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Diagonalization of the generalized Feynman bipolaron model in a magnetic field

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Abstract. The Feynman model Hamiltonian for a polaron is generalized to the case of a *bipolaron* in an external magnetic field. The resulting Hamiltonian is exactly diagonalized and the eigenfrequencies and eigenvectors are found. Numerical results are given as function of the magnetic field and limiting results are obtained in the low- and high-magnetic field limit. The time evolution of the electron position coordinates is derived from which we obtain the optical absorption.

1. Introduction

Conduction electrons in materials repel each other via the screened Coulomb potential, but in very ionic crystals the electron–phonon coupling can be strong enough to overcome the Coulomb repulsion and create a stable electron (or hole) pair. This is the so-called *bipolaron* problem, the concept of which was introduced by Pekar [1]. He suggested that when coupled to a cloud of virtual phonons in a polar crystal, two electrons can form a bound state in spite of the Coulomb repulsion between the two electrons if the attractive interaction due to the electron–phonon coupling is sufficiently large. The latter condition is quite severe and can only be satisfied in very polar materials. Recently, the interest in bipolarons [2, 3, 4, 5, 6, 7, 8] in materials with strong electron–phonon interaction has revived due to the discovery of high-temperature superconductors. In the present paper, we limit ourselves to the case of large bipolarons which are mobile and consequently can contribute to conduction. The theory of large bipolarons using Feynman path-integral techniques was presented by Verbist *et al* [6] in the absence of any external magnetic field. They showed that bipolaron formation is easier in two dimensions (2D) than in three dimensions (in 2D: $\alpha_c \simeq 2.9$ and in 3D: $\alpha_c \simeq 6.9$).

Feynman's path-integral approach to the polaron problem has been very successful to describe the static (i.e. thermodynamic) and dynamic properties of polarons for arbitrary electron–phonon coupling strength [9]. This approach is based on a cumulant expansion in the difference between the actual action and a trial action. The latter is chosen to be a quadratic action such that all path-integrals over it can be done exactly. Corresponding to the Feynman trial action there exists an equivalent Feynman model Hamiltonian which contains extra degrees of freedom. Eliminating these degrees of freedom within a path-integral approach leads to the Feynman trial action [10].

The purpose of the present paper is to generalize Feynman's polaron theory [11] to the case of a bipolaron in the presence of an external magnetic field. In order to do this, we first

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study the generalized Feynman bipolaron model Hamiltonian. In the present paper we limit ourselves to the exact diagonalization of the bipolaron model Hamiltonian and the study of the magnetic field dependence of its different properties. A magnetic field in the z-direction couples the x and y motion of the bipolaron and as a consequence we must deal with a non-separable problem of 16 degrees of freedom. The diagonalization of it turns out to be technical rather involved.

The outline of the present paper is as follows. We start in section 2 with a discussion of the problem, present a generalization of Feynman's polaron theory to bipolarons. The eigenfrequencies are calculated in section 3. Numerical results are presented and asymptotic results for small and large magnetic fields are derived. The time evolution of the electron coordinates are given in section 4. In section 5, the optical absorption is calculated for the bipolaron model Hamiltonian. Our conclusions are presented in section 6.

2. Hamiltonian

The Hamiltonian that describes two electrons interacting with the vibrational modes of a crystal and a constant uniform magnetic field is given by

$$H = H_{\mathrm{e}} + H_{\mathrm{ph}} + H_{\mathrm{I}} + U(\boldsymbol{r}_1 - \boldsymbol{r}_2) \tag{1}$$

with

$$H_{\mathrm{e}} = \frac{1}{2m}\sum_{j=1}^{2}\left[\boldsymbol{p}_j + \frac{e\boldsymbol{A}_j}{c}\right]^2 \tag{2}$$

the Hamiltonian for two free electrons in a magnetic field $\boldsymbol{B} = \mathrm{rot}\,\boldsymbol{A}$, with band mass m, electric charge $-e$, and conjugate coordinates of the jth electron $(\boldsymbol{r}_j, \boldsymbol{p}_j)$.

$$H_{\mathrm{ph}} = \sum_{\boldsymbol{k}} \hbar\omega_{\boldsymbol{k}}(a_{\boldsymbol{k}}^{\dagger}a_{\boldsymbol{k}} + \tfrac{1}{2}) \tag{3}$$

is the Hamiltonian describing the bulk phonons, where $a_{\boldsymbol{k}}^{\dagger}$ ($a_{\boldsymbol{k}}$) is the creation (annihilation) operator for a phonon with wave vector $\boldsymbol{k}$ and frequency $\omega_{\boldsymbol{k}}$. The interaction between the electrons and phonons is described by

$$H_{\mathrm{I}} = \sum_{j=1}^{2}\sum_{\boldsymbol{k}}\left(V_{\boldsymbol{k}}a_{\boldsymbol{k}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_j} + V_{\boldsymbol{k}}^{*}a_{\boldsymbol{k}}^{\dagger}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_j}\right) \tag{4}$$

where $V_{\boldsymbol{k}}$ is the electron–phonon interaction coefficient and $U(\boldsymbol{r})$ is the repulsive potential between the electrons. In the following the magnetic field is taken along the z axis, and the vector potential is written in the symmetrical Coulomb gauge

$$\boldsymbol{A}_j = \frac{B}{2}\left(-y_j, x_j, 0\right). \tag{5}$$

For longitudinal-optical (LO) phonon scattering one usually assumes dispersionless phonons $\omega_{\boldsymbol{k}} = \omega_{\mathrm{LO}}$, with ω_{LO} the frequency of the longitudinal optical phonons. The interaction coefficient in 3D is given by $V_{\boldsymbol{k}} = \mathrm{i}(\hbar\omega_{\mathrm{LO}}/k)(4\pi\alpha/V)^{1/2}(\hbar/2m\omega_{\mathrm{LO}})^{1/4}$, where $\alpha = (1/\hbar\omega_{\mathrm{LO}})(e^2/2\epsilon_{\mathrm{e}})(2m\omega_{\mathrm{LO}}/\hbar)^{1/2}$ is the electron–LO phonon coupling constant where ϵ_{e} is the effective dielectric constant defined in terms of the high frequency dielectric constant ϵ_∞ and the static dielectric constant ϵ_0 as ${\epsilon_{\mathrm{e}}}^{-1} = {\epsilon_\infty}^{-1} - {\epsilon_0}^{-1}$. The electron–phonon coupling constant α, which measures the attractive part, and the strength of the Coulomb repulsion $U(\boldsymbol{r}_1 - \boldsymbol{r}_2) = U/|\boldsymbol{r}_1 - \boldsymbol{r}_2|$ are two relevant parameters that determine the bipolaron formation.

The original idea of the Feynman polaron model is to replace the virtual phonon cloud surrounding the electron by a fictitious particle which is bound to the electron through a spring [10]. The mass of the fictitious particle and the coupling (i.e. spring constant) between the electron and the fictitious particle are a measure for the effective electron–phonon interaction. In a bipolaron system we have two electrons each with their own phonon cloud and consequently the Feynman bipolaron model will consist of four particles, described by the following Hamiltonian

$$H_F = \sum_{j=1}^{2}\left[\frac{1}{2m}\left(\boldsymbol{p}_j + \frac{e\boldsymbol{A}_j}{c}\right)^2 + \frac{\boldsymbol{P}_j^2}{2M} + \frac{\kappa}{2}(\boldsymbol{r}_j - \boldsymbol{R}_j)^2\right] + \frac{\kappa'}{2}\left[(\boldsymbol{r}_1 - \boldsymbol{R}_2)^2 + (\boldsymbol{R}_1 - \boldsymbol{r}_2)^2\right] - \frac{K}{2}(\boldsymbol{r}_1 - \boldsymbol{r}_2)^2. \tag{6}$$

In analogy with the Feynman model for a free polaron, each electron interacts quadratically with a fictitious particle with conjugate coordinates $(\boldsymbol{R}_j, \boldsymbol{P}_j)$ of mass M and oscillator strength κ. Each of the electrons interact with the fictitious particle (phonon cloud) of the other electron with oscillator strength κ'. For the case of harmonic phonons, as is usually assumed in polaron physics, the polarization clouds of overlapping polarons are additive and as a consequence there is no direct interaction between the fictitious particles $(\boldsymbol{R}_1, \boldsymbol{R}_2)$. The Coulomb repulsion between the electrons is approximated by a quadratic repulsion with strength K. Consequently, the model is determined by the four parameters M, κ, κ', and K. which is illustrated in figure 1. In this quadratic model the motion along the magnetic field does not couple with the motion perpendicular to the magnetic field. For motion along the magnetic field, the problem is equivalent to the one-dimensional (1D) Feynman bipolaron model Hamiltonian in the absence of any magnetic field which was diagonalized in [6]. Therefore we limit ourselves to the electron motion perpendicular to the magnetic field.

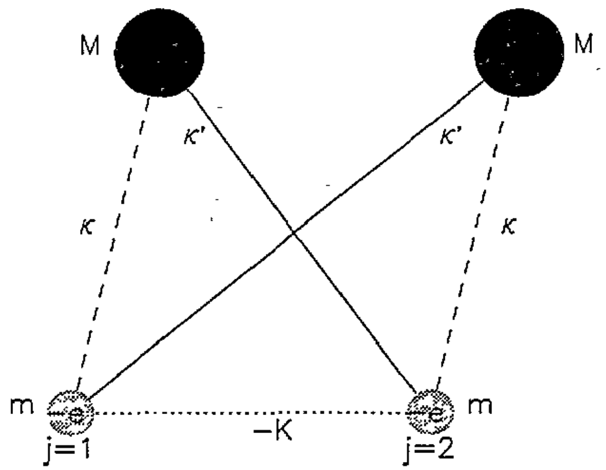

Figure 1. Graphical representation of the bipolaron model.

3. The eigenfrequencies

From now on we will use units such that $\hbar = m = \omega_{LO} = 1$. The Hamiltonian H_F in two dimensions (2D) has sixteen degrees of freedom, and its diagonalization is equivalent to the diagonalization of a 16×16 matrix. An alternative approach [11] is to consider the *equations of motion*

$$\dot{p}_j = -\frac{\partial H_F}{\partial r_j} \qquad \dot{P}_j = -\frac{\partial H_F}{\partial R_j} \tag{7a}$$

$$\dot{r}_j = \frac{\partial H_F}{\partial p_j} \qquad \dot{R}_j = \frac{\partial H_F}{\partial P_j} \tag{7b}$$

which leads to a set of sixteen linear first-order differential equations. The solution of this set of equations is rather lengthy. Therefore only a brief outline of the calculation will be given. After eliminating the momentum variables the sixteen coupled first-order linear differential equations reduce to eight coupled second-order linear differential equations. Taking the Laplace transform of these equations results in eight coupled non-homogeneous algebraic equations, which in principle can be solved analytically. The eigenfrequencies of the system are given by the zeros of the determinant of the homogeneous problem

$$\det A = \begin{vmatrix} s^2+\eta & s\omega_c & \gamma_3 & 0 & -\gamma_1 & 0 & -\gamma_2 & 0 \\ -s\omega_c & s^2+\eta & 0 & \gamma_3 & 0 & -\gamma_1 & 0 & -\gamma_2 \\ \gamma_3 & 0 & s^2+\eta & s\omega_c & -\gamma_2 & 0 & -\gamma_1 & 0 \\ 0 & \gamma_3 & -s\omega_c & s^2+\eta & 0 & -\gamma_2 & 0 & -\gamma_1 \\ -\delta_1 & 0 & -\delta_2 & 0 & s^2+\zeta & 0 & 0 & 0 \\ 0 & -\delta_1 & 0 & -\delta_2 & 0 & s^2+\zeta & 0 & 0 \\ -\delta_2 & 0 & -\delta_1 & 0 & 0 & 0 & s^2+\zeta & 0 \\ 0 & -\delta_2 & 0 & -\delta_1 & 0 & 0 & 0 & s^2+\zeta \end{vmatrix} \tag{8}$$

where $\eta = \gamma_1 + \gamma_2 - \gamma_3$ ($\gamma_1 = \kappa/m$, $\gamma_2 = \kappa'/m$, $\gamma_3 = K/m$), $\zeta = \delta_1 + \delta_2$ ($\delta_1 = \kappa/M$, $\delta_2 = \kappa'/M$) and $\omega_c = eB/mc$ is the cyclotron frequency of a free electron in a magnetic field. In equation (8) 's' is the Laplace variable and the condition $\det A(s^2) = 0$ results in the algebraic equation

$$s^2\left\{-s^2(s^2-\upsilon^2)^2 + \omega_c^2(s^2-\nu^2)^2\right\} \times \left\{[s^4 + (2\gamma_3 - \upsilon^2)s^2 + \varrho^4 - 2\gamma_3\nu^2]^2 - s^2\omega_c^2(s^2-\nu^2)^2\right\} = 0 \tag{9}$$

which leads to the set of eight eigenfrequencies: $\omega_j = \sqrt{s_j}$, $j = 1, \ldots, 7$ and $\omega_8 = 0$. In equation (9) we defined $\upsilon^2 = \gamma_1 + \gamma_2 + \delta_1 + \delta_2 = (\kappa + \kappa')/\mu$, $\nu^2 = \delta_1 + \delta_2 = (\kappa + \kappa')/M$, and $\varrho^4 = 2(\gamma_1\delta_2 + \gamma_2\delta_1) = 4\kappa\kappa'(mM)^{-1}$, where $\mu^{-1} = m^{-1} + M^{-1}$.

The polaron limit is obtained by decoupling the two electrons from each other, i.e. $\kappa = \kappa' = 0$ or equivalently by substituting $\gamma_2 = \gamma_3 = \delta_2 = 0$ in equation (9). This results in the equation

$$s^2(s^2 - \gamma_1 - \delta_1)^2 - \omega_c^2(s^2 - \delta_1)^2 = 0 \tag{10}$$

for the eigenfrequencies which was first obtained in [11]. Next we consider the zero-magnetic field limit of equation (9) and find

$$s^2\left\{-s^2(s^2-\upsilon^2)^2\right\}\left\{[s^4 + (2\gamma_3 - \upsilon^2)s^2 + \varrho^4 - 2\gamma_3\nu^2]^2\right\} = 0 \tag{11}$$

which results in the four eigenfrequencies: $s = 0$ and

$$\Omega_1^2 = \frac{M+m}{Mm}(\kappa + \kappa') = \upsilon^2, \tag{12a}$$

$$\Omega_{2,3}^2 = \frac{1}{2}\left\{\Omega_1^2 - \frac{2K}{m} \pm \left[\left[\frac{M-m}{Mm}(\kappa+\kappa') - \frac{2K}{m}\right]^2 + \frac{4}{Mm}(\kappa - \kappa')^2\right]^{1/2}\right\} \tag{12b}$$

as obtained in [6].

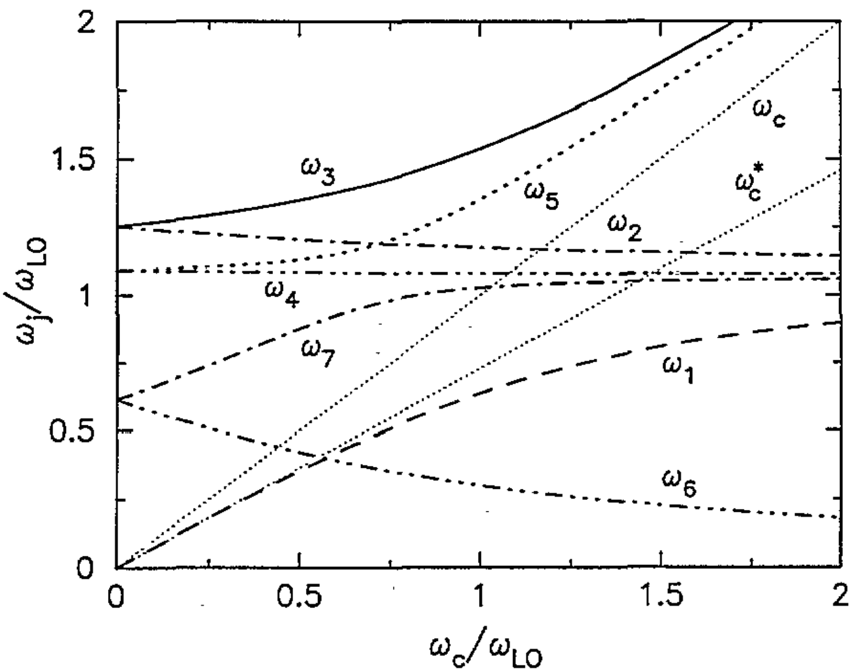

Figure 2. The eigenfrequencies of the bipolaron model for the parameters: $\kappa = 0.269$, $\kappa' = 0.154$, $K = 0$ and $M = 0.369$ as a function of the magnetic field. We also show $\omega_c = eB/mc$ and $\omega_c^* = \omega_c/(m+M)$ by the dotted lines.

Equation (9) was solved numerically. In figure 2 the eigenfrequencies ω_j are depicted as a function of the magnetic field for $\kappa = 0.269$, $\kappa' = 0.154$, $K = 0$ and $M = 0.369$, which are the parameters for a weak coupling polaron in the absence of any Coulomb repulsion. The Feynman parameters for this case are $\upsilon = [(\kappa+\kappa')(1+1/M)]^{1/2} = 1.25$ and $w = [(\kappa+\kappa')/M]^{1/2} = 1.07$. The equivalent results for a strongly coupled polaron are shown in figure 3. We took the following parameters: $\kappa = 269.68$, $\kappa' = 154.32$, $K = 0$ and for the mass of the fictitious particle $M = 369.01$ which are the parameters obtained in [6] for $\alpha = 12$ in the absence of an external magnetic field. The corresponding one-polaron Feynman parameters are $\upsilon = 20.61$ and $w = 1.07$. The discussion of the physical significance of the different roots will be given while discussing the different limiting behaviours.

In the following we will derive explicit analytic results for the eigenfrequencies, for a restrictive range of ω_c-values. We consider $K = 0$, in order to make the expressions sufficiently attractive. First, we will analyse the small magnetic field limit $\omega_c \ll 1$ where we obtained the following results

$$\omega_1 = \omega_c^* - \frac{\nu(\upsilon^2-\nu^2)}{\upsilon^5}\omega_c^{*3} + \frac{\nu(3\upsilon^4-5\nu^2\upsilon^2+2\upsilon^4)}{\upsilon^9}\omega_c^{*5} + O\left(\omega_c^7\right), \qquad (13a)$$

$$\omega_{2,3} = \upsilon \pm \frac{\upsilon^2-\nu^2}{2\upsilon^2}\omega_c + \frac{\upsilon^4-3\nu^4+2\upsilon^2\nu^2}{8\upsilon^5}\omega_c^2 \pm \frac{\nu^4(\upsilon^2-\nu^2)}{2\upsilon^8}\omega_c^3 + O\left(\omega_c^4\right), \qquad (13b)$$

$$\omega_{4,5} = \Omega_2 \pm \frac{\Omega_+}{2\sqrt{2}\Omega_2\sqrt{\upsilon^4-4\varrho^4}}\omega_c + O\left(\omega_c^2\right), \qquad (13c)$$

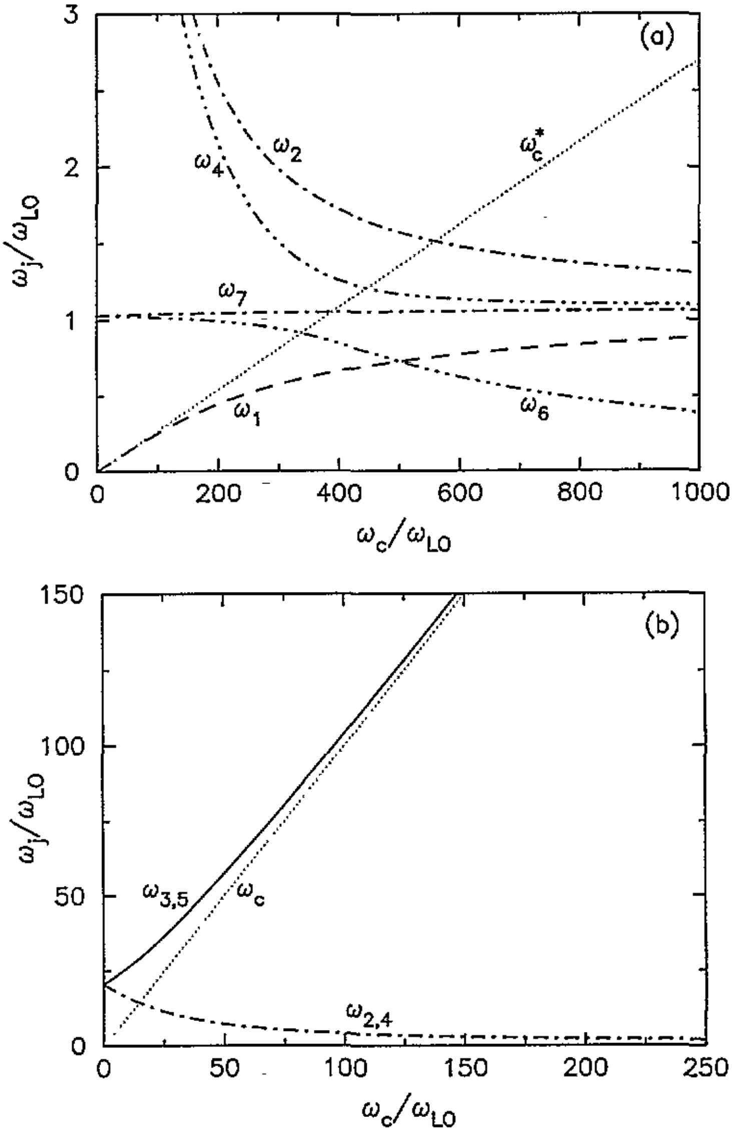

Figure 3. (a) The eigenfrequencies $\omega_{1,2,4,6,7}$, and (b) the eigenfrequencies $\omega_{2,3,4,5}$, as a function of the magnetic field for: $\kappa = 269.68$, $\kappa' = 154.32$, $K = 0$ and $M = 369.01$ which corresponds to the strongly coupled bipolaron system.

$$\omega_{6,7} = \Omega_3 \pm \frac{\Omega_-}{2\sqrt{2}\Omega_3\sqrt{\upsilon^4 - 4\varrho^4}}\omega_c + O\left(\omega_c^2\right), \qquad (13d)$$

where $\omega_c^* = \omega_c \nu^2/\upsilon^2 = \omega_c m/(m+M)$ is the cyclotron frequency for a particle with mass $m+M$ which is equal to the polaron mass, $\Omega_{2,3}^2 = (\upsilon^2 \pm \sqrt{\upsilon^4 - 4\varrho^4})/2$ is the square of the frequencies given by equation (12*b*) for $K = 0$, and $\Omega_\pm^2 = \upsilon^2(\upsilon^2 - \nu^2)^2 \pm \sqrt{\upsilon^4 - 4\varrho^4}[(\upsilon^2 - \nu^2)^2 - \varrho^4] + \varrho^4(4\nu^2 - \upsilon^2)$. The above limiting behaviour is clearly apparent in figures 2 and 3. ω_I is the cyclotron motion of a polaron (= *electron + fictitious particle*) with mass $m+M$ in a magnetic field, or in the present case of a bipolaron with charge $2e$ and mass $2(m+M)$.

At zero magnetic field, ω_2 and ω_3 become equal to the frequency υ for relative motion of the electrons and the fictitious particles in the Feynman polaron model which for non-zero magnetic field splits into two, for clockwise and counter clockwise rotational motion. The frequencies $\omega_{4,5}$ and $\omega_{6,7}$ are pure bipolaron modes which equals equation (12*b*) in the zero magnetic field limit. These internal vibrational modes of the bipolaron split into two when $\omega_c \neq 0$ for the same reason as mentioned for $\omega_{2,3}$.

For large magnetic fields $\omega_c \gg 1$ one finds the following asymptotic expansions

$$\omega_{1,2} = \nu \mp \frac{\upsilon^2 - \nu^2}{2}\frac{1}{\omega_c} + \frac{\upsilon^4 - 6\nu^2\upsilon^2 + 5\nu^4}{8\nu}\frac{1}{\omega_c^2} + \mathrm{O}\left(\frac{1}{\omega_c^3}\right) \tag{14a}$$

$$\omega_3 = \omega_c + (\upsilon^2 - \nu^2)\frac{1}{\omega_c} - (2\nu^4 - 3\nu^2\upsilon^2 + \upsilon^4)\frac{1}{\omega_c^3} + +\mathrm{O}\left(\frac{1}{\omega_c^5}\right) \tag{14b}$$

$$\omega_{4,7} = \nu \pm \left(\frac{\upsilon^2 - \nu^2}{2} - \frac{\varrho^4}{2\nu^2}\right)\frac{1}{\omega_c} \pm \frac{\nu^2(\upsilon^4 + 5\nu^4) + 2\upsilon^2\varrho^4(\varrho^4 - 3\nu^4)(2\nu^4 - 3\rho^4)}{8\nu^3}\frac{1}{\omega_c^2} + \mathrm{O}\left(\frac{1}{\omega_c^3}\right) \tag{14c}$$

$$\omega_5 = \omega_c + (\upsilon^2 - \nu^2)\frac{1}{\omega_c} - (2\nu^4 - 3\upsilon^2\nu^2 + \upsilon^4 + \varrho^4)\frac{1}{\omega_c^3} + \mathrm{O}\left(\frac{1}{\omega_c^5}\right) \tag{14d}$$

$$\omega_6 = \frac{\rho^4}{\nu^2}\frac{1}{\omega_c} + \frac{\varrho^8(\varrho^4 - \upsilon^2\nu^2)}{\nu^8}\frac{1}{\omega_c^3} - \frac{\varrho^{12}(\varrho^4 - \upsilon^2\nu^2)^2}{2\nu^{12}}\frac{1}{\omega_c^5} + \mathrm{O}\left(\frac{1}{\omega_c^7}\right). \tag{14e}$$

Two of the frequencies (ω_3 and ω_5) reache the free electron cyclotron frequency (ω_c) from above when $\omega_c \to \infty$. In this limit the electrons move so fast that the fictitious particles cannot follow the electron motion and the eigenmode of a free electron in a magnetic field is recovered. Several of the other eigenfrequencies, i.e. $\omega_{1,2}$ and $\omega_{4,7}$, approach $\nu = \sqrt{(\kappa + \kappa')/M}$ which is the eigenfrequency of the fictitious particle connected to a fixed electron. i.e. $m \to \infty$. ω_6 is the frequency of a particle moving counter clockwise in a magnetic field, which is similar to the behaviour of skipping orbits in a quantum dot.

4. The eigenvectors

In the process of diagonalization equation (6), two canonically conjugate constants of motion enter

$$\Pi_1 = \frac{1}{4}(x_1 + x_2) - \frac{1}{2\omega_c}(p_{1y} + p_{2y}) - \frac{1}{2\omega_c}(P_{1y} + P_{2y}), \tag{15a}$$

$$\Pi_2 = \frac{1}{4}(y_1 + y_2) + \frac{1}{2\omega_c}(p_{1x} + p_{2x}) + \frac{1}{2\omega_c}(P_{1y} + P_{2x}), \tag{15b}$$

which satisfy the commutation relation $[\Pi_1, \Pi_2] = -i/2\omega_c$. They are related to the position of the classical orbit center. The explicit time evolution of the electron position coordinates are found to be

$$x_1(t) = \Pi_1 + \mathrm{i}\sum_{j=1}^{7} d_j(C_j \mathrm{e}^{\mathrm{i}s_j t} + C_j^\dagger \mathrm{e}^{-\mathrm{i}s_j t}), \tag{16a}$$

$$y_1(t) = \Pi_2 - \mathrm{i}\sum_{j=1}^{7} d_j(C_j \mathrm{e}^{\mathrm{i}s_j t} + C_j^\dagger \mathrm{e}^{-\mathrm{i}s_j t}) \tag{16b}$$

where C_j, ($C_j^\dagger$) are annihilation (creation) operators for quantized motion of the internal degrees of freedom and which satisfy $[C_j, C_l^\dagger] = \delta_{j,l}$. Similar expressions are obtained for the coordinates of the second electron.

For the actual path-integral calculation [6] of the bipolaron energy at zero magnetic field with the trial action obtained from the model Hamiltonian (6), it turned out that taking $K = 0$ does not alter the results appreciably. Therefore, in the following we will take $K = 0$ in order to keep the formulas tractable. The coefficients d_j are given by

$$d_j^2 = \frac{s_j^8 + a_1 s_j^6 + a_2 s_j^4 + a_3 s_j^2 + a_4}{4s_j(3s_j^4 + a_5 s_j^2 + a_6)^2} \qquad j = 1, \ldots, 3 \tag{17a}$$

with

$$a_1 = -2(2+M)\nu^2$$
$$a_2 = (6 + 7M + M^2)\nu^4 + M\omega_c^2\nu^2$$
$$a_3 = -4(1+M)^2\nu^6 - 2M\omega_c^2\nu^4$$
$$a_4 = (1 + 3M + 3M^2 - M^3)\nu^8 + M\omega_c^2\nu^6$$
$$a_5 = -4(1+M)\nu^2 - 2\omega_c^2$$
$$a_6 = (1-M)^2\nu^4 + 2\omega_c^2\nu^2$$

and

$$d_j^2 = \frac{Ms_j^{12} - 2M(2+M)\nu^2 s_j^{10} + b_1 s_j^8 + b_2 s_j^6 + b_3 s_j^4 + b_4 s_j^2 + b_5}{4s_j M(-4s_j^6 + b_6 s_j^4 + b_7 s_j^2 + b_8)^2} \qquad j = 4, \ldots, 7 \tag{17b}$$

with

$$b_1 = M\varrho^4 + M(6 + 7M + M^2)\nu^4 + M^2\nu^2\omega_c^2$$
$$b_2 = 2M(\omega_c^2 - 2M\nu^2)\varrho^4 - 4(1 + 2M^2 + M^3)\nu^6 - 2M^2\nu^4\omega_c^2$$
$$b_3 = -(3M^2 + 8M + 26)\varrho^8/8 + (M(5 + 7M - 4M^2)\nu^4 + 5M\nu^2\omega_c^2 + 13/4)\varrho^4 + M^2(3 + M^2 + 3M^3)\nu^8 + M^2\omega_c^2\nu^6$$
$$b_4 = -M\varrho^4\nu^2(M\varrho + 4\nu^2\omega_c^2)$$
$$b_5 = M\nu^8 + M\varrho^8(M\nu^4 - \varrho^4)$$
$$b_6 = 6(1+M)\nu^2 + 3\omega_c^2$$
$$b_7 = -4\varrho^4 - 2M(2+M)\nu^4 - 4\nu^2\omega_c^2$$
$$b_8 = 2M\varrho^4\nu^2 + \nu^4.$$

For future purposes we give the limiting behaviour of these coefficients d_j for $\omega_c \ll 1$ and $\omega_c \to \infty$.

In the small magnetic field limit the coefficients d_j are given by

$$d_j^2 = \frac{(s_j^2 - \nu^2)^2 + M\nu^4}{4s_j(3s_j^2 - \nu^2)^2} + \mathrm{O}\left(\omega_c^2\right) \qquad j = 1, \ldots, 3 \tag{18a}$$

$$d_j^2 = \frac{(s_j^2 - \nu^2)^2 + M(\nu^4 M - \varrho^4)}{16s_j(2s_j^2 - \nu^2)^2} + \mathrm{O}\left(\omega_c^2\right) \qquad j = 4, \ldots, 7. \tag{18b}$$

In the asymptotic limit of large magnetic fields the expansion coefficients d_j are given by

$$d_j^2 = \frac{M\nu^2}{16s_j}\frac{1}{\omega_c^2} + \mathrm{O}\left(\frac{1}{\omega_c^4}\right) \qquad j = 1, \ldots, 3 \tag{19a}$$

$$d_j^2 = \frac{M^2\nu^2 s_j^8 + c_1 s_j^6 + c_2 s_j^4 + c_3 s_j^2 + c_4}{4s_j(3s_j^4 - 4\nu^2 s_j^2 + \nu^4)^2}\frac{1}{\omega_c^2} + \mathrm{O}\left(\frac{1}{\omega_c^4}\right) \qquad j = 4, \ldots, 7 \tag{19b}$$

with $c_1 = -2(M\nu^4 + \varrho^4)$, $c_2 = M\nu^2(M\nu^4 + 5\varrho^4)$, $c_3 = -4\varrho^4\nu^4$, and $c_4 = M\varrho^4\nu^6$.

5. Optical absorption

In order to investigate the importance of the different eigenfrequencies to the physical properties of the bipolaron we have calculated the velocity auto-correlation function. The real part of the latter is a measure for the optical absorption spectrum. The oscillator strength of the different peaks is a measure of the contribution of the different frequencies to the total optical absorption. In fact, it was shown by Feynman *et al* [12] that the optical absorption spectrum of polarons calculated within the path-integral approach of Feynman [10] consists of two parts. The first part comes from the Feynman polaron model itself which leads to the zeroth order approximation to the spectrum. The same holds still for the present case of bipolarons. The second part results from the difference between the bipolaron and the trial action.

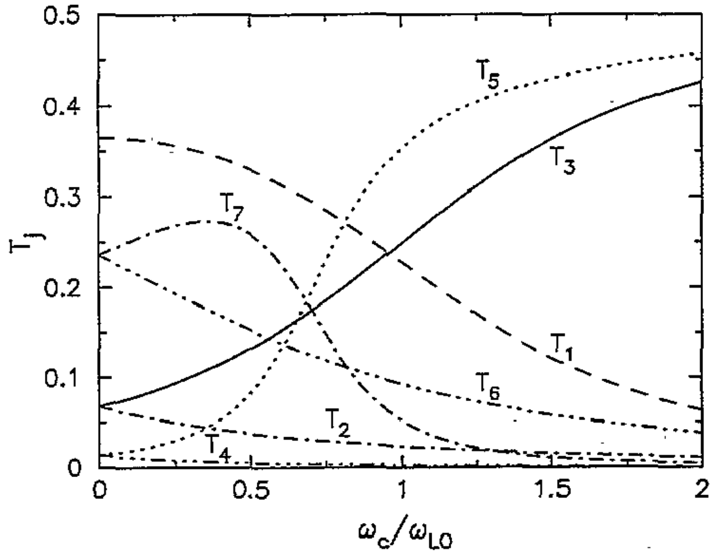

Figure 4. The oscillator strength T_j as function of the magnetic field corresponding to the weak coupling case of figure 2.

Within linear response theory [13, 14] the velocity auto-correlation function relevant for cyclotron resonance absorption (i.e. the Faraday active mode) is given by

$$\sigma(\omega) = -\frac{e^2}{\omega}\int_0^\infty \mathrm{d}t\, e^{i\omega t}\langle[(\dot{x}_1(t) + i\dot{y}_1(t))^\dagger, (\dot{x}_1(0) + i\dot{y}_1(0))]\rangle \tag{20}$$

which is the Fourier transform of the (complex) velocity auto-correlation function. For the bipolaron model Hamiltonian in the presence of an external magnetic field we can easily calculate this quantity by making use of the time evolution, equations (16*a*) and (16*b*), for the electron coordinates. The present model is non-dispersive and consequently the magneto-optical absorption spectrum consists of a series of δ-functions

$$\Re\frac{\sigma(\omega)}{\sigma_0}=\sum_{j=1}^{7}2s_jd_j^2\delta(\omega-s_j) \tag{21}$$

each with an oscillator strength $T_j=2s_jd_j^2$. The oscillator strength satisfy the sum rule $\sum_{j=1}^{7}T_j=1$. Notice that we can easily broaden these δ-functions into Lorentzians by introducing an *ad hoc* broadening. This can be done by replacing ω in equation (20) by $\omega+\mathrm{i}\Gamma$.

The oscillator strength corresponding to the different eigenmodes are depicted in figure 4 for the weak coupling case correspondig to figure 2, and in figure 5 for the strongly coupled polaron system corresponding to figure 3. Notice that for the strong coupling case four frequencies carry almost all the oscillator strength. The four frequencies (see figure 3(b)) are well represented by two-fold degenerate eigenfrequencies. In the strong coupling limit the frequencies ω_2 and ω_3 are obtained from the first part of the RMS of equation (9) in the limit $M\to\infty$, or equivalently $\nu\to 0$. This leads to

$$\omega_{2,3}^2=\upsilon^2+\frac{\omega_c^2}{2}\pm\omega_c\sqrt{\upsilon^2+\frac{\omega_c^2}{4}-2\nu^2} \tag{22}$$

which is valid for all ω_c in the region where T_j is not too small. For the corresponding oscillator strength we obtain from equation (17*a*)

$$T_j=2s_jd_j^2=\frac{1}{2}s_j^4\omega_c^2\frac{s_j^2+\upsilon^2}{(s_j^2(2\upsilon^2+\omega_c^2)-2\upsilon^4)^2}. \tag{23}$$

Note that in the $\omega_c\to 0$ limit we have $\omega_{2,3}=\upsilon\pm\omega_c/2$ for $\nu=0$ which gives us $T_{2,3}=1/4$ and which agrees with figure 5(b).

6. Conclusion

In summary, we studied the properties of a system of two electrons interacting with each other by the direct Coulomb force and by optical phonons in the presence of an external magnetic field. In the present paper we limited ourselves to the study of the Feynman bipolaron model in which the different forces are replaced by springs and the virtual phonon field by a fictitious particle. The resulting Hamiltonian was exactly diagonalized. The diagonalized form is given by

$$H_F=\sum_{j=1}^{7}\hbar\omega_j\left(C_j^\dagger C_j+\tfrac{1}{2}\right) \tag{24}$$

where the different frequencies are determined by the solution of the non-linear algebraic equation (9). The energy levels are consequently given by

$$E=\sum_{j=1}^{7}\hbar\omega_j\left(n_j+\tfrac{1}{2}\right) \tag{25}$$

in which a bipolaron state is now characterized by the 7 discrete quantum numbers $(n_1,\ldots,n_7)$.

After the exact diagonalization of this model bipolaron Hamiltonian we also obtained the time evolution of the electron coordinates which is necessary in order to calculate the electron density-density auto-correlation function. The latter is a basic quantity in the calculation of the bipolaron thermodynamic properties and dynamical quantities. These calculations, within the Feynman path-integral approach, is left for future work.

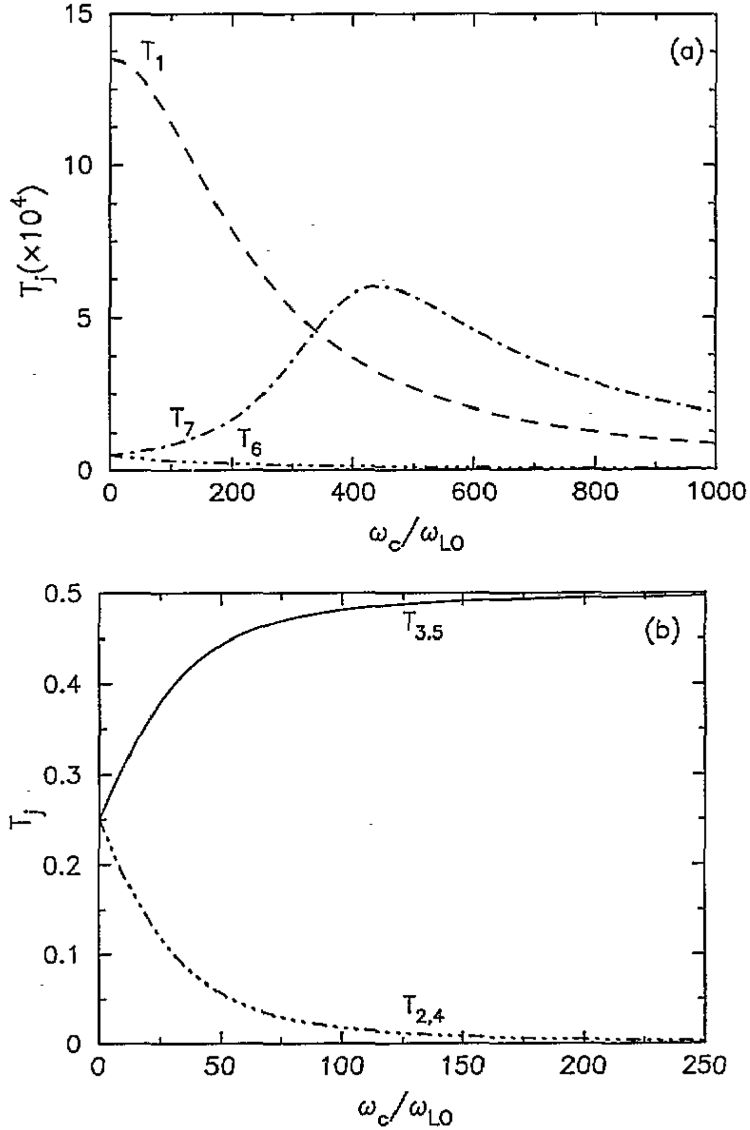

Figure 5. The oscillator strengths $T_{1,6,7}$ and $T_{2,3,4,5}$ as function of the magnetic field for the strong coupling case corresponding to the eigenfrequencies ω_j of figures 3(a) and 3(b).

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