FTAs) are shown in Fig. 4. From the overall behavior of $M(N, h)$, we can see that the amplitudes of the oscillations of α (β) are smaller (larger) as h increases, which is due to the magnetic breakdown.

In the FTAs of $M(N, h)$ there exit the β-α oscillation and a small peak of β+α oscillation in addition to the large peaks of α and β oscillations at $t_z = 0$. In Fig. 5, we show the t_z-dependence of these FTAs. As t_z increases, the α, β and β-α oscillations are strongly suppressed. The three-dimensionality plays a role of the decreasing amplitude of the oscillation. Nevertheless, the β+α oscillation is enhanced clearly and has a maximum at $t_z/t \simeq 0.025$. The damping of the oscillation of μ is closely related to this maximum of the $\beta + \alpha$ oscillation.

§4. Conclusion

We have studied the dHvA oscillation in the quasi-two-dimensional system. In the intermediate region ($0 < 2t_z/\hbar\omega < 1.0$), the effect of the smooth damping of the oscillation of μ appears in the dHvA oscillation. This interesting physical picture has never been shown until now. One can see an anomalous maximum of the amplitude of the β+α oscillation in the quasi-two-dimensional magnetic breakdown system. It will be observed in κ-

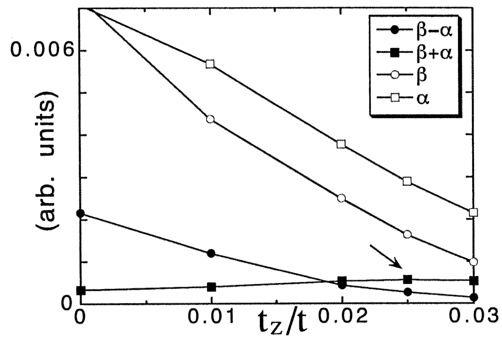

Fig. 5. Main FTAs of $M(N, h)$ as a function of t_z/t. An arrow indicates a maximum.

(BEDT-TTF)$_2$Cu(NCS)$_2$ by the experiments under the uniaxial stress.[30)]

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