

# Quantum magnetic oscillation in the quasi-two-dimensional multi-band systems

Keita Kishigi<sup>a,1</sup>, Timothy Ziman<sup>b</sup>, Hitoshi Ohta<sup>a,c</sup>

<sup>a</sup> *Venture Business Laboratory, Kobe University, Rokkodai 1-1, Nada, Kobe 657-8501, Japan*

<sup>b</sup> *Institut Laue Langevin, BP156, 38042 Grenoble, Cedex 9, France*

<sup>c</sup> *Molecular Photoscience Research Center, Kobe University, Rokkodai 1-1, Nada, Kobe 657-8501, Japan*

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## Abstract

For the analysis of the de Haas-van Alphen (dHvA) oscillation, the Lifshitz and Kosevich (LK) formula is used. However, it is known that the LK formula is not suitable to the analysis of the dHvA oscillation in quasi-two-dimensional (Q2D) and two-dimensional (2D) systems. Recently, the formula for dHvA oscillations in the 2D and Q2D multi-band systems has been derived. We apply this Q2D formula to the Q2D material  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub>. As a result, we obtain that the temperature ( $T$ )-dependencies of amplitudes of  $\alpha$  (resp.  $\beta$ ) oscillations of the Q2D formula are slightly (substantially) different from those of the LK formula below 0.4 [K] although the  $T$ -dependencies of the Q2D formula are the same as those of the LK formula above 0.4 [K]. This means that a good fit for the  $T$ -dependence of amplitudes of the dHvA experiments below 0.4 [K] in that compound would be obtained only by the Q2D formula.

*Key words:* dHvA; quasi-two-dimensional multi-band system;  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub>

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## 1. Introduction

In metals, the magnetization ( $M$ ) periodically oscillates as a function of the inverse magnetic field ( $1/H$ ). This oscillation is known as the de Haas-van Alphen (dHvA) oscillation, and the experiments have been fitted by the Lifshitz and Kosevich (LK) formula[1]. However, it has been noticed that the LK formula cannot be applied in the two-dimensional (2D)[2–4] and quasi-two-dimensional (Q2D)[5] systems, because the oscillation of the chemical potential ( $\mu(N, H)$ ) is neglected.

We consider the eigenvalue in the Q2D multi-band system under the perpendicular field as follows:  $\epsilon_{n,k_z,\sigma,j} = \hbar\omega_{c,j}(n + \frac{1}{2}) - 2t_{z,j}(\cos(c_j k_z) - 1) + g_j\sigma\mu_B H + E_{b,j}$ , where  $\omega_{c,j} = eH/cm_j$ ,  $\rho_j = m_j/(2\pi c_0 \hbar^2)$ ,  $t_{z,j}$  ( $c_j$ ) are the transfer integral (lattice constant) along  $z$ -axis,  $E_{b,j}$  is the band edge,  $c_0$  is the common unit cell length along  $z$ -axis and  $j$  is the band

suffix. Here,  $\mu_B = e\hbar/(2m_0c)$  is the Bohr magneton with a free electron mass ( $m_0$ ) and the velocity of light ( $c$ ). Hereafter, we set  $\hbar = c = k_B = c_0 = 1$ . The formula of the dHvA oscillation has been shown as[5],

$$\tilde{M}_N(N, H) \simeq - \sum_j \sum_{r=1}^{\infty} \frac{2e\rho_j(\mu - E_{b,j})}{\pi r m_j} R_{Y,r,j} R_{D,r,j} R_{S,r,j} \times R_{T,r,j} \sin \left[ 2\pi r \left( \frac{\mu - E_{b,j}}{\omega_{c,j}} + \frac{1}{2} \right) \right] \Big|_{\mu=\mu(N,H)}. \quad (1)$$

with

$$R_{Y,r,j} = J_0 \left( 2\pi r \frac{t_{z,j}}{\omega_{c,j}} \right), \quad R_{D,r,j} = \exp \left( -2\pi r \frac{\Gamma_j}{\omega_{c,j}} \right), \\ R_{T,r,j} = \frac{2\pi^2 r T / (\omega_{c,j})}{\sinh(2\pi^2 r T / (\omega_{c,j}))}, \quad R_{S,r,j} = \cos \left( r\pi \frac{g_j m_j}{2m_0} \right),$$

where  $\Gamma_j = 1/(2\tau_j)$  and  $\tau_j$  is the lifetime of the electron. The chemical potential is given by numerically solving the transcendental equation[3,5]:

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<sup>1</sup> Corresponding author. E-mail: k.kishigi@aist.go.jp

$$\mu(N, H) - \mu_0 = -\frac{1}{\rho_s + \rho_R} \sum_j \sum_{r=1}^{\infty} \frac{\rho_j \omega_{c,j}}{\pi r} R_{Y,r,j} R_{D,r,j} R_{S,r,j} \times R_{T,r,j} \sin \left[ 2\pi r \left( \frac{\mu(N, H) - E_{b,j}}{\omega_{c,j}} + \frac{1}{2} \right) \right] \quad (2)$$

, where  $\rho_s = \sum_j \rho_j$ ,  $\rho_R$  is the density of states of an additional unquantized reservoir and  $\mu_0$  is the chemical potential at  $H = T = 0$ . This Q2D formula (Eqs. (1) and (2)) without the impurity scattering, reservoirs and quasi-two-dimensionality is the same as the 2D formula obtained by one of the authors[3].

In the 2D multi-band system, it was shown by numerical calculations[2] that the interference oscillations such as  $\beta$ - $\alpha$  and  $\beta$ + $\alpha$  oscillations occur. From the 2D formula[3,4] and the Q2D formula[5], it has also been shown that the interference oscillations exist due to the chemical potential oscillation. In fact, the interference oscillations have been confirmed by the dHvA experiments of  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub>[6,7] which is known as a Q2D material. In the LK formula, the interference frequencies are absent.

Although the Q2D formula is considered to be a useful tool for Q2D materials, this formula has not yet been applied to actual materials. Therefore, in this study, we apply the Q2D formula to the dHvA oscillation of  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub> at high fields ( $H \sim 30$  [T]), although strictly speaking the orbit of  $\beta$  is not an independent orbit of the Fermi surface but is formed from the magnetic breakdown between the open and closed sheets. We focus here on the temperature ( $T$ )-dependence of the oscillation amplitudes.

## 2. Results and Discussions

We consider the effects of varying the Dingle temperature. Thus, for simplicity we set that  $T_D = T_{\alpha,D} = 1/(2\pi\tau_{\alpha})$  equal to  $T_{\beta,D} = 1/(2\pi\tau_{\beta})$ . For the two cases of  $T_D = 0.35$  [K] and  $T_D = 0.5$  [K], in Fig. 1 we show the dHvA oscillation of  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub> the parameters[6,7]:  $m_{\alpha} = 3.5m_0$ ,  $m_{\beta} = 6.9m_0$ ,  $g_{\alpha} = g_{\beta} = 1.73$ ,  $f_{\alpha} = 600$  [T],  $f_{\beta} = 3600$  [T],  $T = 200$  [mK],  $\rho_R = 0$  and  $t_z = 0$ [8].

In Fig. 2 we show the  $T$ -dependencies of the Fourier transform intensities (FTIs) for fixed  $T_D = 0.2$  [K] as estimated by Uji et al.[7]. (In fact this was estimated for the  $\beta$  orbit, for  $\alpha$  they obtained  $T_{\alpha,D} = 0.55$  [K].) Below 0.4 [K], the  $T$ -dependencies of the FTIs of  $\alpha$  (resp.  $\beta$ ) oscillations of the Q2D formula are slightly (substantially) different from those of the LK formula. On the other hand, above 0.4 [K], this disagreement becomes small. This is caused by the chemical potential oscillation becoming large only below 0.4 [K].

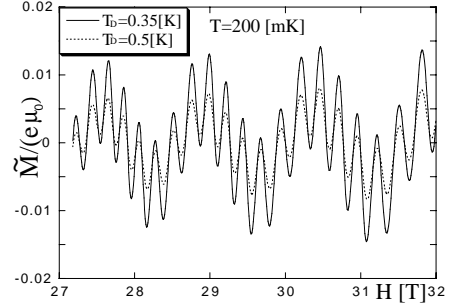


Fig. 1. Calculated dHvA oscillation in  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub> for  $T = 200$  [mK].

In  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub>, Uji et al.[7] fitted the  $T$ -dependencies of the dHvA oscillation amplitude for each frequencies by use of the LK formula in the field range of Fig. 2. We conclude that their good agreement with the LK formula was found because their experiment was done above a cross-over temperature that we estimate from Fig. 2 as 0.4 [K], but below this temperature the amplitude should be fitted correctly only with the Q2D formula. The cross-over temperature can be increased by increasing the magnetic field.

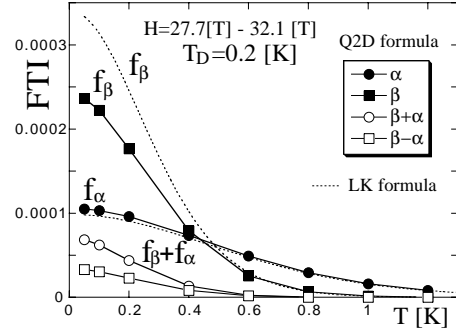


Fig. 2. The  $T$ -dependence of the FTIs. Dots (dotted lines) are for the Q2D (LK) formula, respectively.

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- [8] We can consider the Q2D system as an essentially 2D system by choosing the Yamaji-angle. In  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub>[6], the Yamaji angle is about 20°.