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Cyclotron Resonance of Piezoelectric Polarons in the Quantum Limit*

SATORU J. MIYAKE†
Department of Physics, University of Illinois, Urbana, Illinois 61801

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The shift of the cyclotron resonance frequency of electrons in piezoelectric semiconductors at finite temperature is calculated for the case of such a strong magnetic field that the energy separation of the Landau levels is larger than thermal energy. The thermal Green-function method is used to calculate the energy shifts of the two lowest Landau levels between which the transition occurs; the Dyson equation for the electron self-energy part is solved in an approximate way, taking into account the broadening and the shift of electronic states self-consistently. The shift obtained agrees in sign, and roughly in magnitude, with that given by a semiclassical theory, and with that observed in CdS by Baer and Dexter.

I. INTRODUCTION

CYCLOTRON resonance of electrons in CdS was observed by Sawamoto,[1] and by Baer and Dexter.[2] They found that the frequency of cyclotron resonance of electrons in this substance is about 15% higher than the value expected from the effective mass obtained by other experiments. Cyclotron-resonance measurements show a peak which corresponds to an effective mass of about $0.17m_0$ (m_0 being the electron mass in vacuum). On the other hand, the values of the effective mass obtained from various different experiments lie between $0.19m_0$ and $0.21m_0$.[2]

Mahan and Hopfield[3] noticed the importance of the effect of piezoelectric electron-phonon interaction upon the properties of low-energy electrons. They suggested that in the cyclotron-resonance experiments performed at low temperature, the piezoelectric-polaron effect produces the observed shift in cyclotron frequency, but that in other experiments at high temperature or high frequencies, the effects are negligible. Unfortunately the calculation by Mahan and Hopfield is based on a semiclassical argument. The experiments by Sawamoto, and by Baer and Dexter were done at low temperature and strong field. If we write the temperature T and the microwave frequency ω, the ratio $\hbar\omega/kT$ (k, Boltzmann constant) is 1.4 for Sawamoto's experiment and 2.6 for Baer and Dexter's. It seems an open question whether the semiclassical argument applies for the case $\hbar\omega > kT$, i.e., in the quantum limit.

Larsen[4] undertook a quantum-mechanical calculation of cyclotron-frequency shift at zero temperature in the quantum limit condition. He calculated the frequency shift taking into account such processes in which a phonon is spontaneously emitted by an electron. It was found that the shift in the cyclotron-resonance frequency begins to differ drastically from that expected from the semiclassical theory when $\hbar\Omega_c > \frac{1}{2}ms^2$, where $\hbar\Omega_c$ is the separation in energy of the unperturbed magnetic levels, m is the band mass of the electron, and s is the velocity of sound in the crystal. When $2\hbar\Omega_c/ms^2 = 30$ as in Baer and Dexter's experiment, Larsen's calculation gives a shift which is less than $\frac{1}{5}$ of the magnitude of the correction predicted by the semiclassical theory and of opposite sign. It is apparent that a semiclassical treatment is inappropriate in this case. Larsen did not give a result at finite temperature, at which the absorption and induced emission of phonons by an electron are much more important than the spontaneous emission of phonons by an electron.

Under the conditions of Sawamoto's and Baer and Dexter's experiments, the energy of phonons which contribute much to the piezoelectric-polaron effect is much smaller than the thermal energy kT. It is interesting, therefore, to carry out a quantum-mechanical calculation of the effect at finite temperature, and to compare with the experimental results.

In the present paper, we will present a quantum-mechanical calculation of the shift in cyclotron-resonance frequency in quantum limit at finite temperature. We use an isotropic interaction model which is represented by the Hamiltonian

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_1\,, \\
\mathcal{H}_0 &= [\mathbf{p} + (e/c)\mathbf{A}(\mathbf{r})]^2/2m + \textstyle\sum_{\mathbf{q}} \hbar s q b_{\mathbf{q}}^\dagger b_{\mathbf{q}}\,, \qquad (1.1)\\
\mathcal{H}_1 &= (2\pi\alpha\hbar e^2 s/\kappa V)^{1/2} \textstyle\sum_{\mathbf{q}} q^{-1/2}(b_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} + b_{\mathbf{q}}^\dagger e^{-i\mathbf{q}\cdot\mathbf{r}})\,.
\end{aligned}$$

Here e is the magnitude of the electron charge, c is the velocity of light, $\mathbf{A}(\mathbf{r})$ is the vector potential describing the applied magnetic field, m is the electron band mass, $b_{\mathbf{q}}^\dagger$ and $b_{\mathbf{q}}$ are, respectively, creation and annihilation operator for phonons of wave number $\mathbf{q}$, s is the velocity of sound, α is a dimensionless coupling constant which is equal to $\langle K^2 \rangle_{\mathrm{av}}$, the spherical average of the square of the electromechanical coupling,[5] κ is the dielectric constant, and V is the volume of the crystal.

In the next section, we briefly discuss inadequacy of the second-order perturbational calculation when the quantization of electronic levels due to magnetic field is taken into account. In Sec. III, the method of the

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† On leave of absence from Department of Physics, Tokyo Institute of Technology, Tokyo, Japan.

[1] K. Sawamoto, J. Phys. Soc. Japan **19**, 318 (1964).

[2] W. S. Baer and R. N. Dexter, Phys. Rev. **135**, A1388 (1964).

[3] G. D. Mahan and J. J. Hopfield, Phys. Rev. Letters **12**, 241 (1964).

[4] D. M. Larsen, Phys. Rev. **142**, 428 (1966).

[5] A. R. Hutson, J. Appl. Phys. **32**, 2287 (1961).

present calculation will be described; approximations used in the computation will be discussed. The result of the calculation and some discussions will be given in the last section. The appendix contains some preliminaries to Sec. III.

II. SECOND-ORDER PERTURBATIONAL CALCULATION

An unperturbed electronic state in magnetic field is specified by quantum numbers N, p_z, and X, where N is the quantum number of the cyclotron motion, p_z is the component of momentum in the direction of magnetic field, and X is the center coordinate of the cyclotron orbit.[6] The unperturbed energy of a state (N,p_z,X) is given by

$$\begin{aligned} E^{(0)}(N,p_z,X) &= (N+\tfrac{1}{2})\hbar\Omega_c + p_z^2/2m, \\ \Omega_c &= eH/mc. \end{aligned} \tag{2.1}$$

In the quantum limit where $\hbar\Omega_c > kT$, almost all electrons are in the $N=0$ states. Hence, the most important contribution to the absorption of microwave power comes from transitions between the Landau levels of $N=0$ and 1. The shift of cyclotron-resonance frequency will be determined from the difference of the energy shifts for states of $N=0$ and 1.

The second-order energy shift of the state (N,p_z,X) is given by

$$\begin{aligned} &\Delta E^{(2)}(N,p_z,X) \\ &\quad = P\sum_{N'p_z'X'}\sum_{\mathbf{q}}\left(\frac{2\pi\alpha\hbar e^2 s}{\kappa V q}\right)|(N',p_z',X'|e^{i\mathbf{q}\cdot\mathbf{r}}|N,p_z,X)|^2 \\ &\qquad \times\{N_q(B^-)^{-1}+(N_q+1)(B^+)^{-1}\}, \end{aligned} \tag{2.2}$$

$$B^\pm = E^{(0)}(N,p_z,X) - E^{(0)}(N',p_z',X') \mp \hbar sq,$$

where $N_q = (e^{\hbar sq/kT}-1)^{-1}$ is the number of phonons of wave number q in thermal equilibrium. The matrix elements for $N=0$ and 1 are given as

$$\begin{aligned} &|(N',p_z',X'|e^{i\mathbf{q}\cdot\mathbf{r}}|0,p_z,X)|^2 \\ &\quad = \delta_{p_z',p_z+\hbar q_z}\delta_{X',X-l^2q_y}(N'!)^{-1}\exp(-\tfrac{1}{2}l^2q_\perp^2)(\tfrac{1}{2}l^2q_\perp^2)^{N'}, \\ &|(N',p_z',X'|e^{i\mathbf{q}\cdot\mathbf{r}}|1,p_z,X)|^2 \\ &\quad = \delta_{p_z',p_z+\hbar q_z}\delta_{X',X-l^2q_y}(N'!)^{-1}\exp(-\tfrac{1}{2}l^2q_\perp^2) \\ &\qquad \times(\tfrac{1}{2}l^2q_\perp^2)^{N'-1}(N'-\tfrac{1}{2}l^2q_\perp^2)^2, \end{aligned} \tag{2.3}$$

where $l=(m\Omega_c/\hbar)^{-1/2}$ is the radius of the lowest Landau orbit.

Among the terms on the right-hand side of Eq. (2.2), the one which is independent of N_q was treated by Larsen.[4] We restrict our discussion in this section to the contribution which is linear in N_q.

As we shall see later, we are interested in terms with $N'=N$. We see from Eqs. (2.2) and (2.3) that the wave numbers of phonons which make an appreciable contribution to these terms are such as $q\lesssim 1/l$. At high temperature, where kT is much larger than the energy of typical phonons, $\hbar s/l=(ms^2\hbar\Omega_c)^{1/2}$, we can use the high-temperature approximation:

$$N_{\mathbf{q}} \approx kT/(\hbar sq). \tag{2.4}$$

We can also neglect the energy of phonons in the denominators $B^\pm$ in Eq. (2.2). This approximation is invalid for $p_z\lesssim(2m\hbar s/l)^{1/2}$ but at high temperatures, the number of such electrons is negligible compared with the total number of electrons.

Using these approximations, we obtain the shifts of energy levels for the states $(0,p_z,X)$ and $(1,p_z,X)$:

$$\begin{aligned} \Delta E^{(2)}(0,p_z,X) &= \frac{\sqrt{2}\alpha lkT}{\pi a_B}\sum_N\frac{1}{N!}P\int_0^\infty du\int_{-\infty}^\infty d\xi \\ &\quad\times\frac{e^{-u^2}u^{2N+1}}{(u^2+\xi^2)[x^2-(x+\xi)^2-N]}, \end{aligned} \tag{2.5a}$$

$$\begin{aligned} \Delta E^{(2)}(1,p_z,X) &= \frac{\sqrt{2}\alpha lkT}{\pi a_B}\sum_N\frac{1}{N!}P\int_0^\infty du\int_{-\infty}^\infty d\xi \\ &\quad\times\frac{e^{-u^2}u^{2N-1}(N-u^2)^2}{(u^2+\xi^2)[x^2-(x+\xi)^2-(N-1)]}, \end{aligned} \tag{2.5b}$$

where $a_B=(me^2/\hbar^2\kappa)^{-1}$ is the Bohr radius in the crystal, and we put $x^2=p_z^2/(2m\hbar\Omega_c)$. These shifts show a singular behavior as a function of x as $x\rightarrow 0$. For example, take a term of $N=0$ on the right-hand side of Eq. (2.5a).

$$\begin{aligned} &P\int_0^\infty du\int_{-\infty}^\infty d\xi\frac{e^{-u^2}u}{(u^2+\xi^2)[x^2-(x+\xi)^2]} \\ &\qquad = \int_0^\infty du\, e^{-u^2}u\left[\frac{\pi}{u}\frac{1}{u^2+4x^2}-\tfrac{1}{2}\pi^2\frac{1}{u^2}\delta(x)\right]. \end{aligned} \tag{2.6}$$

The first term in the bracket on the right-hand side is positive and behaves as x^{-1} when x is small, while the second term is proportional to $\delta(x)$ with a negative divergent coefficient. Of course, Eq. (2.5) cannot apply for $|p_z|\lesssim(2m\hbar s/l)^{1/2}$ as mentioned before. If we take account of inelasticity in the scattering process, the singular behavior will be regularized. This singularity is regularized also if we take into account the finite width of the energy of the electronic states. If the width of the electronic energy is larger than the typical phonon energy $(ms^2\hbar\Omega_c)^{1/2}$, a dominant role in regularizing the singularity is played by the broadening of the electronic energy rather than by the inelasticity of the scattering. The situation seems analogous to that of determining the cutoff energy for the logarithmic divergence in the static magnetoconductivity.[7] As we shall see later, in the case of CdS the width of the

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[6] R. Kubo, H. Hasegawa, and N. Hashitsume, Phys. Rev. Letters 1, 279 (1958); J. Phys. Soc. Japan 14, 56 (1959).

[7] R. Kubo, S. J. Miyake, and N. Hashitsume, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1965), Vol. 17, p. 269.

electronic state is larger than the typical phonon energy under experimentally interesting circumstances.

In order to treat the energy broadening of electronic states, we must investigate the imaginary part of the self-energy along with the real part, Eq. (2.2). As pointed out by Larsen,[4] the inverse of the lifetime of the state, which is proportional to the imaginary part of the second-order self-energy, is divergent even if the inelasticity of the scattering is taken into account. Thus, in order to obtain the real part, as well as the imaginary part, of the self-energy, it is necessary to go beyond the lowest perturbational calculation. It is necessary to include the self-energy in a self-consistent manner, since the self-energy of a state is appreciably affected by the self-energy of other states.

III. HIGHER APPROXIMATION FOR ENERGY SHIFT

To a better approximation, we use the formalism of the thermal Green function, which can be found in standard textbooks.[8] Definitions of the Green function and some of its fundamental properties will be given in Appendix.

The self-energy function is given as

$$\begin{aligned}\Sigma(N,p_z,X;\zeta_n) &= -\frac{1}{\beta}\sum_{\omega_j}\sum_{\mathbf{q}}\sum_{N',p_z',X'}\left(\frac{4\pi\alpha\hbar^2e^2s^2}{\kappa V}\right)G(N',p_z',X';\zeta_n-\omega_j)\\ &\quad\times D(\mathbf{q};\omega_j)|(N',p_z',X'|e^{i\mathbf{q}\cdot\mathbf{r}}|N,p_z,X)|^2\Gamma_{\mathbf{q}}, \qquad (3.1)\end{aligned}$$

where $\beta=(kT)^{-1}$, $\zeta_n=\mu+(2n+1)\pi/(-i\beta)$, $\omega_j=2j\pi/(-i\beta)$, G is the one-particle electron Green function, D is the phonon Green function, and $\Gamma_{\mathbf{q}}$ is the vertex function.

Since we are considering a situation in which the number of electrons is small, the self-energy of phonons is negligible. We replace the phonon Green function by the unperturbed one.

$$D(q,\omega_j)\approx D^{(0)}(q,\omega_j)=[\omega_j^2-(\hbar sq)^2]^{-1}. \qquad (3.2)$$

At high temperature ($kT\gg\hbar sq$), $D^{(0)}(q,\omega_j)$ is appreciable only when $j=0$. Thus, we use a high-temperature approximation for the phonon Green function:

$$D(q,\omega_j)\approx-\delta_{j,0}(\hbar sq)^{-2}. \qquad (3.3)$$

Further we replace $\Gamma_{\mathbf{q}}$ by its lowest approximation, i.e., one.

Analytically continuing the variable ζ_n to the real axis, we obtain the self-energy function.

$$\begin{aligned}\Sigma(N,p_z,X;E\pm i\delta) &= \frac{1}{\beta}\sum_{\mathbf{q}}\sum_{N'p_z'X'}\frac{4\pi\alpha e^2}{\kappa Vq^2}\\ &\quad\times\frac{|(N',p_z',X'|e^{iq\cdot r}|N,p_z,X)|^2}{E\pm i\delta-E^{(0)}(N',p_q',X')-\Sigma(N',p_z',X';E\pm i\delta)}. \qquad (3.4)\end{aligned}$$

The energy of a quasiparticle state (N,p_z,X) is given by a real solution of the equation

$$\begin{aligned}E&=E^{(0)}(N,p_z,X)+\Delta(N,p_z,X;E),\\ \Delta(N,p_z,X;E)&\equiv\mathrm{Re}\Sigma(N,p_z,X;E\pm i\delta).\end{aligned} \qquad (3.5)$$

Equations (3.4) and (3.5) constitute a complicated set of simultaneous integral equations. In order to solve these equations, we make the following approximations: (1) We assume that the broadening of a level is large compared with the thermal energy kT. If this is the case, the dependence of $\Sigma(N,p_z,X;E)$ on p_z is not appreciable as far as those states are concerned which participate in the cyclotron-resonance absorption, or which contribute much to the self-energy of states. We neglect the dependence of $\Sigma(N,p_z,X;E)$ on p_z and replace Σ by its value at $p_z=0$. Since $\Sigma(N,p_z,X;E)$ does not depend on X, we have Σ which depends on only N and E. We write this quantity as $\Sigma_N(E)$. (2) The effect of the presence of Σ in the denominator in

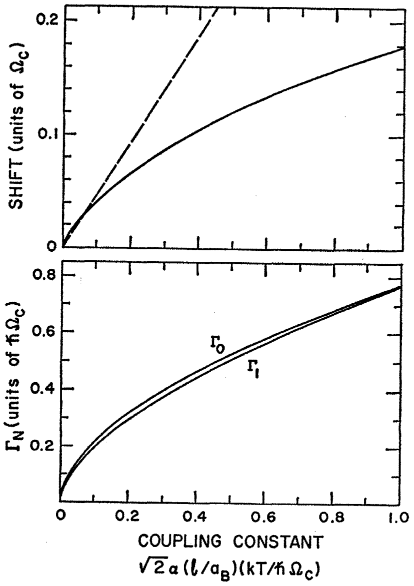

FIG. 1. Shift of cyclotron-resonance frequency $\Delta\omega$ and the imaginary part of the self-energy part Γ_N for the Landau states of $N=0$ and $N=1$ versus a coupling constant $\sqrt{2}\alpha(l/a_B)(kT/\hbar\Omega_c)$. Here, α is the square of electromechanical coupling, l is the radius of the lowest Landau orbit, a_B is the Bohr radius in the crystal, and Ω_c is the unperturbed cyclotron frequency. Solid lines represent the result of the present calculation. A broken line in the upper figure shows the shift calculated according to a semiclassical theory.

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[8] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1963); A. A. Abrikosvo, L. P. Gorkov, and I. E. Dzyaloshinski, *Method of Quantum Field Theory in Statistical Physics*, translated by R. A. Silverman (Prentice-Hall, Inc., Englewood Cliffs, N. J., 1963).

Eq. (3.4) is essential only when the denominator would become zero if Σ were absent. We retain the self-energy function in the energy denominator only if $N' \leq N$. Otherwise, the energy denominators are replaced by their lowest approximation, i.e., the difference of the unperturbed energies.

After these simplifying assumptions, we obtain equations for the self-energy function at $E_N = E^{(0)}(N, p_z = 0) + \Delta_N(E_N)$.

$$d_0 + ig_0 = -\lambda \left\{ \int_0^\infty \frac{du e^{-u^2}}{(ig_0)^{1/2}[(ig_0)^{1/2}+u]} + S_1 \right\}, \tag{3.6a}$$

$$d_1 + ig_1 = -\lambda \left\{ \int_0^\infty \frac{du e^{-u^2} u^2}{(ig_0' - w - 1)^{1/2}[(ig_0' - w - 1)^{1/2}+u]} + \int_0^\infty \frac{du e^{-u^2}(1-u^2)^2}{(ig_1)^{1/2}[(ig_1)^{1/2}+u]} + S_2 \right\}, \tag{3.6b}$$

where $d_i = \Delta_i(E_i)/\hbar\Omega_c$, $g_i = \Gamma_0(E_i)/\hbar\Omega_c = \mathrm{Im}\,\Sigma_i(E_i)/\hbar\Omega_c$,

$$w = [E_1 - \tfrac{3}{2}\hbar\Omega_c - \Delta_0(E_1)]/\hbar\Omega_c, \quad g_0' = \Gamma_0(E_1)/\hbar\Omega_c,$$

$$\lambda = \sqrt{2}\alpha(l/a_B)(kT/\hbar\Omega_c),$$

$$S_1 \equiv \frac{1}{\pi} \sum_{N=1}^{\infty} \frac{1}{N!} \int_0^\infty dk k^2 \int_{-1}^{1} d\mu \frac{1}{k^2} \frac{[k^2(1-\mu^2)]^N e^{-k^2(1-\mu^2)}}{k^2\mu^2 + N},$$

$$S_2 \equiv \frac{1}{\pi} \sum_{N=2}^{\infty} \frac{1}{N!} \int_0^\infty dk k^2 \int_{-1}^{1} d\mu \frac{1}{k^2} \times \frac{[k^2(1-\mu^2)]^{N-1}[N - k^2(1-\mu^2)]^2 \exp[-k^2(1-\mu^2)]}{k^2\mu^2 + (N-1)}.$$

For the square-root function in the above, we have drawn a branch cut from 0 to $-\infty$ and taken the branch the real part of which is positive.

The sums, S_1 and S_2, can be transformed into a more convenient form for computation, as shown by Larsen.[4]

$$S_1 = \frac{1}{\pi} \int_0^\infty dk \int_{-1}^{1} d\mu \int_0^\infty dt \exp[-k^2(1-\mu^2+\mu^2 t)] \times \{\exp[k^2(1-\mu^2)e^{-t}] - 1\}$$

$$= \int_0^\infty dt F_1(t),$$

$$S_2 - S_1 = \frac{1}{\pi} \int_0^\infty dk \int_{-1}^{1} d\mu \int_0^\infty dt k^2(1-\mu^2) \times \exp[-k^2(1-\mu^2+\mu^2 t)]\{\exp[k^2(1-\mu^2)e^{-t}] \times (e^{t/2}-e^{-t/2})^2 - (e^t - 2) - k^2(1-\mu^2)\}$$

$$= \int_0^\infty dt F_2(t),$$

where

$$F_1(t) = (\pi)^{-1/2} \left[\frac{1}{2(t-1+e^{-t})^{1/2}} \times \ln \frac{t^{1/2} + (t-1+e^{-t})^{1/2}}{t^{1/2} - (t-1+e^{-t})^{1/2}} - G(t) \right]$$

$$F_2(t) = \frac{1}{2(\pi)^{1/2}} \left\{ \frac{(e^{t/2}-e^{-t/2})^2}{t-1+e^{-t}} \left[\frac{t^{1/2}}{1-e^{-t}} - \frac{1}{2(t-1+e^{-t})^{1/2}} \times \ln \frac{t^{1/2} + (t-1+e^{-t})^{1/2}}{t^{1/2} - (t-1+e^{-t})^{1/2}} \right] - \frac{e^t - 2}{t-1}[t^{1/2} - G(t)] - \frac{3}{2(t-1)^2} \left[-\frac{t^{1/2}(2t-5)}{3} - G(t) \right] \right\},$$

and

$$G(t) = \frac{1}{(1-t)^{1/2}} \arcsin(1-t)^{1/2}, \qquad (t<1)$$

$$= \frac{1}{2(t-1)^{1/2}} \ln \frac{t^{1/2} + (t-1)^{1/2}}{t^{1/2} - (t-1)^{1/2}}. \qquad (t>1)$$

The results of numerical calculation are as follows:

$$S_1 = 0.611207, \quad S_2 - S_1 = 0.042158.$$

The Eqs. (3.6a) and (3.6b) are not closed since we have unknowns w and g_0' besides d_0, g_0, d_1, and g_1. To facilitate the calculation, we put $w = 0$, and $g_0' = g_1$. Fortunately, the integral which contains w and g_0' is not sensitive to the change of w and g_0', and its magnitude is much smaller than that of other terms. Then Eqs. (3.6a) and (3.6b) are closed equations for g_0 and g_1, respectively. By numerical calculation, we obtain g_0 and g_1 as functions of λ, and also $d_0(\lambda)$ and $d_1(\lambda)$.

IV. RESULTS AND DISCUSSIONS

In Fig. 1 the result of the calculation described in the previous section is shown. The shift of cyclotron-resonance frequency is given by

$$\Delta\omega = [\Delta_1(E_1) - \Delta_0(E_0)]/\hbar = (d_1 - d_0)\Omega_c. \tag{4.1}$$

Along with the present result, the result of a semiclassical calculation, $(\Delta\omega)_{sc}$ is plotted for the sake of comparison. According to the semiclassical theory, the shift of cyclotron-resonance frequency is given by

$$(\Delta\omega)_{sc} = [\Delta E(p_1) - \Delta E(p_0)]/\hbar, \tag{4.2}$$

where $\Delta E(p)$ is the energy shift of the electron of momentum p in the absence of magnetic field, p_0 and p_1 being momenta of electron for the states $N = 0$ and 1, respectively. The second-order energy shift in no magnetic field is given by[9]

$$\Delta E(p) = \tfrac{1}{2}\pi\alpha kT(\hbar/a_B p). \tag{4.3}$$

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[9] Here, we used the result of usual second-order perturbational calculation. Y. Osaka [J. Phys. Soc. Japan **19**, 2347 (1964)] obtained a result just twice as large as that given by Eq. (4.3) by means of the Green-function method, taking account of the simplest self-energy part. If we use Osaka's result, the right-hand side of Eq. (4.3) should be multiplied by 2.

If we take $p_z=0$, we may put $p_0=[2m(\hbar\Omega_c/2)]^{1/2}$ and $p_1=[2m(3\hbar\Omega_c/2)]^{1/2}$. Then we have

$$(\Delta\omega)_{sc}=-\tfrac{1}{2}\pi\alpha kTa_B^{-1}[(3m\hbar\Omega_c)^{-1/2}-(m\hbar\Omega_c)^{-1/2}]$$
$$=-2^{-3/2}\pi(3^{-1/2}-1)\lambda\Omega_c=0.470\lambda\Omega_c. \qquad (4.4)$$

In Baer and Dexter's experiment on cyclotron resonance of electrons in CdS,[2] the temperature is 1.3°K and $\hbar\Omega_c/k$ equals to 2.8°K ($m=0.20m_0$, and $B=4.1$ kG). If we use the values $a_B=25$ Å and $\alpha=0.035$,[5] we obtain $\lambda=0.37$. The present calculation gives 0.10 for the relative shift of cyclotron-resonance frequency, while the semiclassical theory gives 0.17. The latter theory will give a smaller shift when the distribution of electrons in various p_z states is taken into account. These values are in a reasonable agreement with the experimental result. The observed cyclotron mass is anisotropic; the average cyclotron mass is $(0.165\pm0.03)\times m_0$. There is a scatter among the observed values of the band mass; they lie between $0.19m_0$ and $0.21m_0$.[2] Thus the relative shift of resonance frequency seems to be between 0.15 and 0.27. The present calculation gives the shift of the same sign and comparable in magnitude with that obtained by the experiment and the semiclassical argument.

The present result is obtained in the high-temperature approximation (3.3), with which the contribution from the spontaneous emission of phonons is neglected. Larsen calculated this contribution to the shift of the cyclotron-resonance frequency. From his result, we obtain $(\Delta\omega)_{\text{spontaneous}}/\Omega_c=0.02$ for the experiment by Baer and Dexter. This value is small compared with the present result but not negligible, as expected from the ratio of the typical phonon energy (∼0.5°) to the temperature (1.3°K).

The approximation (3.3) implies the elastic-scattering approximation as well as the high-temperature approximation mentioned above. As discussed in Sec. II, the role of the inelasticity in the scattering is expected to be less important than that of the electronic level broadening so long as the typical phonon energy is smaller than the level width. In the example above, the typical phonon energy (∼0.5°K) is smaller than Γ_0 and Γ_1 which are both about 1.2°K.

Next, we compare the present result with that obtained from the second-order perturbational calculation. The latter result is obtained from Eq. (2.2). If we let p_z tend to zero in order to compare with the present result, the shifts diverge, but the difference between the shifts of the $N=0$ and $N=1$ states is finite. We compare the results in Table I for the case of $\lambda=0.37$. In Table I, the contributions to the energy shifts from the states of $N'=0$ and $N'=1$ are shown separately from others. Note that the symbol δ_0 stands for a common positive divergent contribution. We notice that the contributions from the terms $N'=N$ which are positive and divergent in the second-order perturbational calculation, change sign and become finite if we include the level broadening of states. As we mentioned in Sec. II, the contribution from transitions in which the quantum number N does not change, takes a positive value for finite p_z and tends to $+\infty$ as $p_z\to0$ in the second-order perturbation energy. This positive contribution, however, is compensated by a singular negative contribution at $p_z=0$ upon including the level broadening of states, so that the net result becomes negative. This change of the contributions from the terms of $N'=N$ accounts for the change of the sign of the cyclotron-resonance frequency shift.

TABLE I. Energy shifts of Landau levels $\Delta_N(N=0$ and 1) and shift of cyclotron-resonance frequency $(\Delta_1-\Delta_0)/\hbar$, calculated for electrons in CdS[a] at $B=4.1$ kG and $T=1.3$°K.

	Present calculation		Second-order perturbation	
Contributions[b]	$\Delta_0/\hbar\Omega_c$	$\Delta_1/\hbar\Omega_c$	$\Delta_0/\hbar\Omega_c$	$\Delta_1/\hbar\Omega_c$
$N'=0$	-0.121	0.047	δ_0[c]	0.079
$N'=1$	-0.081	-0.084	-0.081	δ_0[c]-0.491
$N'\geq2$	-0.145	-0.210	-0.145	-0.210
Total	-3.347	-0.247	$\delta_0-0.226$	$\delta_0-0.622$
$(\Delta_1-\Delta_0)/\hbar\Omega_c$	$+0.100$		-0.396	

[a] We have used the data $m=0.20m_0$, $(me^2/\hbar^2\kappa)^{-1}=25$ Å, and the square of electromechanical coupling $\alpha=0.035$.

[b] Contributions to the energy shifts which come from mixing of the Landau states $N'=0$, $N'=1$, and $N'\geq2$, are separately shown.

[c] These terms are divergent. But we can subtract a common divergent term, δ_0, from both $\Delta_0/\hbar\Omega_c$ and $\Delta_1/\hbar\Omega_c$.

The dependence of the cyclotron-resonance frequency shift on the temperature and the magnitude of magnetic field is of some interest. The shift depends on the temperature and the magnetic field through the parameter λ. The shift obtained in the present calculation is approximately proportional to $\lambda^{2/3}$ (within 3% error) between $\lambda=0.05$ and 0.8. Since λ is proportional to $TH^{-3/2}$, the present result predicts

$$\Delta\omega/\Omega_c\propto T^{2/3}H^{-1},$$

while the semiclassical result (4.2) which includes the effect of the quantization of orbits semiclassically, gives

$$(\Delta\omega)_{\text{sc}}/\Omega_c\propto TH^{-3/2},$$

and Mahan and Hopfield's result which entirely neglects the quantization effect would give

$$(\Delta\omega)_{MH}/\Omega_c\propto T\langle p^{-3}\rangle_T\propto T^{-1/2},$$

where p is the electron momentum and $\langle\ \rangle_T$ represents the thermal average.

Sawamoto observed the cyclotron resonance of electrons in CdS under a different experimental condition.[1] Unfortunately, the theory for the quantum limit does not seem to apply for his result, since the temperature and the cyclotron-resonance frequency are comparable ($\hbar\omega/kT=1.4$).

In the present calculation, we neglect the dependence of the self-energy on p_z and replace the self-energy by its value at $p_z=0$, assuming that if Γ is large compared with kT, the dependence is not appreciable. Under the condition of Baer and Dexter's experiment, $\Gamma_0(E_0)/k$

TABLE II. The dependence of the self-energy on p_z when the coupling parameter $\lambda=\sqrt{2}(l/a_B)(kT/\hbar\Omega_c)=0.37$. These results are obtained by replacing the self-energy involved in the energy denominator by the self-consistent solution in Sec. III.

$p_z^2/2m\hbar\Omega_c$	$\Delta(0,p_z;E_0)/\hbar\Omega_c$	$\Gamma(0,p_z;E_0)/\hbar\Omega_c$	$\Delta(1,p_z;E_1)/\hbar\Omega_c$	$\Gamma(1,p_zE_1)/\hbar\Omega_c$
0.0	−0.347	0.448	−0.247	0.426
0.23	−0.415	0.369	−0.318	0.364
0.45	−0.435	0.294	−0.342	0.307

($=1.2$°K) and $\Gamma_1(E_1)/k$ ($=1.2$°K) are comparable with the temperature (1.3°K), contrary to the assumption above. To make an estimate of the error introduced by this approximation, we calculate the dependence of the self-energy on p_z in an iterative process. By replacing Σ in the denominator of Eq. (3.4) by the value obtained in the present calculation, we find $\Sigma(N,p_z;E_N)$ for $p_z\neq 0$. The results for $p_z^2/2m=0.23\hbar\Omega_c(\sim\frac{1}{2}kT)$ and 0.45 $\hbar\Omega_c(\sim\Gamma_0)$ are shown in Table II. The dependence on p_z is found far from negligible. We may take account of the dependence on p_z in calculating the cyclotron-resonance frequency shift by replacing Σ in the denominator of Eq. (3.4) by a certain average value of Σ rather than by its value at $p_z=0$. However, the dependence of the cyclotron-resonance frequency shift on the variation of Σ in the energy denominator, is extremely complicated. We cannot hope to determine the appropriate average value to replace Σ in the energy denominator. We arbitrarily assume that the average self-energy is given by the self-energy of a certain representative state. If we use the self-energy for $p_z^2/2m=0.23\hbar\Omega_c$ and $0.45\hbar\Omega_c$ as the average self-energy which replaces Σ in the denominator of Eq. (3.4), the cyclotron-resonance frequency shift practically does not change for both cases compared with the present result described earlier. (If we use the self-energy for $p_z^2/2m=0.23\hbar\Omega_c$ as the average, the shift increases by 1% of the present result; for $p_z^2/2m=0.45\hbar\Omega_c$, the shift increases by 3%.) Although this observation is not decisive, we anticipate that the neglect of the dependence of Σ on p_z does not introduce a serious error.

As seen from Fig. 1, Γ_0 and Γ_1 are fairly large. In fact, they are comparable with the resonance frequency ($\Gamma_0/\hbar\omega$ and $\Gamma_1/\hbar\omega\sim 0.4$ in the example above). These large Γ values raise two questions to be considered.

(1) When Γ is so large that the quasiparticle approximation does not seem to hold, how can we interpret the result obtained above?

The energy obtained from Eq. (3.5) gives the position of the peak of the spectral weight function $A(E)$ if $\Gamma(E)$ varies slowly as a function of E, irrespective of whether the quasiparticle approximation is valid or not. The variation of $\Gamma(E)$ near the peak energy is found very slow. The shape of the absorption curve could be obtained only after working out the calculation of the spectral weight functions for the states of $N=0$ and 1, and the calculation of the oscillator strength which connects these two states. However, we expect that the difference of these peak energies for $N=0$ and 1 will give a good approximate value for the cyclotron-resonance frequency.

(2) How can we observe a sharp resonance line when $\Gamma/\hbar$ is comparable with the resonance frequency?

Baer and Dexter's experimental result shows $\omega\tau\sim 6$, whereas the quantity $\hbar\omega/(\Gamma_0+\Gamma_1)$ is about 1.3. If $(\Gamma_0+\Gamma_1)/\hbar$ would represent the width of the resonance line, the line would be very broad and hardly observable. As pointed out by Saitoh and Kawabata,[10] however, the linewidth is different from the inverse of the lifetime to which the present Γ is related. They showed that to the second order with respect to the perturbation, the expression for the linewidth contains a correction term besides the inverse of the lifetime, and that owing to the presence of the correction term the linewidth is finite whereas the inverse of the lifetime diverges in the second-order perturbational calculation. The situation is analogous to that in the calculation of the conductivity by piezoelectric polarons in the absence of magnetic field. There, in the second-order perturbational calculation, the inverse of the lifetime is divergent; but the inverse of the scattering time contains an extra weighting factor $(1-\cos\theta)$ in its expression (where θ is the deflection angle at the scattering), and is therefore finite. The remarkable difference between the linewidth and the inverse of the lifetime comes from the long-range character of the piezoelectric interaction. It is expected that even to higher orders in the perturbation, the linewidth would be smaller than $(\Gamma_0+\Gamma_1)/\hbar$ on account of the long-range nature of the interaction.

Finally, we discuss the relation between Larsen's calculation of the probability of decay of electronic states[4] and the present calculation of the self-energy. Larsen pointed out that the usual Fermi "Golden-rule" expression for the transition probability per unit time is logarithmically divergent for piezoelectric polarons at finite temperature. He showed that this situation is remedied if one uses a more fundamental expression for the total transition probability of a state [Eq. (21) of Ref. 4]. In this expression, the factor guaranteeing the conservation of energy has a finite width of the order of the energy uncertainty $\hbar/t$, t being the time after the interaction is turned on. The divergence which is the result of replacing the energy conserving factor by a δ function, is removed; the cutoff is given by the energy uncertainty $\hbar/t$. Hence, the rate of change is time-dependent; the amplitude shows a nonexponential decay.

This result is applicable so long as t is much smaller than the lifetime of the state, τ, because in the perturbational calculation the total probability of decay is assumed to be small compared with unity. If we want to discuss the transition probability for $t>\tau$, we must

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[10] M. Saitoh and A. Kawabata, J. Phys. Soc. Japan 23, 1006 (1967).

take into account the broadening of energy levels which is of the order of $\hbar/\tau$. When $t>\tau$, the energy uncertainty $\hbar/t$, becomes smaller than the broadening of energy levels. Hence the cutoff of the logarithmic divergence will be given by $\hbar/\tau$ rather than $\hbar/t$. The decay rate will be time-independent and the amplitude will decay exponentially for a long time.

The time dependence of the amplitude for $t\ll\tau$ is related to the behavior of the self-energy as a function of E in the tail part of the spectral weight function. We can show that when the interaction is sufficiently weak, Larsen's result for the transition probability of the ν state can be obtained from the behavior of the self-energy for $|E-E_\nu^{(0)}|\gg|\Sigma_\nu|$. The value of the self-energy around the peak of the spectral weight function (for $|E-E_N|\lesssim\Gamma$) is irrelevant to the time dependence of the amplitude for $t\ll\tau$.

Thus in terms of the self-energy function, Larsen's calculation for a short-time behavior is related to the behavior of the self-energy function in the tail part of the spectral weight function. On the other hand, the present calculation is concerned with the value of the self-energy function at the peak, which reflects the long-time behavior of the amplitude. Two calculations are not contradictory, but complementary.

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APPENDIX

In this section, we will give definition of the Green functions and their properties used in the text. In the formalism of second quantization, our Hamiltonian (1.1) is rewritten as

$$\begin{aligned}\mathcal{H}_0&=\sum_\nu E^{(0)}(\nu)a_\nu^\dagger a_\nu+\sum_{\mathbf{q}}\hbar sq b_{\mathbf{q}}^\dagger b_{\mathbf{q}},\\ \mathcal{H}_1&=\sum_{\mathbf{q}}\sum_{\nu,\nu'}(4\pi\alpha\hbar^2e^2s^2/\kappa V)^{1/2}(e^{i\mathbf{q}\cdot\mathbf{r}})_{\nu\nu'}a_\nu^\dagger a_{\nu'}\\ &\quad\times(2\hbar sq)^{-1/2}(b_{\mathbf{q}}+b_{-\mathbf{q}}^\dagger),\end{aligned}\tag{A1}$$

where a Greek letter ν stands for a set of quantum numbers (N,p_z,X) and $a_\nu^\dagger$ and a_ν are, respectively, creation and annihilation operators of an electron in a state ν, and

$$(e^{i\mathbf{q}\cdot\mathbf{r}})_{\nu\nu'}=(\nu|e^{i\mathbf{q}\cdot\mathbf{r}}|\nu').\tag{A2}$$

We define the one-particle electron Green function

$$G(\nu,t-t')\equiv-i\langle Ta_\nu(t)a_\nu^\dagger(t')\rangle,\tag{A3}$$

and the phonon Green function

$$\begin{aligned}D(\mathbf{q},t-t')\equiv-i(2\hbar sq)^{-1}\langle T[b_{\mathbf{q}}(+)+b_{-\mathbf{q}}^\dagger(t)]\\ \times[b_{\mathbf{q}}^\dagger(t')+b_{-\mathbf{q}}(t')]\rangle.\end{aligned}\tag{A4}$$

Here t and t' are "imaginary time" variables and T is the Wick time-ordering operator; we used the definition

$$\begin{aligned}\langle A\rangle=\mathrm{Tr}\{\exp[-\beta(\mathcal{H}-\mu N)]A\}/\\ \mathrm{Tr}\exp[-\beta(\mathcal{H}-\mu N)],\end{aligned}\tag{A5}$$

$$N=\sum_\nu a_\nu^\dagger a_\nu,\tag{A6}$$

μ being the chemical potential of an electron.

Noticing the relations

$$G(\nu,-i\beta)=-G(\nu,0)e^{-\beta\mu},\tag{A7}$$

$$D(\mathbf{q},-i\beta)=D(\mathbf{q},0),\tag{A8}$$

we expand G and D in Fourier series:

$$\begin{aligned}G(\nu,t)=(-i\beta)^{-1}\sum_n e^{-i\zeta_nt}G(\nu,\zeta_n),\\ \zeta_n=\mu+(2n+1)\pi(-i\beta)^{-1},\end{aligned}\tag{A9}$$

$$\begin{aligned}D(\mathbf{q},t)=(-i\beta)^{-1}\sum_j e^{-i\omega_jt}D(\mathbf{q},\omega_j),\\ \omega_j=2j\pi(-i\beta)^{-1}.\end{aligned}\tag{A10}$$

If we solve the Dyson equation formally, we obtain the Fourier coefficient of the electron Green function as follows:

$$\begin{aligned}G(\nu,\zeta_n)&=[\zeta_n-E^{(0)}(\nu)-\Sigma(\nu,\zeta_n)]^{-1},\\ \Sigma(\nu,\zeta_n)&=(-i\beta)^{-1}\sum_j\sum_{\mathbf{q}}\sum_{\nu'}G(\nu',\zeta_n-\omega_j)\\ &\quad\times D(\mathbf{q},\omega_j)(4\pi\alpha\hbar^2e^2s^2i/\kappa V)\\ &\quad\times|(e^{i\mathbf{q}\cdot\mathbf{r}})_{\nu\nu'}|^2\Gamma_{\mathbf{q}}(\nu;\nu';\zeta_n,\omega_j),\end{aligned}\tag{A11}$$

where $\Gamma_{\mathbf{q}}$ is the vertex function. We have normalized $\Gamma_{\mathbf{q}}$ so that the lowest-order term is equal to 1.

The quasiparticle energy is determined from the zero of the real part of the denominator of the electron Green function which is analytically continued to the real axis,

$$E-E^{(0)}(\nu)-\mathrm{Re}\Sigma(\nu,E)=0.\tag{A12}$$

This energy gives the position of the peak of the spectral weight function

$$A(\nu,E)=i[G(\nu;E+i\epsilon)-G(\nu;E-i\epsilon)],\tag{A13}$$

when the imaginary part of the self-energy function is a slowly varying function of E near the peak.