Spin factor of de Haas–van Alphen oscillations in two-dimensional systems: Effect of background density of states and chemical-potential oscillations

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(Received 13 July 1999)

We study the spin-split de Haas–van Alphen oscillations in two-dimensional (2D) conductors whose density of states (DOS) is made of two parts: one is a set of sharp Landau levels and another is a DOS unaffected by the magnetic field. We call the latter the background DOS and denote it by $\rho_{\rm BG}$. We report the analytical formula for the spin factors of all the harmonic components at absolute zero temperature; the formula is valid for any $\rho_{\rm BG}$ and for any g value of the quantized band. The obtained spin factors, in particular the ones of the higher-harmonic components, depend complicatedly on $\rho_{\rm BG}$ and g, and differ drastically from those in the Lifshitz-Kosevich formula: the values of g (or the magnetic field angles) for which the spin factors become zero vary with $\rho_{\rm BG}$.

The de Haas–van Alphen (dHvA) effect in strongly two-dimensional (2D) conductors is attracting much attention, because such systems have been realized in several molecular conductors or in other kinds of substances such as Sr_2RuO_4, and because the dHvA effect in those systems shows some peculiarities which are beyond the applicability of the standard Lifshitz-Kosevich (LK) formula.[1,2]

Although the LK formula has been successful in analyzing the dHvA effect in ordinary three-dimensional (3D) conductors, it cannot be applied to the 2D systems, because the formula is derived by neglecting the chemical potential oscillation (CPO). While the CPO is negligibly small in ordinary 3D systems, it is always substantial and cannot be neglected in 2D systems (even far from the quantum limit, i.e. , even if the number of occupied Landau levels is not small).[3,4] For example, in 2D systems having multiple closed bands, novel combination frequency components appear solely owing to the CPO: this phenomenon has been noticed first in Ref. 5, and investigated further recently.[6–10]

In this paper, we consider a perfectly 2D system[11] having multiple bands but only one fundamental frequency; i.e., only a single band of this system is Landau quantized, while the other bands are unaffected by the magnetic field. The latter gives the density of states (DOS) independent of the field, which we call *the background DOS* and designate by $\rho_{\rm BG}$. (The model with $\rho_{\rm BG}$ was first introduced in Ref. 8, and has been used often in succeeding studies on the effect of the CPO.[10,12–14])

The spin effect on the dHvA oscillation in this simple 2D system is unexpectedly complicated and drastically different from the one expressed in the LK formula, owing to the CPO. We report the exact analytical expression for the spin effect of this system at absolute zero temperature ($T=0$) in the form of spin factors of all the harmonic components.

The CPO and, hence, the spin factors are sensitive to $\rho_{\rm BG}$, which serves as an electron reservoir. The two limits (i) $\rho_{\rm BG}\to 0$ and (ii) $\rho_{\rm BG}\to\infty$ correspond, respectively, to the cases of a single quantized band (i) with a fixed electron number and (ii) with a fixed chemical potential. The spin effect in case (i) at $T=0$ is given in Ref. 3. In case (ii), it is expressed by the standard spin factors in the LK formula, irrespective of the dimensionality.

The results in the two limits are completely different. The purpose of this paper is to show the crossover of the spin effect, which occurs in an extremely complicated manner, with varying $\rho_{\rm BG}$ from 0 to ∞, by giving the exact analytic expression for the spin factors of all the harmonic components at $T=0$. The applicability of our results is wider than expected from the simplicity of our model and the restriction to $T=0$, as explained later.

The same model as ours is investigated in Ref. 14, which gives approximate analytical expressions for the magnetization at $T\neq 0$, but not in the form of spin factors. Spin factors have been familiar and convenient tools in the analyses of the experimental results. Thus, our work, while restricted to $T=0$, giving the exact spin factors, is useful and complements Ref. 14.

We consider the following simple 2D two-band model: One band has a simple parabolic dispersion given by

$$\mathcal{E}(\mathbf{k})=\frac{(\hbar k_x)^2}{2m_x}+\frac{(\hbar k_y)^2}{2m_y}, \tag{1}$$

where $\mathbf{k}=(k_x,k_y)$ is the 2D k vector. The masses m_x and m_y must have the same sign, and we assume, without loss of generality, that they are positive, i.e., that the band is an electron (not a hole) band.[16] In the absence of a magnetic field, the DOS (per unit area) of this band for each spin is given by

$$\rho(\varepsilon)=\rho_0 \quad (\text{const for } \varepsilon>0), \tag{2}$$

where

$$\rho_0=m/(2\pi\hbar^2), \quad m=\sqrt{m_x m_y}. \tag{3}$$

We will concern ourselves only with the ratio of ρ_0 to $\rho_{\rm BG}$; hence only note that $\rho_0\propto m$.

Under a magnetic field whose strength is B and whose angle from the z axis is θ, this band is quantized; the Landau levels are given by

$$\mathcal{E}(n,\sigma)=\hbar\omega_c\left(n+\frac{1}{2}+\sigma\gamma\right)$$
$$(\text{for } n=0,1,2,\ldots, \quad \text{and } \sigma=\pm\tfrac{1}{2}), \tag{4}$$

where

$$\hbar\omega_c=\left|\frac{\hbar eB\cos\theta}{m}\right|, \quad \gamma=\left|\frac{g}{2}\frac{m}{m_0\cos\theta}\right| \tag{5}$$

are the Landau level spacing (the cyclotron frequency multiplied by $\hbar$) and the normalized dimensionless gyromagnetic ratio, with g being the g value of this band and m_0 the bare electron mass.

The other band is assumed to be unaffected by magnetic field, except for the Zeeman effect, i.e., not to be Landau quantized. The DOS of this band for each spin ($\sigma=\pm 1/2$) is given by

$$\rho(\varepsilon)=\rho_{\rm BG} \quad (\text{const for } \varepsilon>\mathcal{E}_{\rm b}+\sigma\tilde{\gamma}\hbar\omega_c), \tag{6}$$

where $\mathcal{E}_{\rm b}$ is the band bottom energy at $B=0$, and $\tilde{\gamma}=|mg_{\rm BG}/2m_0\cos\theta|$, with $g_{\rm BG}$ being the g value of this unquantized band. The mass of this unquantized band, $m_{\rm BG}$, is given by $\rho_{\rm BG}=m_{\rm BG}/2\pi\hbar^2$.

The most important parameter in this work is the ratio

$$G=\rho_{\rm BG}/\rho_0=m_{\rm BG}/m. \tag{7}$$

Also important is γ (or θ and g). The crucial condition in our analysis is that the total electron number N must always be kept constant.

The chemical potential at $T=0$ and at $B=0$ for a given N, designated by μ_0, is determined by

$$2\rho_0\mu_0+2\rho_{\rm BG}(\mu_0-\mathcal{E}_{\rm b})=N. \tag{8}$$

In this work, we treat only the case far from the quantum limit; i.e. , we assume that μ_0 and $\mu_0-\mathcal{E}_{\rm b}$ are much greater than $\hbar\omega_c$, $\gamma\hbar\omega_c$, and $\tilde{\gamma}\hbar\omega_c$; thus, the final results do not depend on $\mathcal{E}_{\rm b}$ and $\tilde{\gamma}$.

It is convenient to measure the magnetic field by

$$x=2\mu_0/\hbar\omega_c=2F/B, \tag{9}$$

where

$$F=\left|\frac{\hbar S_0}{2\pi e\cos\theta}\right|, \quad S_0=\frac{2\pi m\mu_0}{\hbar^2} \tag{10}$$

are the oscillation frequency and the cross-sectional area of the cylindrical Fermi surface.

The magnetization along the field direction is defined by

$$M(B,N)=-\frac{\partial\Delta E_{\rm tot}}{\partial B}, \tag{11}$$

where $\Delta E_{\rm tot}$ is the variation of the ground-state energy of the system: $\Delta E_{\rm tot}=E_{\rm tot}(\mathbf{B},N)-E_{\rm tot}(0,N)$. It is convenient to define a normalized magnetization as

$$\tilde{M}=C\cdot M, \quad \text{where } \frac{1}{C}=\frac{2\rho_0\mu_0\hbar e\cos\theta}{m}. \tag{12}$$

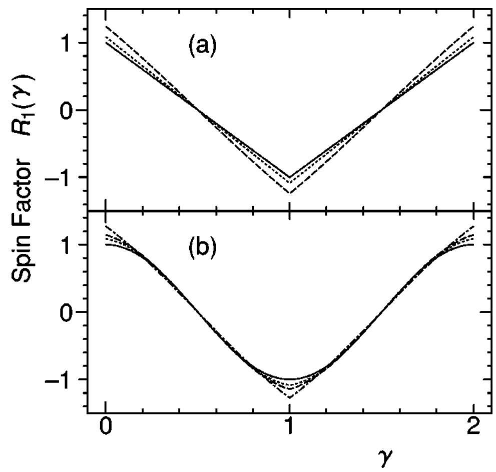

FIG. 1. $R_1(\gamma)$ for seven values of G. (a) Solid line for $G=0$, dotted line 0.1, and dashed line 0.5 and (b) dash-dotted line 1.0, dashed line 2.0, dotted line 10.0, and solid line ∞.

After some calculation, we obtain the following formula for the oscillatory part of $\tilde{M}$, with the spin factor R_n given below:

$$\tilde{M}_{\rm osc}(x)=\sum_{n=1}^{\infty}\frac{-1}{n\pi}R_n(\gamma)\sin n\pi(x-1) \tag{13a}$$

$$=\sum_{n=1}^{\infty}\frac{-1}{n\pi}R_n(\gamma)\sin 2n\pi\left(\frac{F}{B}-\frac{1}{2}\right), \tag{13b}$$

This equation and Eq. (22), the formula for $R_n(\gamma)$, with some definitions in Eqs. (17), (19), and (23) constitute the main result of this work. To demonstrate the complicated manner of the crossover with varying G from 0 to ∞, we depict R_1, R_2, and R_3 as a function of γ for several values of G in Figs. 1–3.

Now, we briefly describe the derivation. First, the ground-state energy is obtained as

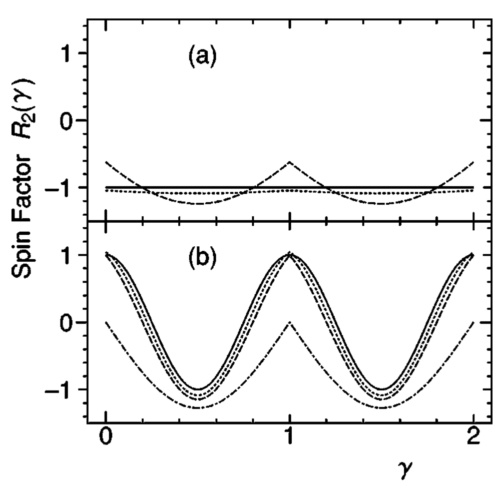

FIG. 2. $R_2(\gamma)$ for seven values of G. (a) Solid line for $G=0$, dotted line 0.1, and dashed line 0.5 and (b) dash-dotted line 1.0, dashed line 2.0, dotted line 10.0, and solid line ∞.

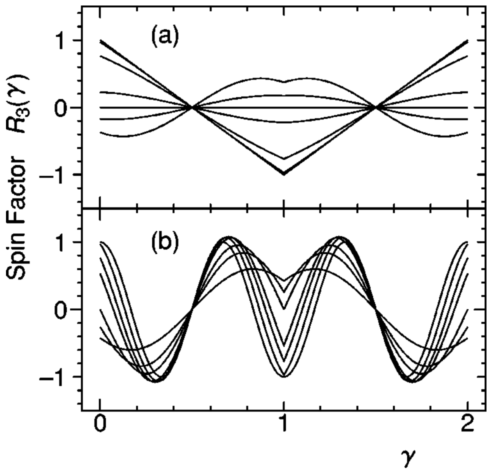

FIG. 3. $R_3(\gamma)$ for 14 values of G. (a) The larger $R_3(0)$, the smaller G, for $G=0$, 0.1, 0.2, 0.4, 0.5, 0.6, and 0.8: For $G=0.5$, $R_3(\gamma)=0$ (const); the lines for 0 and 0.1 are difficult to distinguish. (b) The smaller $R_3(0)$, the smaller G, for $G=1.0$, 1.5, 2.0, 3.5, 5.0, 10.0, and ∞.

$$\Delta E_{\text{tot}}=\rho_0\hbar\omega_c^2 L_\gamma(x)-\frac{\rho_0(\gamma\hbar\omega_c)^2}{4}-\frac{\rho_{\text{BG}}(\tilde{\gamma}\hbar\omega_c)^2}{4}, \tag{14}$$

where the last two terms are the Zeeman energy gain of the respective bands; the function $L_\gamma(x)$ is described below. Second, the normalized magnetization is derived as

$$\tilde{M}=\left\{L'_\gamma(x)-\frac{\hbar\omega_c}{\mu_0}\left(L_\gamma(x)-\frac{\gamma^2+G\tilde{\gamma}^2}{4}\right)\right\}, \tag{15}$$

and third, its oscillatory part is well approximated by

$$\tilde{M}_{\text{osc}}=L'_\gamma(x), \tag{16}$$

because we are assuming that the number of occupied Landau levels is large, i.e., $\hbar\omega_c/\mu_0 \ll 1$, while $L_\gamma(x)$ and $L'_\gamma(x)=dL_\gamma/dx$ are of order unity.

The function $L_\gamma(x)$ is an even periodic function of x with period 2, and is also a periodic function of γ with period 2. We denote the integer part of γ by $[\gamma]$, and denote its fractional part by

$$\delta=\gamma-[\gamma]. \tag{17}$$

If $[\gamma]$ is *even*,

$$4L_\gamma(x)=\delta^2+\frac{G+1}{G}x^2 \quad (\text{for } x\in[0,\eta]) \tag{18a}$$

$$=\delta^2+(1-\delta)^2-(G+1)\{x-(1-\delta)\}^2 \quad (\text{for } x\in[\eta,1-\xi]) \tag{18b}$$

$$=(1-\delta)^2+\frac{G+1}{G}(x-1)^2 \quad (\text{for } x\in[1-\xi,1]), \tag{18c}$$

where

$$\xi=\frac{G}{G+1}\delta, \quad \eta=\frac{G}{G+1}(1-\delta). \tag{19}$$

If $[\gamma]$ is *odd*, we obtain $L_\gamma(x)$ by replacing δ with $1-\delta$ and exchanging ξ for η in Eq. (18).

The Fourier coefficients defined by

$$L_\gamma(x)=\frac{a_0(\gamma)}{2}+\sum_{n=1}^{\infty}a_n(\gamma)\cos(n\pi x), \tag{20a}$$

$$a_n(\gamma)=2\int_0^1 L_\gamma(x)\cos(n\pi x)dx, \tag{20b}$$

are obtained as follows[17] for $n\geqslant 1$:

$$a_n(\gamma)=(-1)^n(n\pi)^{-2}R_n(\gamma), \tag{21}$$

where

$$R_n(\gamma)=\frac{-1}{(n\pi)}\frac{(G+1)^2}{G}S_n(\gamma) \tag{22}$$

and

$$S_n(\gamma)=\sin(n\pi\xi)+(-1)^n\sin(n\pi\eta) \quad (\text{for even } [\gamma]) \tag{23a}$$

$$=(-1)^n\sin(n\pi\xi)+\sin(n\pi\eta) \quad (\text{for odd } [\gamma]). \tag{23b}$$

Note that R_n, as well as a_n and S_n, is a periodic function of γ with period 2, while their absolute values have period 1 and depend only on δ. One might think that it is better to define the spin factors as $R_S^n(\gamma)\equiv R_n(\gamma)/R_n(0)$. This does not work well, however, since it happens that $R_n(0)=0$ for some G generally [only for $n=1$, $R_n(0)\approx 1$ for any G]. Hence, our definition of R_n and our representation of formula (13) seem the most appropriate ones.

In the limits $G\to 0$ and $G\to\infty$, we obtain

$$\lim_{G\to 0}R_n(\gamma)=-\{\delta+(-1)^n(1-\delta)\} \quad (\text{for even } [\gamma]) \tag{24a}$$

$$=-\{(-1)^n\delta+(1-\delta)\} \quad (\text{for odd } [\gamma]), \tag{24b}$$

which completes the partial result in Ref. 15, and

$$\lim_{G\to\infty}R_n(\gamma)=\cos(n\pi\gamma), \tag{25}$$

which reproduces the well-known spin factor for each n in the LK formula.

As a function of γ, $\lim_{G\to 0}R_n(\gamma)$ and $\lim_{G\to\infty}R_n(\gamma)$ are similar only for $n=1$ (Fig. 1). [In the figures, the spin factors $R_n(\gamma)$ are depicted only for one period, $0\leqslant\gamma\leqslant 2$.] For $n\geqslant 2$, they are qualitatively different (Figs. 2 and 3). For example, $\lim_{G\to 0}R_2(\gamma)=-1$ (const), whereas $\lim_{G\to\infty}R_2(\gamma)=\cos 2\pi\gamma$. Between the two limits, we can see that $R_2(\gamma)$ and $R_3(\gamma)$ change their form continuously but drastically. In particular, note that the values of γ which satisfies $R_n(\gamma)=0$ varies generally with varying G (the exceptions are $\gamma=0.5$ and 1.5 for $n=$ odd): this fact is specifically important in analyzing the experimental results.

Now we begin a discussion. The constant N condition has been crucial in our analysis. This condition is realized, within a bulk 2D conductor, by the long-range Coulomb interaction which strongly keeps electrical neutrality. Thus, even if a sample is grounded, this condition holds in the bulk. This implicitly incorporated Coulomb interaction and the Pauli exclusion principle make things complicated and interesting, whereas our model is only a one-body problem.

The spin effect can be investigated most systematically by the angular dependence of the oscillation amplitudes, because $\gamma \propto (\cos\theta)^{-1}$. However, in the real strongly 2D substances, not only the spin effect, but also the Yamaji effect affects the angular dependence.[10,18,19] Hence, we must be careful to be aware of both effects in practical analyses. (The Yamaji effect is an effect caused by the very weak but finite three dimensionality of the systems.[20]) With this care, our results enable us to obtain the g value of the quantized band by analyzing the angular dependence of the spin factors.

The origin of finite G can be not only the coexisting open bands, but also the coexisting closed bands whose masses are much heavier than that of the lightest band. Let us denote the temperature and lifetime by T and τ. If $\hbar/\tau$ and k_BT are much less than the Landau level spacing of the lightest band but are much greater than those of the other bands, then it is possible that $1/\tau$ and T are small enough for them to be approximated by zero for the lightest band, but are large enough to wipe out the quantized structure in the DOS of the heavier bands. Therefore, the results of this work can be applied to the interpretation of many of the dHvA experiments on strongly 2D conductors at appropriate temperatures, and enable us to determine the g value of the lightest band.

In future studies, however, we must incorporate T and τ legitimately. It is certain that we cannot factorize the effect of spin and temperature as in the LK formula like $R_S^n(\gamma,\mathbf{B})\cdot R_T^n(T,\mathbf{B})$, but that we can only obtain a single factor $R_n(\gamma,T,\mathbf{B})$.

Finally, whereas no electronic correlation is incorporated in our model, what is pointed out in this work is of great significance also in the study of correlated systems. For an investigation of correlated systems can be performed only after a complete understanding of uncorrelated systems.

In conclusion, we have obtained an exact analytical formula for the spin factors $R_n(\gamma)$ for an arbitrary background density of states ρ_{BG} at $T=0$. Our results indicate that, in analyzing the experimental results, one must always pay close attention to the fact that the spin factors in the 2D systems are completely different from those in the LK formula and complicatedly and sensitively depend on the values of ρ_{BG} and $\gamma \propto g/\cos\theta$.

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$$2a_0(\gamma)=\delta^2+(1-\delta)^2-\frac{2G+1}{G+1}\left\{\frac{1}{3}-\delta(1-\delta)\right\}.$$

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