Cyclotron resonance in uniaxial polar crystals with complex structure

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Using a variational approach, the energy spectrum of the optical polaron in a uniaxial crystal with complex structure, placed in a weak dc magnetic field directed along the optical axis is obtained. In performing the minimization of the system energy, the mean of the z component of the total angular momentum is considered as a constraint. The obtained expression of both the cyclotron mass and the effective mass of motion along the direction of the magnetic field are used to discuss the results of the cyclotron resonance experiment performed in the layered compound α-HgI_2. [S0163-1829(98)06306-1]

I. INTRODUCTION

In order to assure a theoretical basis for the analysis of the cyclotron resonance phenomenon in polar crystals, a lot of work[1–6] concerning the energy spectrum of the polaron in magnetic field, for the cases of weak, intermediate, and strong coupling has been done.

Excluding the paper of Larsen,[7] in which the cyclotron resonance of polarons in ellipsoidal bands is discussed in the context of the Haga approximation, all other theoretical studies deal with isotropic systems.

Suitable to analyze the cyclotron resonance of holes in some cubic polar insulators having a multivalley valence band, the results obtained by Larsen do not apply to the case of a uniaxial crystal with a complex structure due to the presence of supplemental sources of anisotropy that are contained in both the electron-optical phonon interaction and the frequencies of the phononic modes. Though there are few papers[8–10] devoted to the problem of the energy spectrum of anisotropic optical polaron in uniaxial crystals in the absence of the magnetic field, a model discussing the cyclotron resonance in such an anisotropic system, taking into account all sources of anisotropy, is still missing.

The studies of the cyclotron resonance in layered crystals HgI_2 (Refs. 11 and 12) and InSe (Ref. 13) deal with the anisotropic features of the system in a simplified manner, either considering the corresponding Fröhlich Hamiltonian restricted to the one oscillator model,[8] or introducing two anisotropic polaron coupling constants[13] $\alpha_\perp$ and $\alpha_\parallel$ for motions perpendicular, respectively, parallel to the optical axis. In the second approach the forms of $\alpha_\perp$ and $\alpha_\parallel$ are not entirely based on the anisotropic properties of the system.

In this paper, based on the idea used by Evrard, Kartheuser, and Devreese (EKD)[14] to exploit the existence of the constants of motion induced by the symmetry of the problem, we develop a variational approach strongly related to the one of Lee, Low, and Pines,[15] allowing a discussion of the cyclotron resonance for the magnetic field directed along the optical axis of a polar crystal with complex structure. This peculiar geometry permits us to treat the z component of the total angular momentum as a constant of motion as EKD[14] have considered it for an isotropic system.

It is in our intention to observe what happens to the energy of an anisotropic optical polaron of a crystal with complex structure in the range of weak magnetic fields, obtaining both the form of the cyclotron mass and the form of the effective mass for motion along the direction of the magnetic field.

II. THE HAMILTONIAN

In the absence of the magnetic field and with the z axis of the trihedron directed along the optical axis of the crystal, the form of the Hamiltonian of the system is[9]

$$H_F=\frac{p_z^2}{2m_\parallel}+\frac{p_\perp^2}{2m_\perp}+\sum_{\mathbf{q},\mu}\hbar\omega_\mu(\mathbf{q})b_{\mathbf{q},\mu}^{+}b_{\mathbf{q},\mu}+\sum_{\mathbf{q},\mu}\left[\frac{V_\mu(\mathbf{q})}{\sqrt{V}}\,b_{\mathbf{q},\mu}e^{i\mathbf{q}\cdot\mathbf{r}}+\text{H.c.}\right], \tag{1}$$

where $m_\parallel$, $m_\perp$, and $\omega_\mu(\mathbf{q})$ are the components of the diagonal mass tensor for the conduction ''bare'' electron and the frequencies of the ''true'' normal phononic modes, respectively; the symbols $\parallel$ and $\perp$ correspond to a direction that is either parallel or orthogonal to the optical axis. The concrete form of the coupling constant $V_\mu(\mathbf{q})$, suitable for anisotropic crystals with complex structure, was obtained by Toyozawa.[16]

To preserve the axial character of the problem's symmetry, an important point of subsequent developments, the external dc magnetic field $\mathbf{B}_0$ will be assumed directed along the optical axis.

Considering the problem of the electron magnetic-field interaction in the symmetrical Coulomb gauge, we shall introduce the operators (A,A^+) and (B,B^+) related to those considered in Ref. 17 by the equations

$$A=(2\hbar m_\perp\Omega)^{-1/2}\Pi, \tag{2a}$$

$$B=\left(\frac{2\hbar}{m_\perp\Omega}\right)^{1/2}X_+, \tag{2b}$$

where, by $\Omega=(eB_0/m_\perp)$ we have denoted the cyclotron frequency of the ''bare'' electron.

Using these operators that verify the following commutation relations: $[A,A^+]=[B,B^+]=1$ and $[A,B]=[A,B^+]$

$=0$, both, the electronic contributions to the Hamiltonian and to the z component of the angular momentum have the expressions

$$H_e=\frac{p_z^2}{2m_\parallel}+\hbar\Omega(A^+A+\tfrac{1}{2}), \tag{3}$$

$$L_{e,z}=\hbar(A^+A-B^+B). \tag{4}$$

According to EKD,[14] we shall consider the following constants of motion: the z component of the total momentum

$$\hat{P}_Z=p_z+\sum_{\mathbf{q},\mu}\hbar q_z b^+_{\mathbf{q},\mu}b_{\mathbf{q},\mu}, \tag{5}$$

and the z component of the total angular momentum

$$L_Z=L_{e,Z}+i\hbar\sum_{\mu,\mathbf{q},\mathbf{q}'}b^+_{\mathbf{q},\mu}b_{\mathbf{q},\mu}\frac{\partial}{\partial\varphi'}\left[\frac{1}{V}\int d\mathbf{r}e^{i\mathbf{r}\cdot(\mathbf{q}'-\mathbf{q})}\right], \tag{6}$$

where the expression of the contribution of the optical phonons to the z component of the total angular momentum diagonal in μ index is obtained as a generalization of the form presented by EKD.[14] In the expression (6), φ' is the azimuthal angle in the $\mathbf{q}'$ space.

III. THE VARIATIONAL APPROACH OF THE POLARON PROBLEM

We shall apply the LLP[15] theory, suitable to discuss the polaron problem for the intermediate coupling range, to our anisotropic system in the presence of the magnetic field.

In order to eliminate the electronic coordinates from the Hamiltonian, according to Ref. 15, we introduce the following unitary transformation:

$$S=S_Z S_\perp, \tag{7}$$

where

$$S_Z=\exp\left[\frac{i}{\hbar}\left(P_Z-\sum_{\mathbf{q},\mu}\hbar q_z b^+_{\mathbf{q},\mu}b_{\mathbf{q},\mu}\right)z\right] \tag{8}$$

and

$$S_\perp=\exp\left[-\frac{i}{\hbar}\sum_{\mathbf{q},\mu}\hbar(xq_x+yq_y)b^+_{\mathbf{q},\mu}b_{\mathbf{q},\mu}\right], \tag{9}$$

P_Z, being the eigenvalue of the operator $\hat{P}_Z$. Taking into account the possibility of replacing the electron coordinates x and y by the operators A and B, for the transformed Hamiltonian S^+HS one obtains the form

$$\begin{aligned}\widetilde{H}\equiv S^+HS=&\frac{1}{2m_\parallel}\left(P_Z-\sum_{\mathbf{q},\mu}\hbar q_z b^+_{\mathbf{q},\mu}b_{\mathbf{q},\mu}\right)^2\\&+\hbar\Omega\left[A^+-\left(\frac{\hbar}{2m_\perp\Omega}\right)^{1/2}\sum_{\mathbf{q},\mu}q_+b^+_{\mathbf{q},\mu}b_{\mathbf{q},\mu}\right]\\&\times\left[A-\left(\frac{\hbar}{2m_\perp\Omega}\right)^{1/2}\sum_{\mathbf{q},\mu}q_-b^+_{\mathbf{q},\mu}b_{\mathbf{q},\mu}\right]\\&+\frac{\hbar\Omega}{2}+\sum_{\mathbf{q},\mu}\hbar\omega_\mu(\mathbf{q})b^+_{\mathbf{q},\mu}b_{\mathbf{q},\mu}\\&+\sum_{\mathbf{q},\mu}\left[\frac{V_\mu(\mathbf{q})}{\sqrt{V}}b_{\mathbf{q},\mu}+\frac{V^*_\mu(\mathbf{q})}{\sqrt{V}}b^+_{\mathbf{q},\mu}\right],\end{aligned} \tag{10}$$

provided that $p_Z=0$, where

$$q_\pm=q_x\pm iq_y. \tag{11}$$

It is our intention to treat on the same basis the electron in magnetic field and the system of optical phonons. In this respect, the trial state is chosen of coherent[15,17] type

$$|\{g\}\rangle=|\xi,\zeta\rangle\otimes\Pi_{\mathbf{q},\mu}|f_\mu(\mathbf{q})\rangle, \tag{12}$$

where $|\xi,\zeta\rangle$ and $|f_\mu(\mathbf{q})\rangle$ are eigenstates of the operators A, B, and $b_\mu(\mathbf{q})$, respectively.

These states are obtained by acting with the displacement operators $D_A(\xi)$, $D_B(\zeta)$, and $D[f_\mu(\mathbf{q})]$ on the fundamental states of the oscillators, $|0,0\rangle_e$ (the fundamental state of the ''bare'' electron in magnetic field with zero value of z component of angular momentum) and $|0\rangle_{\mathrm{ph}}$ (the phonon vacuum state).

Because a coherent state of an electron in magnetic field[17] is obtained as a superposition of many states with different Landau quantum number n, the expression of the energy spectrum of the polaron that we intend to obtain will be correct in the limit

$$\Omega\to 0 \quad \text{with} \quad n\Omega=\text{const}, \tag{13}$$

allowing a proper treatment of cyclotron resonance phenomenon. Thus, we shall disregard, from the beginning, the constant $\hbar\Omega/2$ in the transformed Hamiltonian, such a choice affecting only the origin of the energy scale and consequently, the expression of the ground-state energy. By comparing our expression of the polaron energy spectrum, reduced to the isotropic case and in the limit of weak magnetic field, with the first order in Ω term of the relation (33) of Ref. 1, in this limit of accuracy, the origin of the energy scale can be established.

Taking into account the effect of the canonical transformations of the displaced-oscillators form on the operators A, B, and $b_{\mathbf{q}\mu}$,

$$D_A^{-1}(\xi)AD_A(\xi)=A+\xi, \tag{14}$$

$$D_B^{-1}(\zeta)BD_B(\zeta)=B+\zeta, \tag{15}$$

$$D^{-1}[f_\mu(\mathbf{q})]b_{\mathbf{q},\mu}D[f_\mu(\mathbf{q})]=b_{\mathbf{q},\mu}+f_\mu(\mathbf{q}), \tag{16}$$

the energy of the polaron that should be minimized has the expression

$$E(\xi,\{f_\mu(\mathbf{q})\})=\langle\{g\}|\widetilde{H}|\{g\}\rangle=\frac{P_Z^2}{2m_\parallel}+\hbar\sum_{\mathbf{q},\mu}\left[\omega_\mu(\mathbf{q})-\frac{P_Z q_z}{m_\parallel}+\frac{\hbar}{2}\left(\frac{q_Z^2}{m_\parallel}+\frac{q_\perp^2}{m_\perp}\right)\right]|f_\mu(\mathbf{q})|^2+\frac{\hbar^2}{2m_\parallel}\sum_{\substack{\mathbf{q},\mathbf{q}'\\ \mu,\mu'}} q'_Z q_Z |f_{\mu'}(\mathbf{q}')|^2|f_\mu(\mathbf{q})|^2$$
$$+\sum_{\mathbf{q},\mu}\left[\frac{V_\mu(\mathbf{q})}{\sqrt{V}}f_\mu(\mathbf{q})+\frac{V_\mu^*(\mathbf{q})}{\sqrt{V}}f_\mu^*(\mathbf{q})\right]+\hbar\Omega\Bigg\{|\xi|^2-\xi\left[\frac{\hbar}{2m_\perp\Omega}\right]^{1/2}\sum_{\mathbf{q},\mu}q_+|f_\mu(\mathbf{q})|^2$$
$$-\xi^*\left[\frac{\hbar}{2m_\perp\Omega}\right]^{1/2}\sum_{\mathbf{q},\mu}q_-|f_\mu(\mathbf{q})|^2+\left[\frac{\hbar}{2m_\perp\Omega}\right]\sum_{\substack{\mathbf{q},\mathbf{q}'\\ \mu,\mu'}}q_+q'_-|f_\mu(\mathbf{q})|^2\cdot|f_{\mu'}(\mathbf{q}')|^2\Bigg\}. \tag{17}$$

The minimizing procedure will be performed considering the mean of the z component of the total angular momentum over the same state $S|\{g\}\rangle$, as a constraint.

With the expressions (4) and (6) of the two contributions of the z component of the total angular momentum, and after a lengthy but straightforward calculation, the form of this mean value has been obtained:

$$\frac{L_Z}{\hbar}=\langle\{g\}|S^+\frac{L_Z}{\hbar}S|\{g\}\rangle=|\xi|^2-|\zeta|^2-i\sum_{\mathbf{q},\mu}f_\mu^*(\mathbf{q})\frac{\partial f_\mu(\mathbf{q})}{\partial\varphi}. \tag{18}$$

As an intermediate result a set of equations for the variational parameters ξ, ζ, and $f_\mu(\mathbf{q})$ is obtained. The form of the equation for $f_\mu(\mathbf{q})$ is a generalization of the usual expression (25) of Ref. 15 permitting the introduction of the magnetic field into the problem. To work out the problem of the polaron energy we have to solve the equation for $f_\mu(\mathbf{q})$, and find out the dependencies of the variational parameters on P_Z and L_Z to obtain the final form of the polaron energy $E(P_Z,L_Z)$.

IV. WEAK MAGNETIC FIELD

In the following, we shall consider the case of weak magnetic-field range $(\Omega/\omega_\mu(\theta)\ll 1)$ and low values of $P_Z\{P_Z\ll[2\hbar m_\parallel\omega_\mu(\theta)]^{1/2}\}$.

In this case, it is a matter of calculation to see that simplifying the expression (18) to

$$L_z/\hbar\approx|\xi|^2, \tag{19}$$

the correct form of the polaron energy spectrum, including the terms of type $(\Omega/\omega_\mu)^2$, $P_z^2/2\hbar m_\parallel\omega_\mu$ and $P_z^2/2\hbar m_\parallel\omega_\mu(\Omega/\omega_\mu)$, is obtained.

If the trial state had been an eigenstate of the corresponding operator, the mean value of the z component of the angular momentum L_z would have been of the form $\hbar n$, n integer. Unfortunately, this is not the case, so that in the following we shall take only approximately

$$L_z\approx\hbar(n+\varepsilon), \tag{20}$$

where ε lies between 0 and 1 and with $n\geqslant 0$ as a result of Eq. (19).

The final form of the energy spectrum of an anisotropic polaron is obtained:

$$\frac{E(P_z,n)}{\hbar}=-\sum_\mu\langle\alpha_\mu(\theta)\omega_\mu(\theta)\rangle+(n+\varepsilon)\Omega A_\perp^{-1}-\frac{9}{64}\nu^2\Omega^2(n+\varepsilon)^2A_\perp^{-4}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\sin^4\theta}{\omega_\mu(\theta)s^2(\theta)}\right\rangle+\frac{P_z^2}{2\hbar m_\parallel}\left[A_\parallel^{-1}-\frac{9}{8}\nu\Omega(n+\varepsilon)A_\perp^{-2}A_\parallel^{-2}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\sin^2\theta\cos^2\theta}{\omega_\mu(\theta)s^2(\theta)}\right\rangle\right], \tag{21}$$

where

$$A_\perp=1+\frac{\nu}{4}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\sin^2\theta}{s(\theta)}\right\rangle \tag{22}$$

and

$$A_\parallel=1+\frac{1}{2}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\cos^2\theta}{s(\theta)}\right\rangle, \tag{23}$$

ν being the anisotropic mass ratio $\nu=m_\parallel/m_\perp$ for the ''bare'' electron. In the above expressions we denote by $\alpha_\mu(\theta)$ the Fröhlich's dimensionless coupling constant[10] corresponding to the phononic branch μ and by $s(\theta)$ the expression $\cos^2\theta+\nu\sin^2\theta$, the symbol $\langle\,\rangle$ meaning an angular average

$$\langle f(\theta)\rangle=\frac{1}{2}\int_0^\pi f(\theta)\sin(\theta)d\theta. \tag{24}$$

In the case of an isotropic crystal with simple structure, the expression (21) of the polaron energy is reduced to the result

$$\frac{E_{\mathrm{is}}(P_z,n)}{\hbar\omega}=-\alpha+(n+\varepsilon)\beta\frac{\Omega}{\omega}-\frac{3}{40}(n+\varepsilon)^2\alpha\beta^4\left(\frac{\Omega}{\omega}\right)^2+\frac{P_Z^2}{2m\hbar\omega}\left[\beta-\frac{3}{20}(n+\varepsilon)\alpha\beta^4\frac{\Omega}{\omega}\right], \tag{25}$$

where ω is the optical phonon frequency and β is the combination $(1+\alpha/6)^{-1}$. This expression is an extension to the intermediate coupling range of the result obtained by Bajaj.[3]

In the limit of small Ω, by choosing $\varepsilon=\frac{1}{2}$, the form of the ground-state energy of Eq. (25) is

$$\frac{E_{\rm is}(0,0)}{\hbar\omega}=-\alpha+\frac{1}{2}\beta\frac{\Omega}{\omega}, \tag{26}$$

also obtained, in the same order in Ω, from the expression (33) of Ref. 1.

The choice of the trial state (12) prevents us from obtaining, in the second order in Ω, the correct contribution to the ground-state energy. However, what is important in the study of cyclotron resonance, the energy difference between two consecutive levels has the same expression,

$$\frac{E_{\rm is}(P_z,n+1)-E_{\rm is}(P_Z,n)}{\hbar\omega}=\beta\frac{\Omega}{\omega}-\frac{3}{20}(n+1)\alpha\beta^4\left(\frac{\Omega}{\omega}\right)^2-\frac{3}{20}\alpha\beta^4\frac{\Omega}{\omega}\frac{P_Z^2}{2m\hbar\omega}, \tag{27}$$

whatever the form, either Eq. (25) of our work or Eq. (33) of Ref. 1 would be used.

As was stated by Larsen,[1] for the weak-coupling limit of the energy difference between the ground state and the first excited magnetic state on obtains the value

$$\left(1-\frac{\alpha}{6}\right)\frac{\Omega}{\omega}-\frac{3}{20}\left(\frac{\Omega}{\omega}\right)^2\alpha, \tag{28}$$

also found in the frame of the perturbation theory.

According to Refs. 1 and 18, the isotropic form (25) of the polaron energy spectrum in the magnetic field, for $\varepsilon=\frac{1}{2}$, can be obtained[19] from the solution

$$E_{\rm is}(P)/\hbar\omega=-\alpha+\beta\frac{P^2}{2m\hbar\omega}-\frac{3}{40}\alpha\beta^4\left(\frac{P^2}{2m\hbar\omega}\right)^2, \tag{29}$$

found in the absence of the magnetic field, $(n+\frac{1}{2})\hbar\Omega+P_z^2/2m$ replacing $P^2/2m$ everywhere.

A similar correspondence between the two polaron energy spectra (i.e., in the absence or in the presence of the magnetic field) also holds for the case of anisotropic uniaxial crystal.

Thus extending the expression[10] of the polaron energy in uniaxial crystal in the absence of the magnetic field by including also the terms of fourth order in P one obtains

$$E^{(4)}(P_\parallel,P_\perp)=E^{(2)}(P_\parallel,P_\perp)+J_\parallel^{(2)}\left(\frac{P_\parallel^2}{2m_\parallel}\right)^2+J_\perp^{(2)}\left(\frac{P_\perp^2}{2m_\perp}\right)^2+J_{\parallel,\perp}^{(1)}\left(\frac{P_\parallel^2}{2m_\parallel}\right)\left(\frac{P_\perp^2}{2m_\perp}\right), \tag{30}$$

where the coefficients J have the forms

$$J_\parallel^{(2)}=-\frac{3}{8}A_\parallel^{-4}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\cos^4\theta}{\hbar\omega_\mu(\theta)s^2(\theta)}\right\rangle, \tag{31a}$$

$$J_\perp^{(2)}=-\left(\frac{3}{8}\right)^2\nu^2A_\perp^{-4}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\sin^4\theta}{\hbar\omega_\mu(\theta)s^2(\theta)}\right\rangle, \tag{31b}$$

$$J_{\parallel,\perp}^{(1)}=-\frac{9}{8}\nu A_\parallel^{-2}A_\perp^{-2}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\sin^2\theta\cos^2\theta}{\hbar\omega_\mu(\theta)s^2(\theta)}\right\rangle, \tag{31c}$$

and

$$E^{(2)}(P_\parallel,P_\perp)=-\sum_\mu\hbar\langle\alpha_\mu(\theta)\omega_\mu(\theta)\rangle+\frac{P_\parallel^2}{2m_\parallel A_\parallel}+\frac{P_\perp^2}{2m_\perp A_\perp}. \tag{32}$$

Now it is obvious that the form (21) of the energy spectrum of an uniaxial polaron in a magnetic field, written for $\varepsilon=\frac{1}{2}$, can be obtained from the relation (30) by substituting $P_z^2/2m_\parallel$ and $\hbar\Omega(n+\frac{1}{2})$ for $P_\parallel^2/2m_\parallel$ and $P_\perp^2/2m_\perp$, respectively. Thus one can obtain both the cyclotron mass M_c^*, defined through the energy difference between two consecutive polaron levels, usually taken at $P_z=0$,

$$\frac{m_\perp}{M_C^*}=A_\perp^{-1}-\frac{9}{32}\nu^2(n+1)\Omega A_\perp^{-4}\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\sin^4\theta}{\omega_\mu(\theta)s^2\theta}\right\rangle \tag{33}$$

and the effective mass of motion along the direction of the magnetic field $M_\parallel$,

$$\frac{m_\parallel}{M_\parallel}=A_\parallel^{-1}-\frac{9}{8}\nu\left(n+\frac{1}{2}\right)\Omega A_\perp^{-2}A_\parallel^{-2}\times\sum_\mu\left\langle\frac{\alpha_\mu(\theta)\sin^2\theta\cos^2\theta}{\omega_\mu(\theta)s^2\theta}\right\rangle. \tag{34}$$

Just like in the case of an isotropic crystal, when at very weak magnetic fields the value of the polaron mass[1] is obtained for both the cyclotron mass and the effective mass of the motion along the direction of the magnetic field, in the anisotropic case the aforementioned quantities are reduced to the components[10] of the polaron effective mass tensor:

$$M_C^*\simeq M_\perp=m_\perp A_\perp, \tag{35a}$$

$$M_\parallel=m_\parallel A_\parallel. \tag{35b}$$

The relations (22), (23), and (35) permit us to obtain the equation

$$\sum_\mu\langle\alpha_\mu(\theta)\rangle=2[(M_\parallel-m_\parallel)/m_\parallel+2(M_\perp-m_\perp)/m_\perp], \tag{36}$$

which is a generalization to this anisotropic case of the well-known result of the intermediate coupling theory

$$M^*=m(1+\alpha/6). \tag{37}$$

Using the expression (21), the corresponding form of a two-dimensional (2D) electron interacting with a 3D anisotropic system of phonons is obtained by taking formally $m_\parallel\to\infty$. In terms of $\tilde{\alpha}_\mu(\theta)$ defined through the relation

$$\tilde{\alpha}_\mu(\theta)=\sin\theta\lim_{m_\parallel\to\infty}\alpha_\mu(\theta), \tag{38}$$

the obtained form (39) is a generalization to the anisotropic uniaxial crystal and to the intermediate coupling case of the expression of the so-called semiclassical contribution to the level shift δE_{SC}, found by Das Sarma[20] for an isotropic system:

$$E(n)/\hbar = -\frac{1}{2}\sum_{\mu}\int_0^{\pi}\tilde{\alpha}_{\mu}(\theta)\omega_{\mu}(\theta)d\theta + \Omega(n+\tfrac{1}{2})(A_{\perp}^{2D})^{-1} - \frac{9}{128}\Omega^2(n+\tfrac{1}{2})^2(A_{\perp}^{2D})^{-4}\sum_{\mu}\int_0^{\pi}\frac{\tilde{\alpha}_{\mu}(\theta)}{\omega_{\mu}(\theta)}d\theta, \quad (39)$$

where

$$A_{\perp}^{2D} = 1 + \frac{1}{8}\sum_{\mu}\int_0^{\pi}\tilde{\alpha}_{\mu}(\theta)d\theta. \quad (40)$$

Similar results are found for the case of an electron interacting with a 3D anisotropic system of phonons and which is confined in a quantum well whose width goes to zero.

V. RESULTS AND DISCUSSION

We discuss the experiments of the cyclotron resonance phenomenon in red mercury iodide (α-HgI_2) performed by Bloch *et al.*[11] and Hodby and co-workers,[12] restricting ourselves to the case of electrons. The aim of such experiment is to obtain the components of the effective mass tensor of the ''bare'' electron. Due to the involved axial symmetry, in addition to the measurement of the cyclotron resonance frequency performed for $\mathbf{B}_0$ directed along the optical axis, a supplemental source of information concerning the polaron spectrum has to be considered. Thus, according to the results obtained from the drift mobility measurements,[21] Bloch *et al.*[11] take for the anisotropic polaron factor $N = M_{\parallel}/M_{\perp}$, the value $N_1 = 0.837$. In the second paper[12] the cyclotron mass obtained for $\mathbf{B}_0$ perpendicular to the optical axis was identified with the expression $(M_{\parallel}M_{\perp})^{1/2}$. Though this result is beyond our frame of the polaron problem, we shall take it into consideration together with the value of the cyclotron mass for $\mathbf{B}_0$ parallel to the optical axis obtaining $N_2 = 1.085$, where, accordingly to Ref. 12, the small nonparabolicity of the polaron spectrum at low magnetic fields was neglected.

Based on the knowledge of the parameters of the optical phonon modes from infrared reflectivity measurements,[22] in order to analyze the results of the experiments we shall consider the curves representing the functions

$$N = \nu\,\frac{1 + \dfrac{1}{2}\sum_{\mu}\left\langle\dfrac{\alpha_{\mu}(\theta)\sin^2\theta}{s(\theta)}\right\rangle}{1 + \dfrac{\nu}{4}\sum_{\mu}\left\langle\dfrac{\alpha_{\mu}(\theta)\cos^2\theta}{s(\theta)}\right\rangle} = f_{m_{\perp}}(\nu) \quad (41)$$

for different values of mass component $m_{\perp}$. For each of the values N_1 and N_2 the expression (41) permits us to obtain a set of values $(m_{\perp}, \nu)$ that leads to the curves $m_{\perp} = m_{\perp}(\nu)$ presented in Fig. 1. This curves present the possible values $m_{\perp}$ and ν determined by the anisotropic properties of the phononic spectra of this material compatible with the corresponding anisotropic factor N of the polaron spectrum. The values of the ''bare'' electron effective masses inferred from the experiments reported in Refs. 11 and 12 correspond in Fig. 1 to the points H_1 ($\nu = 0.862$, $m_{\perp} = 0.29\, m_0$) and H_2 ($\nu = 0.863$, $m_{\perp} = 0.33\, m_0$), respectively. Depending on the specific value of the anisotropic factor of the polaron spectrum, induced by a supplemental measurement, the acceptable effective mass $m_{\perp}$ is obtained by comparing the experimental value of the cyclotron mass with those determined by Eq. (33), $m_{\perp}$ belonging to one of the curves of Fig. 1. Due to the fact that the Fröhlich coupling functions $\alpha_{\mu}(\theta)$ depend on the values of the effective masses of the ''bare'' electron that at their term are derived from the cyclotron resonance measurements, a self-consistent solution has to be found. Using the expression (33) and the values of the effective masses of the ''bare'' electron corresponding to the points H_1 and H_2 shown in Fig. 1, the dashed and the dotted curves marked with (1) in Fig. 2 present the dependence of the cyclotron resonance frequency on the magnetic field. The dot corre-

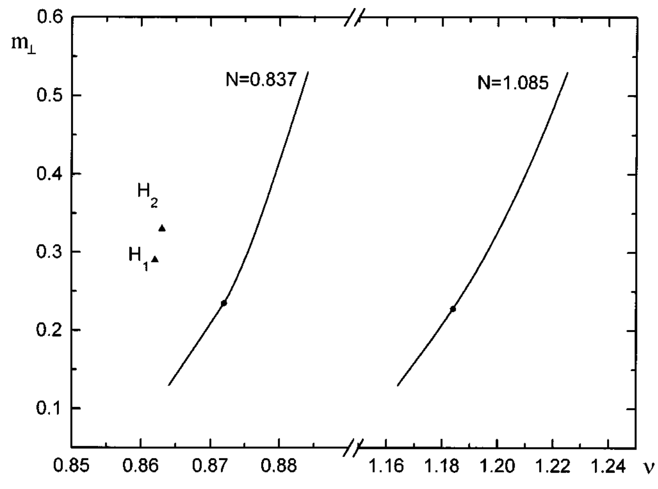

FIG. 1. The curves $m_{\perp} = m_{\perp}(\nu)$ for the two values of the anisotropic polaron factor $N_1 = 0.837$, $N_2 = 1.085$.

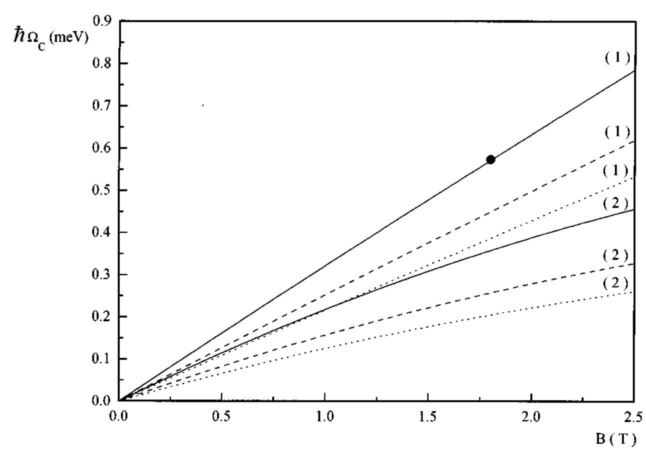

FIG. 2. The cyclotron resonance frequency vs magnetic field. The solid, dashed, and dotted curves marked with (1) correspond to the values ($m_{\perp} = 0.235\, m_0$, $m_{\parallel} = 0.205\, m_0$), ($m_{\perp} = 0.29\, m_0$, $m_{\parallel} = 0.25\, m_0$), and ($m_{\perp} = 0.33\, m_0$, $m_{\parallel} = 0.285\, m_0$), respectively. The curves marked with (2) are obtained, in the weak coupling formulation of the polaron problem, for the same values $m_{\perp}$ and $m_{\parallel}$. The dot marked on the first curve corresponds to the experimental value of the cyclotron resonance frequency found in the experiment discussed in Ref. 11.

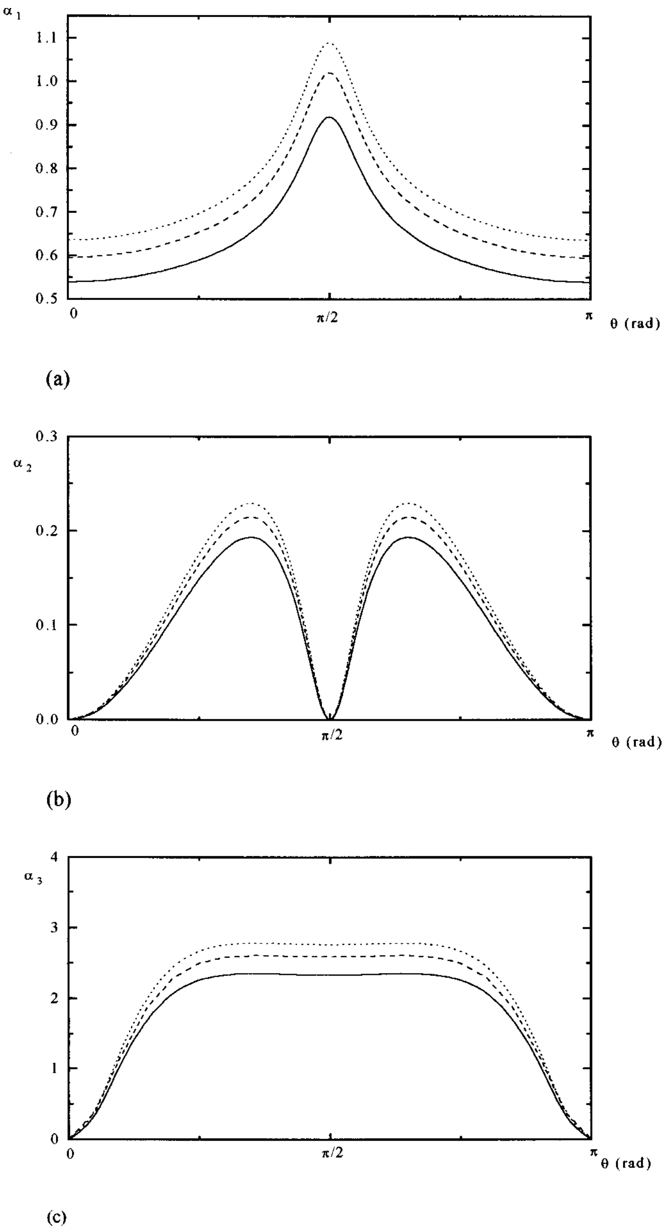

FIG. 3. The angular dependence of the coupling functions $\alpha_\mu(\theta)$ for the three branches of the involved phonon modes. The solid, dashed, and dotted curves correspond to the same values of $m_\perp$ and $m_\parallel$ as those presented in Fig. 2.

sponds to the cyclotron resonance frequency found in the experiment[11] performed in the geometry considered throughout this paper. The solid curve (1) in Fig. 2 was obtained for $m_\perp = 0.235\, m_0$ and $\nu = 0.872$, these values corresponding to the point marked on the curve for $N_1 = 0.837$ in Fig. 1.

Knowing the parameters of the optical phonons from infrared reflectivity measurements[22] and the values of the considered components of the effective mass tensor of the ''bare'' electron, the angular dependencies of the Fröhlich's phonon coupling functions $\alpha_\mu(\theta)$, $\mu = \overline{1,3}$ are plotted in Fig. 3. The dotted, dashed, and solid curves are obtained for the values $m_\perp$ and ν corresponding to the points H_2, H_1, and to that marked on the curve drawn in Fig. 1 for N_1, respectively.

Excepting the contribution of the quasitransverse modes illustrated in Fig. 3(b), for the other contributions ($\mu = 1,3$), due to their values, a perturbational approach to the polaron problem seems to be inadequate.

The curves similar to those with the index (1), obtained in the frame of the weak electron-phonon coupling are marked in Fig. 2 with the index 2.

The observed discrepancy between the curves labeled (1) in Fig. 2 that are obtained in the context of intermediate coupling theory and corresponding curves (2) is due to the large values of Fröhlich's coupling constants. Thus, at very weak magnetic field, denoting the slopes of two corresponding curves (1) and (2) by s_p and s_v, respectively, for the relative variation η_s, one obtains the expression

$$\eta_s = \frac{s_v - s_p}{s_v} = (A_\perp - 1)^2. \tag{42}$$

Also the ratio of the deviations form the linearity of the curves (1) and (2), plotted for the same values of $m_\perp$ and $m_\parallel$, representing the ratio of the coefficients γ_p and γ_v of the terms in B^2 is given by

$$\gamma_p / \gamma_v = A_\perp^4. \tag{43}$$

For the solid, dashed, and dotted curves, the values of $A_\perp$ are 1.51, 1.57, and 1.60, respectively.

Thus, the discrepancy between the behaviors of two curves (1) and (2), especially for large values of B, increases with the strength of the electron-phonon interaction. Nevertheless, for the case of weak electron-phonon interaction the above discrepancy is insignificant and the perturbational approach is an adequate one.

For the anisotropic polaron factor $N_2 = 1.085$ reached from the second experiment,[12] in a similar manner, for the effective masses of the ''bare'' electron one obtains $m_\perp = 0.228\, m_0$ and $m_\parallel = 0.269\, m_0$ determining the point marked on the corresponding curve of the Fig. 1. We believe that the anisotropic features of this material could not support the coexistence of both values $N_2 = 1.085$ and $\nu = 0.863$ proposed in Ref. 12. As concerns the point H_1 shown in Fig. 1, we think that the difference between the values found by Bloch *et al.*[11] for the components of the effective mass tensor of the ''bare'' electron and ours is due to the underestimation of the electron-phonon interaction in the first case.

Our results reflect mainly the strong contribution to the electron-phonon interaction of the branch $\mu = 3$ of the phonon modes with low frequencies, $\omega_3(\theta) \in [17.46\ \mathrm{cm}^{-1}, 32.15\ \mathrm{cm}^{-1}]$.

However in the circumstances of the existence of a large free-electron contribution to the dielectric tensor, the screening effect may be important leading to a reduction of corresponding Fröhlich's coupling functions. It is our intention to discuss this subject in the future.

The central point of the method that we have developed is to consider the mean value of the z component of the total angular momentum, which is a constant of motion, as a constraint in the minimizing procedure of the polaron energy.

As far as in the presence of a magnetic field the axial symmetry of the system is preserved, the method just presented can be applied, allowing the study of the cyclotron resonance in uniaxial crystals, quasi-two dimensional structures, and anisotropic uniaxial quantum wells, as well.

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