

Cyclotron mass of a polaron in two dimensions

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A new calculation of the two-dimensional polaron cyclotron mass, which goes beyond second-order perturbation theory, is presented. The present approach is based on a memory-function formalism and does not rely on a calculation of the Landau levels themselves. A comparison is made with the cyclotron mass obtained from other theories. It is found that the present results are valid for a larger range of electron-phonon coupling constants than are the existing results.

I. INTRODUCTION

Recently¹⁻⁴ there has been interest in the calculation of properties of a two-dimensional (2D) polaron beyond second-order perturbation theory. In the present paper, as in Refs. 1-4, we consider an ideal 2D system in which an electron in a parabolic conduction band interacts with LO phonons. The electron-phonon coupling constant (α) is allowed to have arbitrary values. Such calculations are important, e.g., in order to indicate the range of validity of second-order perturbation theory.

The aim of the present paper is to calculate the cyclotron resonance frequency (or equivalently the cyclotron mass) beyond first order in α in an approximate way. In the existing theories the cyclotron resonance frequency

(ω_c^*) is determined as the difference between the energy of the first (E_1) and the second (E_2) Landau level: $E_2 - E_1 = \hbar\omega_c^*$. The energy of the Landau levels is determined, e.g., by second-order perturbation theory.⁵⁻⁸ The most accurate available treatment is called "improved Wigner-Brillouin perturbation theory" (IWBPT) (Refs. 9 and 10), where the electron-phonon correction ΔE_n to the Landau level E_n has to be calculated self-consistently. Although the calculation is only valid to order α , we recently¹¹ showed in the case of the 3D polaron that the self-consistency induces corrections which are of higher order in α . In 2D a similar conclusion applies as we can demonstrate by solving the self-consistency relation [see Eq. (21) of Ref. 8] for small values of the magnetic field up to order α^2 and found

$$E_n = -\alpha \frac{\pi}{2} \left[1 + \frac{2n+1}{8} \omega_c + \frac{18n(n+1)+1}{128} \omega_c^2 + \frac{5}{1024} (2n+1)[10n(n+1)-1] \omega_c^3 + \dots \right] + \frac{\alpha^2 \pi^2}{32} n \omega_c \left[1 + \frac{3(7n+5)}{16} \omega_c + \frac{1}{64} (97n^2 + 123n + 26) \omega_c^2 + \dots \right], \quad (1)$$

where ω_c is expressed in units of ω_0 and ΔE_n in units of $\hbar\omega_0$ with ω_0 the optical phonon energy. The cyclotron mass can now easily be found ($\omega_c^* = eB/m^*c$)

$$\frac{m^*}{m_b} = 1 + \frac{\alpha\pi}{8} \left(1 + \frac{9}{8} \omega_c + \frac{145}{128} \omega_c^2 + \dots \right) - \frac{\alpha^2 \pi^2}{65} \left(1 + \frac{9}{4} \omega_c + \frac{133}{32} \omega_c^2 + \dots \right) \quad (2)$$

with m_b the electron band mass. Note that the α^2 term gives a negative correction to the polaron mass which is clearly wrong. For example, within the Feynman approximation we know that at zero magnetic field one has² up to order α^2

$$\frac{m^*}{m_b} = 1 + \frac{\pi}{8} \alpha + \frac{\pi^2}{72} \alpha^2. \quad (3)$$

For $\alpha=0.07$ and zero magnetic field IWBPT gives an error of 5% in the polaron correction to the effective mass.

This error increases with increasing α and/or increasing ω_c .

In the present paper we will present a calculation of the 2D polaron cyclotron mass under an approximation that is valid for all values of the electron-phonon coupling strength and for arbitrary values of the magnetic field. The present approximation does not suffer from the above-mentioned inadequacies, i.e., the wrong sign for the α^2 term in the polaron mass. Furthermore, in our approach we do not rely on a calculation of the energy of the Landau levels themselves, but we calculate the cyclotron resonance spectrum which directly gives the cyclotron resonance frequency. The calculation is based on the Feynman polaron model. The calculation itself¹² is a direct generalization of the Feynman-Hellwarth-Iddings-Platzman theory¹³ for the response of a polaron in the case where a magnetic field is present and the polaron motion is limited to two-dimensions. It turns out that the present approach even if limited to second-order perturbation theory is valid for larger values of the electron-phonon coupling constant than is IWBPT.

II. CYCLOTRON RESONANCE

Using the memory-function formalism¹² we find that the cyclotron resonance spectrum is given by

$$\lim_{\epsilon \rightarrow 0} \text{Re} \left[\frac{i}{\omega - \omega_c - \Sigma(\omega + i\epsilon)} \right], \quad (4)$$

where $\Sigma(z)$ is the memory function which is calculated using the Feynman polaron model. This gives

$$\Sigma(z) = \alpha \frac{\sqrt{2\pi}}{8} \frac{1}{z} \int_0^\infty dt (1 - e^{izt}) \text{Im} \left[\frac{(1 + \bar{n})e^{it} + \bar{n}e^{-it}}{[D_H(t)]^{3/2}} \right] \quad (\hbar = m_b = \omega_0 = 1). \quad (5)$$

We introduced the occupation number for the LO phonons $\bar{n} = n(\omega_0) = 1/(e^{\beta\omega_0} - 1)$ and the function ($\beta = 1/kT$)

$$D_H(t) = \sum_{j=1}^3 d_j^2 [1 - e^{is_j t} + 4n(s_j) \sin^2(s_j t/2)], \quad (6)$$

where the frequencies s_j and the constants d_j^2 are given¹⁴ functions of ω_c and of the parameters of the Feynman polaron model (v, w). The latter parameters were determined in Ref. 4 by a variational calculation of the polaron ground-state energy.

In the following we will limit ourselves to the zero-temperature case and to frequencies below the LO-phonon continuum, i.e., $\omega < \omega_0$. For this situation $\text{Im}\Sigma(\omega) = 0$ and the cyclotron resonance spectrum consists of a delta function which is located at the frequency ω_c^* which is determined by the equation

$$\omega_c^* - \omega_c - \text{Re}\Sigma(\omega_c^*) = 0. \quad (7)$$

Under these circumstances, the memory function can be written as

$$\text{Re}\Sigma(\omega) = -\frac{\alpha\sqrt{2\pi}}{4} \int_0^\infty dt \frac{e^{-t} \sinh^2(\omega t/2)}{[D(t)]^{3/2}} \quad (8)$$

with

$$D(t) = \sum_{j=1}^3 d_j^2 (1 - e^{-s_j t}). \quad (9)$$

We have solved Eq. (7) numerically for different values of α and ω_c . The results for the cyclotron mass for a weak electron-phonon coupling constant, i.e., $\alpha = 0.01$, are listed in Table I and are compared with other approaches. The results for RSPT (Rayleigh-Schrödinger perturbation theory), WBPT (Wigner-Brillouin perturbation theory), and IWBPT are obtained from a numerical evaluation of the energy of the first two Landau levels. The results from RSPT and the present approach are very close to each other up to $\omega_c/\omega_0 \approx 0.75$, where the difference due to the polaron correction is 5%. For larger values of the magnetic field the difference starts to increase rapidly. The polaron correction in the IWBPT and the present results differ at most by 3.5%. The WBPT correction for the polaron mass is smaller (for $\omega_c/\omega_0 = 1$ the difference is 17%) than that of the present approximation.

The differences between the various theories become more pronounced for larger values of the electron-phonon

TABLE I. Cyclotron mass for $\alpha = 0.01$ and for different values of the magnetic field. The results of different approaches are given.

ω_c/ω_0	RSPT	WBPT	IWBPT	Present work
0	1.003 94	1.003 82	1.003 94	1.003 94
0.05	1.004 18	1.004 05	1.004 15	1.004 18
0.10	1.004 44	1.004 29	1.004 40	1.004 43
0.15	1.004 73	1.004 56	1.004 68	1.004 72
0.20	1.005 06	1.004 87	1.005 01	1.005 05
0.25	1.005 43	1.005 22	1.005 37	1.005 41
0.30	1.005 86	1.005 61	1.005 79	1.005 84
0.35	1.006 35	1.006 06	1.006 27	1.006 32
0.40	1.006 93	1.006 58	1.006 82	1.006 88
0.45	1.007 61	1.007 20	1.007 48	1.007 55
0.50	1.008 43	1.007 93	1.008 26	1.008 34
0.55	1.009 43	1.008 80	1.009 21	1.009 31
0.60	1.010 68	1.009 88	1.010 38	1.010 50
0.65	1.012 30	1.011 24	1.011 87	1.012 02
0.70	1.014 47	1.012 98	1.013 80	1.014 00
0.75	1.017 52	1.015 30	1.016 41	1.016 68
0.80	1.022 13	1.018 51	1.020 08	1.020 47
0.85	1.029 90	1.023 16	1.025 51	1.026 10
0.90	1.045 81	1.030 28	1.034 00	1.034 95
0.95	1.096 63	1.041 70	1.047 74	1.049 34
1.00		1.060 03	1.069 48	1.072 01

coupling constant as is shown in Fig. 1 for $\alpha = 0.1$ and in Fig. 2 for $\alpha = 1$. Note that for $\omega_c/\omega_0 \lesssim 0.2$ our results are closest to the RSPT results. For $\alpha = 0.1$ the difference between the polaron correction to the effective mass for the IWBPT and for the present result is about 14% when

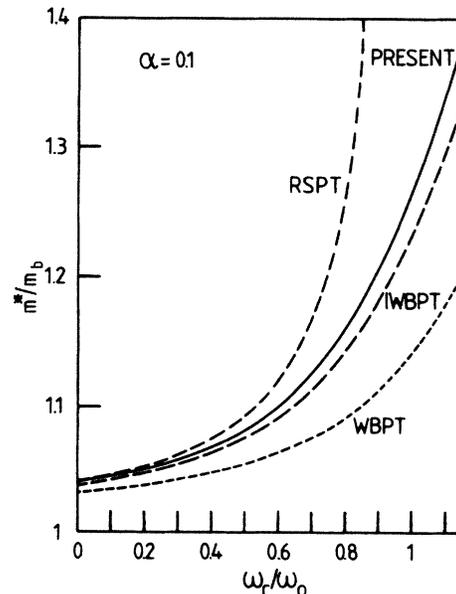


FIG. 1. Cyclotron mass as function of the magnetic field for $\alpha = 0.1$. The present results are compared with (i) RSPT: Rayleigh-Schrödinger perturbation theory, (ii) IWBPT: Improved-Wigner-Brillouin perturbation theory, and (iii) WBPT: Wigner-Brillouin perturbation theory.

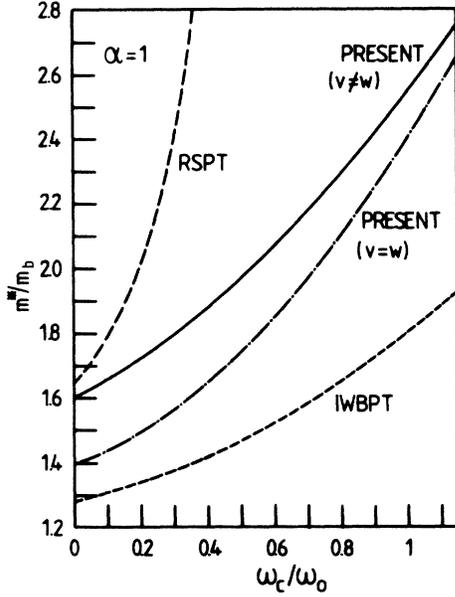


FIG. 2. Same as Fig. 1, but now for $\alpha=1$. The present result with a perturbative (i.e., $v=w$) calculation of the memory function is also presented.

$\omega_c/\omega_0=1$. When $\alpha=1$ this difference is increased to about a factor of 2.

In our calculation we have also considered $v=w$ for the parameters of the Feynman polaron model which is equivalent to a calculation of the memory function $\Sigma(\omega)$ with second-order perturbation theory. For $\alpha=0.1$, the difference with our original calculation (i.e., where $v \neq w$ and v and w are determined by a variational calculation of the polaron ground-state energy) is too small to be seen on the scale of Fig. 1.

In the limit of zero magnetic field the present result for the cyclotron resonance spectrum reduces to the result for the optical absorption as calculated using the FHIP theory.¹³ Consequently the cyclotron mass should reduce to the Feynman polaron mass in this limit. In order to calculate the magnetic field correction to the polaron mass (3) for $\alpha \ll 1$ and $\omega_c/\omega_0 \ll 1$ we expanded Eq. (8) for low frequencies

$$\begin{aligned} \text{Re}\Sigma(\omega) = & -\alpha \frac{\pi}{8} \omega \left[\left[1 + \frac{\pi\alpha}{9} \right] + \omega_c \frac{9}{8} \left[1 + \frac{31}{1944} \pi\alpha \right] \right. \\ & \left. + \omega_c^2 \frac{105}{128} \left[1 - \frac{25147}{34020} \pi\alpha \right] + \dots \right] \\ & - \frac{5\alpha\pi}{128} \omega^3 \left[\left[1 + \frac{209}{1440} \pi\alpha \right] + \dots \right] + \dots, \end{aligned} \quad (10)$$

where use was made of the results for the variational parameters v, w as derived in the Appendix. Inserting this expansion into Eq. (7) the following expression for the cy-

clotron mass of the 2D polaron is found:

$$\begin{aligned} \frac{m^*}{m_b} = & 1 + \frac{\alpha}{8} \left[1 + \frac{9}{8} \omega_c + \frac{145}{128} \omega_c^2 \right] \\ & + \frac{\alpha^2 \pi^2}{72} \left[1 + \frac{31}{192} \omega_c - \frac{13253}{2304} \omega_c^2 \right], \end{aligned} \quad (11)$$

which should be compared with Eq. (2). Note that Eq. (11) has a positive α^2 correction to the polaron mass when $\omega_c/\omega_0 \ll 1$.

Let us consider the memory function within second-order perturbation theory, i.e., $v=w$ and consequently $s_1=\omega_c$, $s_2=s_3=v$, $d_1^2=\frac{1}{2}\omega_c$, $d_2^2=d_3^2=0$. A small magnetic field and small frequency expansion gives

$$\text{Re}\Sigma(\omega) = -\alpha \frac{\pi}{8} \omega \left[1 + \frac{9}{8} \omega_c + \frac{5}{16} \left[\omega^2 + \frac{21}{8} \omega_c^2 \right] + \dots \right] \quad (12)$$

from which we get the cyclotron mass

$$\begin{aligned} \frac{m^*}{m_b} = & 1 + \alpha \frac{\pi}{8} \left[1 + \frac{9}{8} \omega_c + \frac{145}{128} \omega_c^2 + \dots \right] \\ & - \alpha^2 \frac{5\pi^2}{512} \omega_c^2 + \dots \end{aligned} \quad (13)$$

Note that for zero magnetic field $m^*/m_b = 1 + \alpha\pi/8$ and the second-order perturbation version for the memory-function formalism does not induce any α^2 -correction terms into the cyclotron mass. This is the reason why the present approach, even for $v=w$, is superior to IWBPT.

III. CONCLUSION

First we will discuss the main difference between the present approach of calculating the cyclotron frequency and the more conventional approaches based on WBPT or IWBPT. For convenience we take $v=w$ in our expression.^{7,8} In the present calculation the cyclotron frequency is determined by the equation $\omega - \omega_c - \text{Re}\Sigma(\omega) = 0$. For zero polaron coupling $\text{Re}\Sigma(\omega) = 0$ and the cyclotron frequency becomes $\omega = \omega_c^* = \omega_c$. In the presence of electron-phonon coupling $\text{Re}\Sigma(\omega_c^*)$ gives the shift of the cyclotron frequency due to the electron-phonon interaction, i.e., $\omega_c^* = \omega_c + \text{Re}\Sigma(\omega_c^*)$. Consequently our approach amounts to a perturbative calculation of the *shift in the cyclotron frequency*. This is in contrast with WBPT or IWBPT where the *shift in energy of the Landau levels* is calculated perturbatively, i.e., $E_n = \hbar\omega_c(n + \frac{1}{2}) + \Delta E_n$. From it the cyclotron frequency is then derived, $\omega_c^* = (E_1 - E_0)/\hbar$.

In the zero magnetic field limit the present results reduce to the Feynman polaron mass. The latter one provides a good approximation to m^* for all electron-phonon coupling strengths. Because our calculation is a direct generalization to the Feynman polaron theory¹⁵ one may expect (although there is no proof) that the present theory gives a good approximation for magnetic fields at least up to $\omega_c \simeq \omega_0$ and for all values of α . This is in contrast to the IWBPT results which are inaccurate for $\alpha > 0.1$ due to the fact that they lead to an α^2 correction which has the

wrong sign. Note, however, that up to order α and for small magnetic fields IWBPT and the present calculation give exactly the same results.

At this moment there are no two-dimensional electron systems which are embedded in a strongly polar semiconductor. Therefore, at present the present results have a limited practical applicability. We expect that for $\alpha \geq 0.1$ the differences between IWBPT and the present approach will become important.

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APPENDIX

In this Appendix we calculate the nonperturbative corrections to the ground-state energy (E) of the 2D polaron. In particular, we will calculate E up to order α^2 within the Feynman polaron model. Recently the present

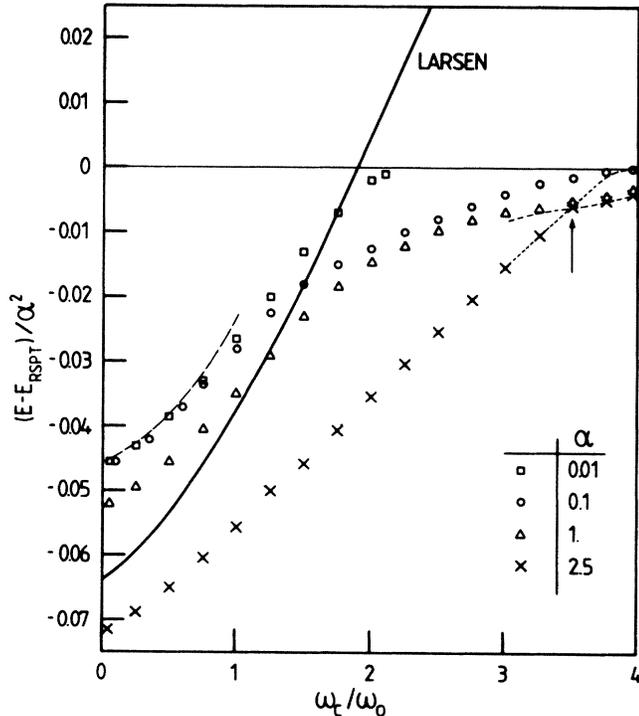


FIG. 3. Difference between the Feynman polaron ground-state energy (E) and the result from second-order perturbation theory (E_{RSPT}) vs the magnetic field for different values of the electron-phonon coupling constant. Larsen's fourth-order perturbation result, i.e., $\alpha \rightarrow 0$, for the 2D polaron ground-state energy is also given (solid curve).

authors applied⁴ an earlier extension¹⁴ of the Feynman polaron theory to nonzero magnetic field, to the case of a 2D polaron. In such a theory two parameters (v, w) are present which were obtained variationally. These parameters are needed in Sec. II and will be determined up to order α for weak magnetic fields, i.e., $\omega_c \ll \omega_0$. Recently Larsen³ has questioned the variational character of the Feynman polaron model for magnetic fields such that $\omega_c/\omega_0 \geq 1.9$. In the present work we limit ourselves to $\omega_c/\omega_0 < 1.2$.

For weak electron-phonon coupling v and w are nearly equal and we have $w = v(1 - \epsilon)$ with ϵ positive and of the order of α . Expanding the ground-state energy to order α^2 for weak magnetic fields results in

$$E = \frac{\omega_c}{2} - \frac{\pi}{2} \alpha \left[1 + \frac{\omega_c}{8} + \frac{\omega_c^2}{128} \right] + \Delta E \quad (\text{A1})$$

with

$$\Delta E = a\epsilon^2 - b\epsilon \quad (\text{A2})$$

of order α^2 and

$$a = \frac{v}{2} \left[1 - 4 \frac{\omega_c}{v} + 9 \frac{\omega_c^2}{v^2} \right], \quad (\text{A3})$$

$$b = \frac{\pi}{2} \alpha \left\{ \left[1 - \frac{2}{v} (\sqrt{1+v} - 1) \right] - \frac{\omega_c}{8} \left[1 + \frac{6}{v} \left[1 - \frac{1}{\sqrt{1+v}} \right] \right] + \omega_c^2 \left[\frac{3}{v^2} - \frac{3}{8} - \frac{6}{v^3} (\sqrt{1+v} - 1) + \frac{1}{8v} \left[1 - \frac{1}{(1+v)^{3/2}} \right] \right] \right\}. \quad (\text{A4})$$

The term of order α in Eq. (A1) was already obtained in Ref. 8. Minimizing E gives $\epsilon = b/2a$ and the correction to E to second order in α become $\Delta E = b^2/4a$. In the limit $\alpha \rightarrow 0$ and $\omega_c \rightarrow 0$ the energy minimum is obtained for $v=3$ and consequently

$$\epsilon = \frac{\pi \alpha}{18} \left[1 + \frac{7}{12} \omega_c + \frac{265}{576} \omega_c^2 + \dots \right] \quad (\text{A5})$$

which gives

$$\Delta E = \frac{\pi^2 \alpha^2}{216} \left[1 - \frac{\omega_c}{6} - \frac{367}{1152} \omega_c^2 + \dots \right]. \quad (\text{A6})$$

Note that the coefficient of the α^2 term at $\omega_c=0$: $\pi^2/216=0.04569$ differs with 28% from the exact result 0.06397 which was obtained earlier by the present authors.² In Fig. 3 we show the nonperturbative correction to the ground-state energy divided by α^2 as a function of the magnetic field for different values of the electron-phonon coupling constant as obtained with the Feynman approximation of Ref. 2. For $\alpha \rightarrow 0$ the result should reduce to the full curve as was recently calculated by Larsen³ with the use of fourth-order perturbation theory.

The dashed line in Fig. 3 gives the limiting behavior as represented by Eq. (A6).

Note that for $\omega_c/\omega_0 < 1$ our result and the exact result of Larsen have a similar qualitative behavior as a function of the magnetic field, although our result is 28% off the exact result for $\omega_c = 0$. With increasing electron-phonon coupling strength α corrections to E of order α^n with $n = 3, 4, \dots$, which are not incorporated in Larsen's calculation, become more and more important. In the limit of large magnetic fields we found $v/w \rightarrow 1$ and the E obtained within the Feynman approximation approaches the result of second-order perturbation theory and consequently $E - E_{\text{RSPT}} \approx 0$. Within our approach $E - E_{\text{RSPT}}$ can never become positive because $E < E_{\text{RSPT}}$. Note also that for $\alpha = 2.5$ the ground-state energy exhibits a discontinuity for $\omega_c/\omega_0 \approx 3.5$. The nature of this discontinuity was examined in Refs. 14 and 2.

Finally we remark that from the above results we are able to define a model mass

$$M = \left(\frac{v}{w} \right)^2 = 1 + \frac{\pi\alpha}{9} \left[1 + \frac{7}{12}\omega_c + \frac{265}{576}\omega_c^2 + \dots \right] + \dots \quad (\text{A7})$$

which in the $\alpha \ll 1$ and $\omega_c/\omega_0 \ll 1$ limit is slightly different from the cyclotron mass. The ground-state energy enables us to define a magnetic mass¹⁶ by noting

$$E = E(\omega_c = 0) + \frac{\omega_c}{2m_H} \quad (\text{A8})$$

which results in

$$\frac{m_H}{m_b} = 1 + \frac{\pi\alpha}{8} + \frac{73\pi^2}{5184}\alpha^2, \quad (\text{A9})$$

where $E(\omega_c = 0) = -\pi\alpha/2 - \pi^2\alpha^2/216$. The coefficient of the α^2 term $73\pi^2/5184 = 0.13898$ differs with 1.4% from the Feynman mass result [Eq. (11)] $\pi^2/72 = 0.13708$.

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