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Statistical properties of polarons in a magnetic field. I. Analytic results

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The free energy of an ideal polaron gas in a static magnetic field is calculated using Feynman's path-integral formalism. The trial action, used in Feynman's polaron theory, is extended to take into account the anisotropy of the effective electron-phonon interaction. This results in a free-energy expression with four variational parameters. According to Feynman's conjecture, the resulting free energy is an upper bound to the exact result. The approximate free energy is expected to provide accurate results for arbitrary electron-phonon coupling strength (α), temperature (T), and magnetic field strength ($\mathscr{H}$). The free energy per polaron is evaluated for limiting values of α, T, and $\mathscr{H}$.

I. INTRODUCTION

Our objective is the calculation of the Helmholtz free energy F for a polaron in an ideal polaron gas[1] in interaction with an external uniform magnetic field $\mathscr{H}$. The magnetization, the magnetic susceptibility, the internal energy, the entropy, and the specific heat are subsequently obtained as derivatives of F. As a supplementary result we obtain an approximation to the polaron mass,[2] which is a function of the magnetic field strength. Furthermore, the polaron mass will be anisotropic because the magnetic field introduces a preferential direction into the system.

A variety of methods have been applied to the calculation of the ground-state energy of a polaron in a magnetic field. Most of them are restricted to the zero-temperature limit. In the weak and intermediate electron-phonon coupling limit Larsen[3] has modified the Lee-Low-Pines (LLP) method[4] to describe the ground-state energy and the low-lying-excited states of a polaron in a weak magnetic field. In the high magnetic field limit a method based on the LLP transformation and the Born-Oppenheimer approximation has been introduced by Evrard *et al.*[5] (EKD). In Ref. 6 Larsen presented a calculation of the polaron-energy spectrum for arbitrary magnetic fields valid in the small coupling limit by using second-order Rayleigh-Schrödinger perturbation theory (RSPT). In the same reference a variational generalization of the Haga ansatz[7] to arbitrary magnetic fields was derived. Bajaj[8] approximated the polaron energy spectrum, the cyclotron mass, and the longitudinal effective mass in a magnetic field, for the case of weak and intermediate electron-phonon coupling, by using an approach given by Onsager[9] that is based on the use of the Bohr-Sommerfeld quantization rule. Although in principle such a method is only valid for large quantum numbers (i.e., the classical limit) he showed that the results are also meaningful for small quantum numbers. The strong electron-phonon coupling limit was first studied by Porsch.[10] He applied the adiabatic approximation (in the polaron problem also called the Landau-Pekar approximation) to calculate the polaron ground-state energy and the longitudinal effective mass as function of the magnetic field. This approximation can be improved slightly by the inclusion of electron-phonon correlation effects as shown by Kartheuser and Negrete[11] (KN). The first systematic analytical and numerical calculation of the polaron ground-state energy for zero temperature, arbitrary electron-phonon coupling strength and arbitrary magnetic field strength was performed by Lépine and Matz.[12] These authors used Green's-function techniques to obtain a variational upper bound to the exact polaron ground-state energy in the Fock approximation. They showed analytically how the weak- and strong-coupling results, for small and large magnetic fields, as derived by previous methods, could be

reobtained.

The validity of the calculations on the magnetic field dependence of the polaron properties reported above is restricted to zero temperature. Extensions to nonzero temperature have been developed using the Feynman path-integral formalism.[13] Hellwarth and Platzman[14] were the first to extend Feynman's polaron theory[15] to nonzero magnetic field and nonzero temperature. Explicit calculations were made within the Feynman two-parameter model (this means an *isotropic* quadratic action) in the limit of small magnetic fields and low temperature. However, both limits were taken such that $\beta\hbar\omega_c \ll 1$ (ω_c is the cyclotron resonance frequency and $\beta=1/k_BT$ with T the lattice temperature and k_B the Boltzmann constant). In this limit they calculated the free energy, the magnetic susceptibility, and the polaron mass. They found that the magnetic field correction to the free energy is quadratic in ω_c, while at zero temperature the correction is linear in the magnetic field. Marshall and Chawla[16] have calculated this linear correction term within the same approach as in Ref. 14. Recently, Saitoh[17,18] used a general quadratic action with an infinite number of variational parameters to calculate the polaron free energy and effective mass in the limit of small[17] and large[18] magnetic fields. However, no numerical results were obtained in this work.

The purpose of the present paper (hereafter referred to as I) is to generalize Feynman's polaron theory[15] to arbitrary magnetic field strength and arbitrary temperature. To do so we shall apply the Feynman inequality.[19,20] Although Feynman's proof of this inequality is only valid if no magnetic field is present, there are intuitive reasons to believe that the inequality is also applicable in our situation. Our arguments in favor of this conjecture, which we call the Feynman conjecture because Feynman[19] had already suggested it in Ref. 19, are listed in the Appendix and are based on a comparison between the Feynman inequality and the Bogolyubov inequality.[21,22]

The trial action S_m used by Feynman is generalized as follows: First a magnetic field is included, and subsequently the quadratic self-interaction is chosen to be anisotropic. This *anisotropy* in the effective interaction is a novel feature not present in other approaches considered so far, with the exception of Ref. 18. The inclusion of the anisotropy in the effective electron-phonon interaction turns out to be very important in describing the high magnetic field properties of the polaron. Furthermore, it leads to interesting physical effects. This will be discussed in more detail in the following paper (hereafter referred to as II).

The outline of the present paper is as follows. We start in Sec. II with a brief discussion of the problem and show that in calculating the free energy along the lines of Ref. 15 it is sufficient to know the Fourier transform of the electron density-density correlation function as described by a trial action (or trial Hamiltonian) and the free energy corresponding with that trial action. In Sec. III we present a generalization of the Feynman trial action and show that it can be obtained from the Hamiltonian of an anisotropic Feynman polaron model. Static and dynamic properties of this Hamiltonian are calculated. We found that this model already exhibits some essential dynamic features, such as noncrossing of Landau levels and the appearance of the pinning effect, which are apparent in more detailed investigations on magneto-optics. The results of Secs. II and III are combined in Sec. IV to obtain an approximation for the polaron free energy. Most of the previous polaron theories are reobtained as limiting cases of the present result. However, the present result can be considered as a special case of Saitoh's[18] result, where the most general form for the quadratic trial action was used. Section V is devoted to the analytic calculation of different limits. The results are compared with other results obtained earlier by others. Finally, Sec. VI contains our concluding remarks where special reference is made to the recent work of Saitoh.[18] Units are used such that $\hbar=m=\omega_0=1$.

II. FORMULATION OF THE PROBLEM AND APPROXIMATION

The Hamiltonian that describes an electron interacting with the vibrational modes of a crystal and a constant uniform magnetic field is given by[23]

$$H=H_e+H_{\rm ph}+H_I \tag{1}$$

with

$$H_e=\frac{1}{2m}\left[\vec{p}+\frac{e\vec{A}}{c}\right]^2, \tag{2}$$

$$H_{\rm ph}=\sum_{\vec{k}}\omega_{\vec{k}}(a^\dagger_{\vec{k}}a_{\vec{k}}+\tfrac{1}{2}), \tag{3}$$

$$H_I=\sum_{\vec{k}}(V_{\vec{k}}a_{\vec{k}}e^{i\vec{k}\cdot\vec{r}}+V^*_{\vec{k}}a^\dagger_{\vec{k}}e^{-i\vec{k}\cdot\vec{r}}). \tag{4}$$

A free electron in a magnetic field $\vec{\mathscr{H}}=\mathrm{rot}\vec{A}$ with band mass m, electric charge $-e$, and conjugate coordinates $(\vec{r},\vec{p})$ is described by the Hamiltonian H_e. In the following the magnetic field is taken along the z axis, and the vector potential is written in the symmetrical Coulomb gauge

$$\vec{A}=\left[-\frac{\mathscr{H}}{2}y,\frac{\mathscr{H}}{2}x,0\right].$$

The operators $a^{\dagger}_{\vec{k}}$ and $a_{\vec{k}}$ are creation and annihilation operators for a phonon with wave vector $\vec{k}$ and frequency $\omega_{\vec{k}}$. The constant $V_{\vec{k}}$ gives the strength of the interaction between the electron and the field mode $\vec{k}$. For longitudinal-optical (LO) phonon scattering one has

$$\omega_{\vec{k}}=\omega_0\,,\qquad V_{\vec{k}}=i\frac{\hbar\omega_0}{k}\left[\frac{4\pi\alpha}{V}\right]^{1/2}\left[\frac{\hbar}{2m\omega_0}\right]^{1/4}, \tag{5}$$

ω_0 is the LO-phonon frequency, V the volume of the crystal, and α the dimensionless Fröhlich coupling constant.

The Helmholtz free energy may be written as

$$F=-\frac{1}{\beta}\ln Z$$

with

$$Z=\mathrm{Tr}\,e^{-\beta H}$$

the partition function. The trace can be split up into two parts, an electron part Tr_e and a phonon part $\mathrm{Tr}_{\mathrm{ph}}$,

$$Z=\mathrm{Tr}_e\circ\mathrm{Tr}_{\mathrm{ph}}(e^{-\beta H})=\int d\vec{r}\langle\vec{r},t\mid\mathrm{Tr}_{\mathrm{ph}}(e^{-\beta H})\mid\vec{r},t\rangle\,,$$

where the space integral is restricted to the crystal volume V. Time translational invariance allows us to take t equal to zero. Owing to the property that the Fröhlich Hamiltonian is quadratic in the phonon coordinates it is possible to perform the trace $\mathrm{Tr}_{\mathrm{ph}}$ exactly. Using a path-integral formulation one obtains[15,24,25]

$$Z=Z_{\mathrm{ph}}\int d\vec{r}\int D\vec{r}(u)\exp\{S[\vec{r}(u)]\}\delta(\vec{r}(\beta)-\vec{r})\delta(\vec{r}(0)-\vec{r}) \tag{6}$$

with $\int D\vec{r}$ an integral over all possible electron paths. The variable u is related to the real time variable t via $u=it$. The partition function of the free-phonon system (which is a set of harmonic oscillators) appears as a factor in Eq. (6), which for LO phonons is equal to

$$Z_{\mathrm{ph}}=\mathrm{Tr}\,e^{-\beta H_{\mathrm{ph}}}=[2\sinh(\beta/2)]^{-N} \tag{7}$$

with N the number of phonon modes. The action $S[\vec{r}]$ in Eq. (6) was obtained after the exact elimination of the phonon coordinates and thus is a functional of the electron position coordinates only. It is given by[24,25]

$$S=S_e+S_I\,, \tag{8a}$$

$$S_e=-\tfrac{1}{2}\int_0^{\beta}du\{\dot{\vec{r}}(u)^2+i\omega_c[x(u)\dot{y}(u)-y(u)\dot{x}(u)]\}\,, \tag{8b}$$

$$S_I=\sum_{\vec{k}}|V_{\vec{k}}|^2\int_0^{\beta}du\int_0^{\beta}ds\,G_{\omega_{\vec{k}}}(u-s)\exp\{i\vec{k}\cdot[\vec{r}(u)-\vec{r}(s)]\}\,, \tag{8c}$$

where

$$G_{\omega}(u)=\tfrac{1}{2}n(\omega)(e^{\omega|u|}+e^{\omega(\beta-|u|)}) \tag{8d}$$

is the phonon Green's function, $\omega_c=e\mathscr{H}/mc$ the cyclotron frequency, and $n(\omega)=(e^{\beta\omega}-1)^{-1}$ the number of phonons with frequency ω.

The path integral in Eq. (6) with the action (8a)–(8c) has not been evaluated exactly. To obtain a reasonable approximation to Eq. (6) we shall proceed along the lines indicated by Feynman.[15] Instead of the action S consider a trial (or model) action S_m that describes the electron evolution in an approximate way. Furthermore, S_m is taken such that path integrals with this action can be done exactly. S_m defines a partition function

$$Z_m=e^{-\beta F_m}\equiv\int d\vec{r}\int D\vec{r}(u)\exp\{S_m[\vec{r}(u)]\}\delta(\vec{r}(\beta)-\vec{r})\delta(\vec{r}(0)-\vec{r}) \tag{9}$$

and an expectation value

$$\langle A[r]\rangle_m=\frac{1}{Z_m}\int d\vec{r}\int D\vec{r}(u)e^{S_m}A[\vec{r}(u)]\delta(\vec{r}(\beta)-\vec{r})\delta(\vec{r}(0)-\vec{r}) \tag{10}$$

for any functional $A[r]$. These notations allow us to write Eq. (6) as follows:

$$Z = Z_{\rm ph} Z_m \langle \exp(S - S_m) \rangle_m \ .$$

If the actions S and S_m are real one can apply the convexity property of the function e^x to establish the inequality

$$\langle \exp(S - S_m) \rangle_m \geq \exp(\langle S - S_m \rangle_m) \ ,$$

which leads to the Feynman variational principle[15,20] for the free energy

$$F \leq F_{\rm ph} + F_m - \frac{1}{\beta} \langle S - S_m \rangle_m \ . \tag{11}$$

For the problem under study the actions S and S_m are complex quantities. However, as argued in the Appendix we accept Feynman's conjecture that Eq. (11) can be applied in the present situation because S and S_m (see next section) are derivable from Hermitian Hamiltonians after the elimination of the appropriate variables.

With the assumption that S_m is derivable from a Hermitian Hamiltonian H_F (with corresponding Lagrangian L_F) after the elimination of the variable $\vec{\mathbf{R}}$ (the generalization to more variables is straightforward) one may write

$$e^{S_m} = \frac{1}{Z_R} \int d\vec{\mathbf{R}} \int d\vec{\mathbf{R}}(u) e^{S_F} \delta(\vec{\mathbf{R}}(\beta) - \vec{\mathbf{R}}) \times \delta(\vec{\mathbf{R}}(0) - \vec{\mathbf{R}}) \ , \tag{12}$$

where the action S_F is given by

$$S_F[\vec{\mathbf{r}}, \vec{\mathbf{R}}] = \int_0^\beta du \, L_F(i\dot{\vec{\mathbf{r}}}, i\dot{\vec{\mathbf{R}}}; \vec{\mathbf{r}}, \vec{\mathbf{R}}) \ ,$$

and L_F is a Lagrangian describing a two-particle problem, with a corresponding Hamiltonian $H_F = H_e + H_R + H_{e,R}$ [the significance of the different terms is similar to those of Eq. (1)]. In Eq. (12) we used the partition function $Z_R = \mathrm{Tr}[\exp(-\beta H_R)]$ [see also Eqs. (6) and (7)]. The partition function Z_F corresponding to the Hamiltonian H_F is given by

$$Z_F = e^{-\beta F_F} = \mathrm{Tr}(e^{-\beta H_F}) = \int d\vec{\mathbf{r}} \int d\vec{\mathbf{R}} \int D\vec{\mathbf{r}}(u) \int D\vec{\mathbf{R}}(s) e^{S_F} \delta(\vec{\mathbf{r}}(\beta) - \vec{\mathbf{r}}) \delta(\vec{\mathbf{r}}(0) - \vec{\mathbf{r}}) \delta(\vec{\mathbf{R}}(\beta) - \vec{\mathbf{R}}) \delta(\vec{\mathbf{R}}(0) - \vec{\mathbf{R}}) \ . \tag{13}$$

Inserting Eq. (12) into Eq. (9) and using Eq. (13) results in

$$Z_F = Z_R Z_m = e^{-\beta(F_R + F_m)} \ ,$$

which implies that

$$F_m = F_F - F_R \ . \tag{14}$$

The expectation value (10) can be written in terms of the action S_F by using Eqs. (12) and (14):

$$\langle A[\vec{\mathbf{r}}] \rangle_m = \frac{1}{Z_F} \int d\vec{\mathbf{r}} \int d\vec{\mathbf{R}} \int D\vec{\mathbf{r}}(u) \int D\vec{\mathbf{R}}(s) e^{S_F} A[\vec{\mathbf{r}}] \delta(\vec{\mathbf{r}}(\beta) - \vec{\mathbf{r}}) \delta(\vec{\mathbf{r}}(0) - \vec{\mathbf{r}}) \delta(\vec{\mathbf{R}}(\beta) - \vec{\mathbf{R}}) \delta(\vec{\mathbf{R}}(0) - \vec{\mathbf{R}}) = \langle A[r] \rangle_F \ . \tag{15}$$

The subscript F in the notation $\langle \ \rangle_F$ refers to the weight function e^{S_F}.

Because S_F contains only equal-time interactions it becomes possible to make the link with the operator formalism. Using Ref. 26 [see formula (18.12) on p. 49] the expectation value (15) may be written as

$$\langle A[\vec{\mathbf{r}}] \rangle_m = \langle T_c A[\hat{\vec{\mathbf{r}}}(u)] \rangle_F \tag{16}$$

with the operator

$$\hat{\vec{\mathbf{r}}}(u) = e^{uH_F} \hat{\vec{\mathbf{r}}}(0) e^{-uH_F} \tag{17}$$

and the expectation value

$$\langle A \rangle_F = \frac{1}{Z_F} \mathrm{Tr}(e^{-\beta H_F} A) \ . \tag{18}$$

The time-ordering operator for imaginary times is labeled by T_c. Using Eqs. (14) and (16) the approximation to the free energy [Eq. (11)] can be written in the operator formalism. To simplify the expectation value $\langle S - S_m \rangle_m$, we choose a trial action of the form

$$S_m = S_e + S_{m,I} \tag{19}$$

with S_e given by Eq. (8b) and $S_{m,I}$ the self-

interaction part of the trial action, which will be chosen quadratic in the electron coordinates (see Sec. III). The expectation value $\langle S-S_m\rangle_m$ splits up into two terms [use Eqs. (8a) and (19)]

$$\langle S-S_m\rangle_m=\langle S_I\rangle_m-\langle S_{m,I}\rangle_m \ . \tag{20}$$

The calculation of the first term, $\langle S_I\rangle_m$, results in evaluating

$$f(\vec{k},u,s)=\langle e^{i\vec{k}\cdot[\vec{r}(u)-\vec{r}(s)]}\rangle_m \tag{21a}$$

or in terms of operators [use Eq. (16)]

$$f(\vec{k},u,s)=\langle T_c(e^{i\vec{k}\cdot\hat{\vec{r}}(u)}e^{i\vec{k}\cdot\hat{\vec{r}}(s)})\rangle_F \ . \tag{21b}$$

If the self-interaction part of the trial action is quadratic, the expectation value $\langle S_{m,I}\rangle_m$ results in evaluating terms like

$$\langle[\vec{r}(u)-\vec{r}(s)]\cdot\overleftrightarrow{G}\cdot[\vec{r}(u)-\vec{r}(s)]\rangle_m$$
$$=-\nabla_{\vec{k}}f(\vec{k},u,s)\cdot\overleftrightarrow{G}\cdot\nabla_{\vec{k}}f(\vec{k},u,s)\,|_{\vec{k}=0} \tag{22}$$

where $\overleftrightarrow{G}$ is a tensor that may depend on u and s but is independent of the electron coordinates.

From Eqs. (21a) and (22) it is apparent that the key quantity to evaluate is $f(\vec{k},u,s)$. This function is related to the Fourier transform of the electron density-density correlation function (for the definition see, e.g., Ref. 27, p. 370)

$$S(\vec{k},t)=\langle e^{-i\vec{k}\cdot\vec{r}(0)}e^{i\vec{k}\cdot\vec{r}(t)}\rangle \tag{23}$$

in the following way [using the property $\mathrm{Tr}(AB)=\mathrm{Tr}(BA)$]:

$$f(\vec{k},u,s)=\begin{cases}S_c(-\vec{k},|u-s|), & u>s\\ S_c(\vec{k},|u-s|), & u<s\end{cases} \tag{24}$$

with

$$S_c(\vec{k},u)=S(\vec{k},iu) \ .$$

With expression (24) in mind, the expectation value $\langle S_I\rangle_m$ can be reduced to a more convenient form by applying the property

$$S_c(\vec{k},u)=S_c(-\vec{k},\beta-u), \ u \text{ real} \tag{25a}$$

which is a direct consequence of the Kubo-Martin-Schwinger (KMS) condition. Indeed, the density matrix is of the form $\rho=e^{-\beta H}/\mathrm{Tr}(e^{-\beta H})$ (in the present case the Hamiltonian H becomes H_F) and thus satisfies the KMS condition, which induces the following properties[28] (the variable z is in general complex):

(i) $S(\vec{k},z)=S(-\vec{k},i\beta-z)$.

(ii) $S(\vec{k},z)=S^*(\vec{k},-z^*)$.

(iii) $S(\vec{k},z)$ is analytic for $0<\mathrm{Im}z<\beta$, and $S(\vec{k},z)$ is continuous and uniform bounded for $0\le\mathrm{Im}z\le\beta$.

The first property (i) implies Eq. (25a), while the second one gives

$$S_c(\vec{k},u)=S_c^*(\vec{k},u), \ u \text{ real} \ . \tag{25b}$$

The above properties and Eqs. (24), (25a), and (25b) will be used to simplify $\langle S_I\rangle_m$ significantly. Define the function

$$g(u)=\sum_{\vec{k}}|V_{\vec{k}}|^2G_{\omega_{\vec{k}}}(u)S_c(\vec{k},u) \ ,$$

which allows us to write Eq. (8c) as

$$\langle S_I\rangle_m=\int_0^\beta du\int_0^\beta ds\, g(|u-s|) \ ,$$

where use has been made of the equalities $|V_{\vec{k}}|^2=|V_{-\vec{k}}|^2$ and $\omega_{\vec{k}}=\omega_{-\vec{k}}$ that follow directly from the time-reversal symmetry of the electron-phonon system. From the property $g(u)=g(\beta-u)$, which is induced by Eq. (25a), it follows that

$$\langle S_I\rangle_m=\beta\int_0^\beta du\, g(u) \ ,$$

and after some simplifications the final expression is obtained:

$$\frac{1}{\beta}\langle S_I\rangle_m=\sum_{\vec{k}}|V_{\vec{k}}|^2[1+n(\omega_{\vec{k}})]$$
$$\times\int_0^\beta du\, S_c(\vec{k},u)e^{-\omega_{\vec{k}}u} \ . \tag{26}$$

To resume the results of this section, given a Hermitian model Hamiltonian H_F one can find an approximation to the exact free energy [see Eq. (11)]. In doing this, one needs to know the free energy corresponding to H_F and the Fourier-transformed density-density correlation function of the electron as described by H_F. Equation (11), which was obtained in the path-integral formalism, is thus expressed in the operator formalism. The choice of the relevant model Hamiltonian H_F, which will be used in the present paper, is discussed in the next section.

III. STATIC AND DYNAMIC STUDY OF THE GENERALIZED FEYNMAN POLARON MODEL IN A MAGNETIC FIELD

First we will discuss the choice of the trial action. In the zero magnetic field case Feynman[20]

introduced a trial action that can be obtained from a two-particle Hamiltonian after elimination of the coordinates of one of the two particles. This Hamiltonian describes an electron that is coupled to a second particle via a harmonic force. This second particle, also called the fictitious particle (because its coordinates must be eliminated to obtain the trial action), simulates the polarization cloud around the electron. The mass of the fictitious particle and the coupling between the electron and the fictitious particle are a measure for the effective electron-phonon interaction. This model system is called the Feynman polaron model.

The application of an external static magnetic field will influence the electron motion. It not only introduces a preferential direction, but it will also influence the efficiency with which the electron interacts with the phonons. Indeed, the mass of the fictitious particle and the strength of the effective interaction will depend on the direction and on the strength of the applied field. As will be seen later, the direction and field dependence of the effective interaction will be of fundamental importance for the appearance of certain physical phenomena.

In view of the foregoing discussion it seems reasonable to generalize the isotropic Feynman polaron Hamiltonian to a Hamiltonian with anisotropy in both the coupling and mass of the fictitious particle. Using the axial symmetry around the direction of the magnetic field we introduce the following generalization of the Feynman polaron Hamiltonian:

$$H_F = H_{||} + H_\perp$$

with

$$H_{||} = \frac{p_z^2}{2m} + \frac{p_z'^2}{2m'_{||}} + \tfrac{1}{2}\kappa_{||}(z-z')^2 ,$$

$$H_\perp = \frac{1}{2m}(p_x - \tfrac{1}{2}m\omega_c y)^2 + \frac{1}{2m}(p_y + \tfrac{1}{2}m\omega_c x)^2 + \sum_{i=x,y}\left[\frac{p_i'^2}{2m'_\perp} + \tfrac{1}{2}\kappa_\perp (r_i - r_i')^2\right] .$$

This Hamiltonian describes an electron with coordinates $(\vec{r},\vec{p})$ and mass $m=1$, subjected to a magnetic field $\vec{\mathcal{H}} = \mathcal{H}\vec{e}_z$ and interacting with a second particle, called the fictitious particle, with coordinates $(\vec{r}',\vec{p}')$ and diagonal mass tensor

$$\begin{bmatrix} m'_\perp & 0 & 0 \\ 0 & m'_\perp & 0 \\ 0 & 0 & m'_{||} \end{bmatrix} .$$

The interaction is quadratic with a coupling tensor

$$\begin{bmatrix} \kappa_\perp & 0 & 0 \\ 0 & \kappa_\perp & 0 \\ 0 & 0 & \kappa_{||} \end{bmatrix} .$$

After eliminating the coordinates of the fictitious particle one obtains an action S_m, which is a functional of the electron coordinates only. This action will be used as our trial action S_m and is given by

$$S_m = S_e + S_{m,I} , \tag{27}$$

where S_e is given by Eq. (8b) and

$$S_{m,I} = -\sum_{i=1}^{3} C_i \int_0^\beta du \int_0^\beta ds\, G_{w_i}(u-s) \times [r_i(u) - r_i(s)]^2 . \tag{28}$$

The constants $C_\perp = C_1 = C_2$, $C_{||} = C_3$ and $w_\perp = w_1 = w_2$, $w_{||} = w_3$ are given by

$$w_i^2 = \frac{\kappa_i}{m_i'} , \quad v_i^2 = \kappa_i \frac{1+m_i'}{m_i'} ,$$

$$C_i = \frac{w_i}{4}(v_i^2 - w_i^2) , \quad i = \perp, || .$$

Note that the action (28) is a function of four parameters namely, $v_\perp, v_{||}, w_\perp, w_{||}$, which will be determined variationally. The original Feynman trial action is obtained if we take $v = v_\perp = v_{||}$, $w = w_\perp = w_{||}$, and $\omega_c = 0$.

A. Exact diagonalization of the Hamiltonian H_F

The Hamiltonian H_F has twelve degrees of freedom. Thus the diagonalization of H_F is equivalent with the diagonalization of a 12×12 matrix. The z component does not couple with the xy components, and therefore the diagonalization of H_F is divided into the diagonalization of $H_{||}$ (four degrees of freedom) and the diagonalization of $H_\perp$ (eight degrees of freedom).

1. *Diagonalization of* $H_{||}$

The Hamiltonian $H_{||}$ has four degrees of freedom, so a 4×4 matrix must be diagonalized. This has been done in Ref. 24. The results can be summarized as follows:

$$H_{||}=\frac{P_{||}^2}{2M_{||}}+s_0(C_0^\dagger C_0+\tfrac{1}{2}) \tag{29}$$

with $R_{||}$ and $P_{||}$ the conjugate variables of the center of mass and $C_0^\dagger$ and C_0, respectively, the creation and annihilation operators for the internal oscillation with frequency $s_0=v_{||}$. The total mass $M_{||}$ is given by

$$M_{||}=1+m'_{||} . \tag{30}$$

The explicit time evolution of the z component of the electron coordinate can be expressed in terms of the normal coordinates

$$z(t)=R_{||}+\frac{P_{||}}{M_{||}}t+d_0(C_0e^{-is_0t}+C_0^\dagger e^{is_0t}) \tag{31}$$

with

$$d_0^2=\frac{m'_{||}}{2M_{||}}\frac{1}{s_0}=\frac{v_{||}^2-w_{||}^2}{2v_{||}^3} . \tag{32}$$

2. *The exact diagonalization of $H_\perp$*

The diagonalization of $H_\perp$ is equivalent with the diagonalization of a real symmetric 8×8 matrix. One of us (J.T.D.) and others[29] have performed a partial diagonalization of $H_\perp$ in the following way. After a canonical transformation the nondiagonal part in the transformed Hamiltonian was handled as a perturbation to the diagonal part. Then with perturbation theory the low-lying energy levels were calculated. In the following, an *exact* diagonalization of $H_\perp$ will be given.

We proceed via the Heisenberg equations of motion, because solving the equations of motion is equivalent with an exact diagonalization of the Hamiltonian. For example, the explicit time dependence of the electron position coordinate provides the eigenfrequencies (and thus the eigenvalues of $H_\perp$) as well as the normal coordinates [see, e.g., Eq. (31)]. The equations of motion for the position and momentum variables form a set of eight linear first-order differential equations because $H_\perp$ is quadratic and has eight degrees of freedom. The solution of this set of equations is rather lengthy but straightforward. Therefore only a brief outline of the calculation will be given.

After eliminating the momentum variables the eight coupled first-order linear differential equations reduce to four coupled second-order linear differential equations. Taking the Laplace transform of these equations results in four coupled nonhomogeneous algebraic equations, which can be solved analytically. One only has to deal with 4×4 matrices. Then the inverse Laplace transform gives the explicit time dependence of the position coordinates in terms of the normal coordinates.

The results of such a calculation can be summarized as follows.

(i) The normal coordinates are:

(a) Two constants of motion (which were already introduced in Ref. 29) Π_1 and Π_2, which are related to the classical orbital center. Namely, in classical mechanics $(-\Pi_2/\omega_c,\Pi_1/\omega_c)$ are the position coordinates of the center of mass.

(b) Three creation and three annihilation operators $\{C_i^\dagger,C_i \mid i=1,2,3\}$ (the approximate calculation of Ref. 29 leads to four creation and annihilation operators) for internal oscillations with frequency $s_1\le s_2\le s_3$, which are given by the positive roots of the equation

$$s^2(s^2-v_\perp^2)^2-\omega_c^2(s^2-w_\perp^2)^2=0 . \tag{33}$$

(ii) The explicit time evolution of the electron position coordinates takes the form

$$x(t)=-\frac{\Pi_2}{\omega_c}-\sum_{j=1}^{3}d_j(C_je^{-is_jt}+C_j^\dagger e^{is_jt}) , \tag{34}$$

$$y(t)=\frac{\Pi_1}{\omega_c}+i\sum_{j=1}^{3}(-1)^jd_j(C_je^{-is_jt}-C_j^\dagger e^{is_jt}) , \tag{35}$$

with

$$d_j^2=\frac{1}{2s_j}\frac{s_j^2-w_j^2}{3s_j^2+2(-1)^j\omega_cs_j-v_\perp^2} , \quad j=1,2,3 . \tag{36}$$

(iii) The diagonalized Hamiltonian becomes

$$H_\perp=\sum_{j=1}^{3}s_j(C_j^\dagger C_j+\tfrac{1}{2}) , \tag{37}$$

which consists of three one-dimensional harmonic oscillators. The energy levels are given by

$$E_\perp(n_1,n_2,n_3)=\sum_{j=1}^{3}s_j(n_j+\tfrac{1}{2}) , \tag{38}$$

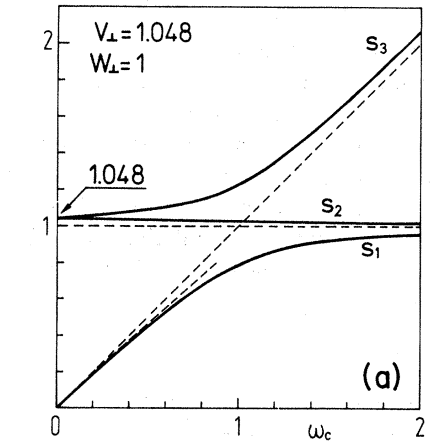
where n_j are positive integers.

B. Physical interpretation of the eigenfrequencies

In Fig. 1(a) the eigenfrequencies s_j, which are given by the roots of Eq. (33), are plotted as a

function of the magnetic field for a particular choice of the parameters $v_\perp$ and $w_\perp$. As an example, we took $w_\perp=1$ and $v_\perp=1.048$. From this figure it is apparent that the eigenfrequencies s_1 and s_3 can be related to the resonance transition energies of free electrons in a magnetic field and in polar semiconductors.[30,31]

Using the same choice of parameters (i.e., $w_\perp=1$ and $v_\perp=1.048$) we have plotted in Fig. 1(b) the ground-state energy $E_\perp(0,0,0)$ and the energy of some excited states [namely $E_\perp(1,0,0)$ and $E_\perp(0,0,1)$] of the model Hamiltonian $H_\perp$. The energy scale is lifted with the zero point energy of $H_\perp$ at zero magnetic field and the unperturbed Landau energy levels are drawn as dashed lines in Fig. 1(b). In a perturbation calculation of the polaron ground-state energy the spectrum of a free electron in a magnetic field is used [dashed lines in Fig. 1(b)] as the unperturbed part, while in the present approach we used the spectrum of $H_\perp$ as the unperturbed part [solid lines in Fig. 1(b)]. This model Hamiltonian $H_\perp$ allows us to take into account the following two effects (which in other approaches results only after a perturbative calculation):



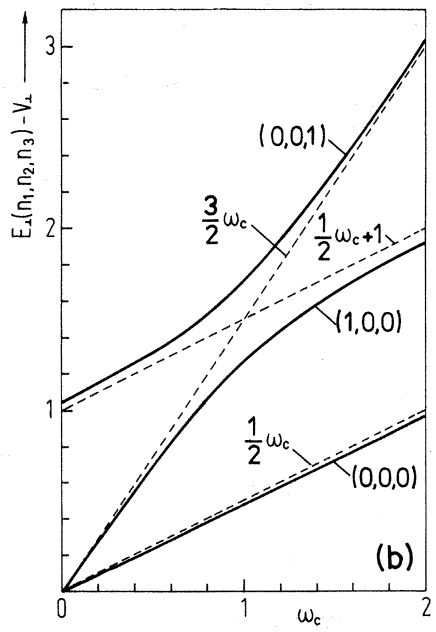


FIG. 1. (a) shows the eigenfrequencies [which are determined by Eq. (33)] of the Feynman polaron Hamiltonian as a function of the magnetic field. The low-lying energy states of the same Hamiltonian [see Eq. (38)] are plotted in (b). The dashed lines indicate the energy levels of the noninteracting system.

(1) The absence of level crossing at $\omega_c=1$. Namely, at $\omega_c=1$ there is a crossing of the unperturbed energy levels $\frac{3}{2}\omega_c$ (no phonons and the first Landau level) and $\frac{1}{2}\omega_c+1$ (one phonon and the zeroth Landau level) that is lifted by the interaction of the electron with the LO phonons. The consequence of this effect is the appearance of a doublet structure in the magneto-optical spectrum.[30–33]

(2) The pinning effect. For $\omega_c\to\infty$ the energy level $E_\perp(1,0,0)$ is pinned[6,34–39] to the unperturbed energy $\frac{1}{2}\omega_c+1$ [see Fig. 1(b)].

C. The free energy

The free energy of the system described by the Hamiltonian $H_F=H_1+H_{||}$ will be calculated. From the diagonalized Hamiltonian [see Eqs. (29) and (37)] one notes that the partition function is the product of the partition function of a one-dimensional free particle with mass $M_\perp$ and the partition function of four one-dimensional harmonic oscillators. Furthermore, one must sum over all allowed values of the constants of the motion Π_1 and Π_2; this sum is equal to $(L_xL_y/2\pi)m\omega_c$ (see Ref. 27, p. 217). Assume that the system is confined to move in a box with dimensions L_x, L_y, and L_z and volume $V=L_xL_yL_z$. Then the partition function is given by

$$Z_F=\frac{V}{2\pi}\omega_c\left[\frac{M_{||}}{2\pi\beta}\right]^{1/2}\prod_{\mu=0}^{3}\frac{1}{2\sinh(\frac{1}{2}s_\mu\beta)} \tag{39}$$

from which the free energy,

$$F_F=-\frac{1}{\beta}\ln Z_F\ ,$$

is easily calculated. At zero temperature the free energy reduces to the zero point energy of the model Hamiltonian H_F [see Eqs. (29) and (37)].

D. Fourier transform of the electron density-density correlation function

As shown in Sec. II the Fourier transform of the density-density correlation function of the electron, whose time evolution is described by the model Hamiltonian H_F, must be calculated. From the diagonalized form of the model Hamiltonian [Eqs. (29) and (37)] and the explicit time dependence of the electron coordinate [see Eqs. (31), (34), and (35)] it is clear that the correlation function $S(\vec{k},t)$ [see Eq. (23)] can be written as a product of five functions:

$$S(\vec{k},t)=S_4(\vec{k},t)\prod_{\mu=0}^{3}S_\mu(\vec{k},t) \tag{40}$$

with

$$S_0(\vec{k},t)=\langle\exp[-id_0k_z(C_0+C_0^\dagger)]\exp[id_0k_z(C_0e^{-is_0t}+C_0^\dagger e^{is_0t})]\rangle_F\ , \tag{41}$$

$$S_j(\vec{k},t)=\langle\exp(id_j\{[k_x-i(-1)^jk_y]C_j+[k_x+i(-1)^jk_y]C_j^\dagger\}) \times\exp(-id_j\{[k_x-i(-1)^jk_y]C_je^{-is_jt}+[k_x+i(-1)^jk_y]C_j^\dagger e^{is_jt}\})\rangle_F\ ,\quad j=1,2,3 \tag{42}$$

and

$$S_4(\vec{k},t)=\left\langle\exp(-ik_zR_{||})\exp\left[ik_zR_{||}+i\frac{k_zP_{||}}{M_{||}}t\right]\right\rangle_F\ . \tag{43}$$

As an example we calculate $S_0(\vec{k},t)$. The operators can be put into normal order by applying the commutation relation twice,

$$e^Ae^B=e^{A+B}e^{[A,B]/2}\ , \tag{44}$$

which is valid if $[A,B]$ commutes with A and B. This gives

$$S_0(\vec{k},t)=\exp[-d_0^2k_z^2(1-e^{is_0t})]\langle\exp[id_0k_zC_0^\dagger(e^{is_0t}-1)]\exp[-id_0k_zC_0(e^{-is_0t}-1)]\rangle_F\ .$$

Using the identity (see, e.g., Ref. 38, p. 374)

$$\langle e^{\vec{q}^*\cdot\vec{c}^\dagger}e^{-\vec{q}\cdot\vec{c}}\rangle=\mathrm{Tr}(e^{-\beta\Omega\vec{c}^\dagger\cdot\vec{c}}e^{\vec{q}^*\cdot\vec{c}^\dagger}e^{-\vec{q}\cdot\vec{c}})/\mathrm{Tr}(e^{-\beta\Omega\vec{c}^\dagger\cdot\vec{c}})=\exp[-|\vec{q}|^2n(\Omega)]\ , \tag{45}$$

one obtains

$$S_0(\vec{k},t)=\exp\left[-k_z^2d_0^2\left[1-e^{is_0t}+4n(s_0)\sin^2\frac{s_0t}{2}\right]\right]\ .$$

The other four functions are calculated in an analogous way (see, e.g., Ref. 39 for a similar calculation). The final result is

$$S(\vec{k},t)=\exp[-k_z^2D^0(t)]\exp[-k_\perp^2D_H^0(t)]\ , \tag{46}$$

with

$$k_\perp^2=k_x^2+k_y^2\ , \tag{47a}$$

$$D^0(t)=\frac{1}{2M_{||}}\left[-it+\frac{t^2}{\beta}\right]+d_0^2\left[1-e^{is_0t}+4n(s_0)\sin^2\frac{s_0t}{2}\right]\ , \tag{47b}$$

$$D_H^0(t)=\sum_{j=1}^{3}d_j^2\left[1-e^{is_jt}+4n(s_j)\sin^2\frac{s_jt}{2}\right]\ . \tag{47c}$$

In the expression for the free energy one needs the function $S(\vec{k},t)$ for imaginary argument:

$$S_c(\vec{k},u)=\exp[-k_z^2 D(u)]\exp[-k_\perp^2 D_H(u)] , \tag{48}$$

where

$$D(u)=\frac{u}{2M_{||}}\left[1-\frac{u}{\beta}\right]+d_0^2\left[1-e^{-s_0 u}-4n(s_0)\sinh^2\frac{s_0 u}{2}\right] , \tag{49a}$$

$$D_H(u)=\sum_{j=1}^{3} d_j^2\left[1-e^{-s_j u}-4n(s_j)\sinh^2\frac{s_j u}{2}\right] . \tag{49b}$$

The last two functions have the property

$$\lim_{\omega_c\to 0} D_H(u)=D(u) .$$

In the special case of an isotropic Feynman model ($v=v_\perp=v_{||}$, $w=w_\perp=w_{||}$) Hellwarth and Platzman[14] calculated the same functions via path-integral techniques [see Eq. (16) in Ref. 14]. The correspondence between the function $G(u)$ in Ref. 14 and the function $D_H(u)$ above is as follows: $D_H(u)=D(u)-\omega_c^2 G(u)$. In Ref. 14 $D(u)$ and $G(u)$ are represented as an infinite sum, while here these functions are given in a closed analytic form.

IV. GENERAL ANALYTIC EXPRESSION FOR THE POLARON FREE ENERGY AND RELATION TO OTHER THEORIES

The results of Secs. II and III will be combined to obtain an explicit expression for the polaron free energy for arbitrary temperature, electron-phonon coupling, and magnetic field strength. The zero-temperature limit of the free energy, which in this limit is equal to the polaron ground-state energy, will be given. Furthermore, the relation between the present result and those derived earlier by other authors will be pointed out.

A. Analytic expression for the polaron free energy

Equation (11) [see also Eq. (20)] gives a general expression for an upper bound to the exact free energy

$$F\le F_{\rm ph}+F_m-\frac{1}{\beta}\langle S_I\rangle_m+\frac{1}{\beta}\langle S_{m,I}\rangle_m . \tag{50}$$

The free energy of the phonons, in the absence of the electron, is obtained from Eq. (7) and is equal to

$$F_{\rm ph}=\frac{N}{\beta}\ln\left[2\sinh\frac{\beta}{2}\right] . \tag{51}$$

The trial action S_m defines the free energy [see Eqs. (9) and (14)]

$$F_m=F_F-F_R , \tag{52}$$

with F_F the free energy of the generalized Feynman polaron model [see Eq. (39)]

$$F_F=\frac{1}{\beta}\sum_{\mu=0}^{3}\ln\left[2\sinh\frac{\beta s_\mu}{2}\right]-\frac{1}{\beta}\ln\left[\frac{v_{||}}{w_{||}}\frac{\omega_c}{2\pi}\frac{1}{\sqrt{2\pi\beta}}\right]-\frac{1}{\beta}\ln V , \tag{53}$$

and F_R is the free energy of the fictitious particle in the generalized Feynman polaron model in the absence of the electron. Equivalently, it is the free energy of the Hamiltonian (see Sec. III)

$$H_R=\sum_{i=1}^{3}\left[\frac{p_i'^2}{2m_i'}+\tfrac{1}{2}\kappa_i r_i'^2\right]$$

which equals

$$F_R=\frac{2}{\beta}\ln\left[2\sinh\frac{\beta w_\perp}{2}\right]+\frac{1}{\beta}\ln\left[2\sinh\frac{\beta w_{||}}{2}\right] . \tag{54}$$

The expectation value of S_I is obtained from Eqs. (26) and (47). For LO phonons and in the limit of an infinite crystal volume one obtains

$$F_I=\frac{1}{\beta}\langle S_I\rangle_m=\frac{\alpha}{2\sqrt{2\pi}}[1+n(\omega_0)]\times\int_0^\beta du\frac{e^{-u}}{\sqrt{H(u)}}\ln\left[\frac{\sqrt{D(u)}+\sqrt{H(u)}}{\sqrt{D(u)}-\sqrt{H(u)}}\right] , \tag{55}$$

where $H(u)=D(u)-D_H(u)$; $D(u)$ and $D_H(u)$ are given by Eqs. (49a) and (49b).

Two different methods can be used to calculate $\langle S_{m,I}\rangle_m$, where $S_{m,I}$ is given by Eq. (28). One can use the expectation value (22) and expressions (24) and (48) to obtain $\langle S_{m,I}\rangle_m$. However, another and more convenient approach uses the equality

$$-\frac{1}{\beta}\langle S_{m,I}\rangle_m = C_\perp \frac{\partial F_m}{\partial C_\perp} + C_{||}\frac{\partial F_m}{\partial C_{||}} , \tag{56}$$

which is obtained from the Eqs. (9), (10), (19), and (28). Inserting Eqs. (52), (53), and (54) into Eq. (56) one obtains

$$\begin{aligned} F_{m,I} &= -\frac{1}{\beta}\langle S_{m,I}\rangle_m \\ &= \frac{C_\perp}{v_\perp w_\perp}\sum_{j=1}^{3}\frac{\partial s_j}{\partial v_\perp}\coth\frac{\beta s_j}{2} \\ &\quad + \frac{C_{||}}{v_{||}w_{||}}\left[-\frac{2}{\beta v_{||}}+\coth\frac{\beta v_{||}}{2}\right] , \end{aligned} \tag{57}$$

where the derivatives $\partial s_j/\partial v_\perp$ are obtained from Eq. (33) and are given by

$$\frac{\partial s_j}{\partial v_\perp} = \frac{2v_\perp s_j}{3s_j^2+2(-1)^j\omega_c s_j - v_\perp^2} . \tag{58}$$

The free energy of the phonons $F_{\rm ph}$ [see Eq. (51)] and the volume contribution $-(1/\beta)\ln V$ in Eq. (53) only give a constant contribution to the free energy. In the following this constant contribution will be subtracted from the right-hand side of Eq. (50). This amounts to shifting the zero point of the free energy. Finally, we obtain the following approximation to the polaron free energy:

$$F_{\rm as} = F_0 - F_{m,I} - F_I \tag{59a}$$

with

$$F_0 = -\frac{1}{\beta}\ln\left[\frac{1}{2\pi}\frac{v_{||}}{w_{||}}\frac{\omega_c}{\sqrt{2\pi\beta}}\frac{2\sinh\frac{\beta w_{||}}{2}}{2\sinh\frac{\beta v_{||}}{2}} \times \frac{\left[2\sinh\frac{\beta w_\perp}{2}\right]^2}{\prod_{i=1}^{3}2\sinh\frac{\beta s_i}{2}}\right] . \tag{59b}$$

Equation (59a) is the central result of the present paper. The subscript "as" in Eq. (59a) indicates that the trial action contains an anisotropic effective electron-phonon interaction. Expression (59a) is valid for all α, T, ω_c and depends on four variational parameters $v_\perp, w_\perp, v_{||}, w_{||}$. Thus we may write

$$F_{\rm as} = F_{\rm as}(\alpha, T, \omega_c; v_\perp, w_\perp, v_{||} w_{||}) ,$$

where the variational parameters will be determined so that $F_{\rm as}$ takes its minimum value. The minimalization of Eq. (59) to the four parameters has to be performed numerically (see paper II) except for some limiting cases where the minimalization can be done analytically (see the next section).

B. Relation to other theories

The relation between the present result, Eq. (59a), and the result of some other theories is represented schematically in Fig. 2. Hellwarth and Platzman[14] extended Feynman's path-integral variational calculation to include the effect of an external magnetic field. As a trial action they choose a general quadratic symmetric action. The general results were presented in terms of infinite series. Explicit analytic results were derived in Ref. 14, within, the isotropic Feynman polaron model, in the limit of small magnetic fields ($\omega_c \ll 1$) and low temperature ($\beta \gg 1$, but such that $\beta\omega_c \ll 1$). We have verified that in the limits considered our result is identical to the one of Ref. 14.

In the zero magnetic field limit one has $v = v_\perp = v_{||}$, $w = w_\perp = w_{||}$ and Eq. (59a) transforms to the result of Osaka.[24] Taking the zero-temperature limit further one obtains the result of Feynman's polaron theory.[15]

Several theoretical studies have been published during the last few years about the polaron in a magnetic field. Almost all of them are concerned with the zero-temperature limit. Below we show how some of these results can be reobtained from the present result [Eq. (59a)]. In the zero-temperature limit the free energy $F_{\rm as}$ [Eq. (59)] is equal to the polaron ground-state energy $E_{\rm as}$,

$$E_{\rm as} = \lim_{T\to 0} F_{\rm as} ,$$

and thus

$$\begin{aligned} E_{\rm as} &= \tfrac{1}{2}\left[\sum_{\mu=0}^{3} s_\mu - 2w_\perp - w_{||}\right] - \frac{C_\perp}{v_\perp w_\perp}\sum_{j=1}^{3}\frac{\partial s_j}{\partial v_\perp} + \frac{C_{||}}{v_{||}w_{||}} \\ &\quad - \frac{\alpha}{2\sqrt{2\pi}}\int_0^\infty du\,\frac{e^{-u}}{\sqrt{H(u)}}\ln\left[\frac{\sqrt{D(u)}+\sqrt{H(u)}}{\sqrt{D(u)}-\sqrt{H(u)}}\right] . \end{aligned} \tag{60}$$

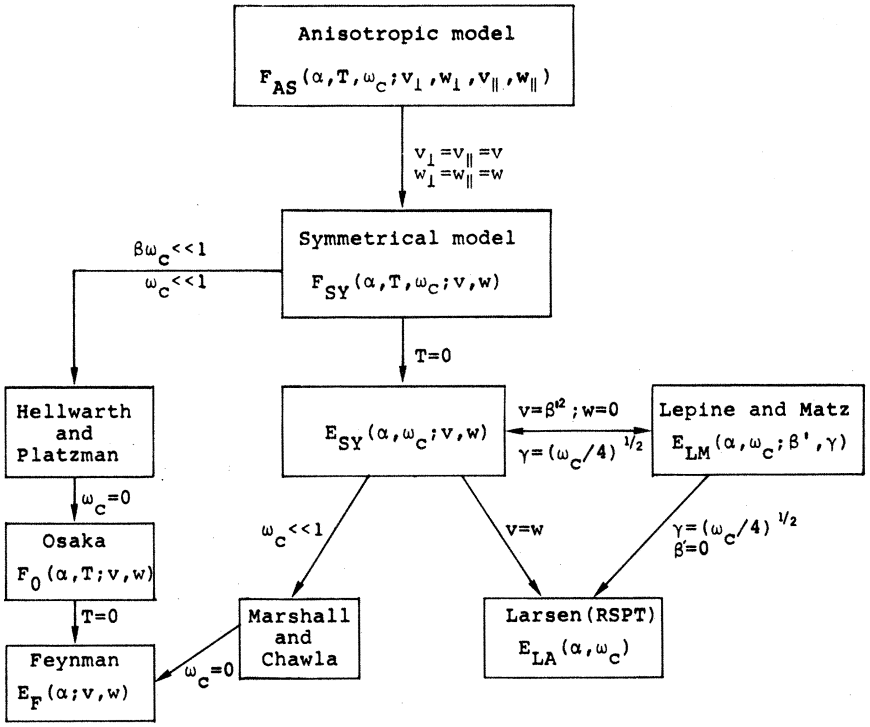


FIG. 2. Relation between different polaron theories.

The above expression is closely related to the result of Lépine and Matz.[12] In Ref. 12 Lépine and Matz presented an expression for the polaron ground-state energy, which was derived by using a nonperturbative Fock-type mean-field theory. Their result, which contains two variational parameters (γ and β'), is an upper bound to the exact polaron ground-state energy. A model Hamiltonian was used to simulate the electron motion. This model Hamiltonian describes an electron in a magnetic field $\mathscr{H}'=4\gamma^2 mc/e$ (which we shall call an internal field) and which is coupled quadratically, with a spring constant $K=\beta'^4$, to a point fixed in space. Note that the internal magnetic field $\mathscr{H}'$ may differ from the external magnetic field $\mathscr{H}$. It can easily be verified that our result [Eq. (60)] coincides with the result of Ref. 12 [Eq. (25) of Ref. 12] if one sets $v_\perp=v_\parallel=\beta'^2$, $w_\perp=w_\parallel=0$ in Eq. (60) and if the internal field in Lépine and Matz's theory is taken equal to the external magnetic field, i.e., $\gamma^2=\omega_c/4$.

The present result for the polaron ground-state energy [Eq. (60)] differs in three respects with the Lépine and Matz[14] result. Firstly, here a trial *action* is used to simulate the electron motion while in Ref. 14 a trial (or model) *Hamiltonian* was used. Secondly, the trial action S [Eqs. (19), (8b), and (28)] describes a *self-interacting* electron, i.e., it includes a memory effect, while the model Hamiltonian of Ref. 17 describes an electron with a *local* (equal-time) interaction. Thirdly, in the present study we allowed the effective electron phonon interaction to be *anisotropic*. No such anisotropy is present in the theory of Ref. 17.

If we take $v_\perp=v_\parallel$, $w_\perp=w_\parallel$ (symmetrical model) and expand Eq. (60) for small magnetic fields, we obtain the result of Marshall and Chawla.[16] These authors calculated the polaron ground-state energy, using the Feynman path-integral approach up to first order in the magnetic field. From the first-order term, which is inversely proportional to the polaron effective mass, these authors[16] calculated the polaron mass.

If we take $v_\perp=v_\parallel=w_\perp=w_\parallel$ [this implies $C_i=0$ in Eq. (28)] the generalized Feynman trial action reduces to the action of a free electron in a magnetic field. Thus the result of Rayleigh-Schrödinger perturbation theory (RSPT) for the polaron ground state, as derived by Larsen,[6] will be obtained. Indeed, one can verify that inserting $v_\perp=v_\parallel=w_\perp=w_\parallel$ in Eq. (60) results in Eq. (69) of Ref. 6.

The comparison between the present result and the more general result of Saitoh[18] is postponed to

the conclusion.

V. EXPLICIT ANALYTIC RESULTS IN LIMITING CASES

In the derivation of Eq. (59a) no restriction on the strength of the electron-phonon coupling (α), temperature ($\beta=1/k_BT$), and magnetic field ($\omega_c=e\mathscr{H}/mc$) was imposed. However, in general, the variational calculation of the free energy [Eq. (59a)] must be performed numerically. In this section it is our goal to derive explicit analytic results for the free energy, and in some cases for the Feynman polaron mass, for a restrictive range of α, β, and ω_c values where it is possible to perform the variational calculation analytically. A systematic study of the most important limits will be made.

A. Small electron-phonon coupling ($\alpha \ll 1$)

For small α the effective electron-phonon interaction will be small and thus $v_\perp$ ($v_\parallel$) will be near to $w_\perp$ ($w_\parallel$). If we write

$$v_\perp = w_\perp(1+\epsilon_\perp)\,, \qquad v_\parallel = w_\parallel(1+\epsilon_\parallel)\,, \tag{61}$$

then $\epsilon_\perp$ and $\epsilon_\parallel$ will be of order α. With this in mind, the three terms in the approximate free energy [Eq. (59a)] may be expanded up to α^2. We found

$$F_0 = F_e + B_\parallel\epsilon_\parallel + B_\perp\epsilon_\perp + E_\parallel\epsilon_\parallel^2 + E_\perp\epsilon_\perp^2 + \cdots\,, \tag{62a}$$

$$F_{m,I} = B_\parallel\epsilon_\parallel + B_\perp\epsilon_\perp + K_\parallel\epsilon_\parallel^2 + K_\perp\epsilon_\perp^2 + \cdots\,, \tag{62b}$$

$$F_I = F_{I,0} + A_\parallel\epsilon_\parallel + A_\perp\epsilon_\perp + \cdots\,, \tag{62c}$$

where F_e is the free energy of a free electron in a magnetic field

$$F_e = \frac{3}{2\beta}\ln(2\pi\beta) - \frac{1}{\beta}\ln\left[\frac{\beta\omega_c}{2}\sinh\left[\frac{\beta\omega_c}{2}\right]\right], \tag{63}$$

and $B_\perp, B_\parallel, E_\perp, E_\parallel, K_\perp, K_\parallel, A_\perp, A_\parallel$ are certain functions of β and ω_c and the two variational parameters $v_\perp$ and $v_\parallel$ [because $w_\perp$ and $w_\parallel$ have been eliminated by using Eq. (61)]. Although it is possible to evaluate $B_\parallel$, $B_\perp$, $E_\parallel$, $E_\perp$, $K_\parallel$, and $K_\perp$ explicitly we will not give the explicit expressions for these functions because they are rather lengthy and are of no direct relevance at the moment. The other functions $F_{I,0}$, $A_\parallel$, and $A_\perp$ have α as a prefactor. They are much more difficult to evaluate because F_I [Eq. (55)] contains an integral that can only be performed analytically in a restricted range of β and ω_c values.

Adding up the different contributions to the free energy [Eqs. (62) and see Eq. (59a)]

$$F_{\rm as} = F_e - F_{I,0} + (E_\parallel - K_\parallel)\epsilon_\parallel^2 + (E_\perp - K_\perp)\epsilon_\perp^2 - A_\parallel\epsilon_\parallel - A_\parallel\epsilon_\parallel + \cdots$$

and minimizing $F_{\rm as}$ with respect to the parameters $\epsilon_\parallel$ and $\epsilon_\perp$ results in

$$\epsilon_\parallel = \frac{A_\parallel}{2(E_\parallel - K_\parallel)}\,, \quad \epsilon_\perp = \frac{A_\perp}{2(E_\perp - K_\perp)}\,, \tag{64}$$

and the free energy becomes

$$F_{\rm as} = F_e - F_{I,0} - \frac{A_\parallel^2}{4(E_\parallel - K_\parallel)} - \frac{A_\perp^2}{4(E_\perp - K_\perp)}\,, \tag{65}$$

where F_e [Eq. (63)] is the free-electron contribution, $F_{I,0}$ is linear in α, and the last two terms of Eq. (65) are of order α^2.

1. $\beta\omega_c \gg 1$

In this limit the electron free energy (63) has the asymptotic expansion

$$F_e = \frac{3}{2\beta}\ln(2\pi\beta) + \frac{\omega_c}{2} - \frac{1}{\beta}\ln\left[\frac{\beta\omega_c}{2}\right] + \cdots\,. \tag{66}$$

a. $\omega_c \ll 1$

This is the small magnetic field and low-temperature limit, but such that $1/\beta \ll \omega_c \ll 1$. In the small magnetic field limit the difference between $D_H(u)$ and $D(u)$ is of order ω_c and thus $H(u)/D(u) \ll 1$ can be considered as an expansion parameter in the integrand of Eq. (55). After evaluating the integral in Eq. (55) we found

$$-F_{I,0} = -\alpha\left[(1+\tfrac{1}{12}\omega_c - \tfrac{1}{240}\omega_c^2 + \cdots) + \frac{1}{12\beta}(1+\tfrac{9}{20}\omega_c + \tfrac{27}{16}\omega_c^2 + \cdots) + \frac{81}{40\beta^2}(1-\tfrac{125}{48}\omega_c + \tfrac{5075}{864}\omega_c^2 + \cdots)\right], \tag{67}$$

which is the first-order correction in α of the polaron free energy relative to the electron free energy. The zero-temperature limit of Eq. (67) is identical to the expansion obtained by Larsen.[3]

The parameters $\epsilon_{||}$ and $\epsilon_{\perp}$ [see Eq. (64)] are, to first order in ω_c and $1/\beta$, given, respectively, by

$$\epsilon_{\perp}=\alpha\left[\epsilon_{\perp}^{0}+\epsilon_{\perp}^{c}\omega_c+\epsilon_{\perp}^{\beta}\frac{1}{\beta}+\cdots\right] \tag{68}$$

with

$$\epsilon_{\perp}^{0}=\frac{2}{3v_{\perp}}\left[1-\frac{2}{v_{\perp}}(\sqrt{1+v_{\perp}}-1)\right], \tag{69a}$$

$$\epsilon_{\perp}^{c}=\frac{2}{15v_{\perp}}\left[-1+\frac{1}{v_{\perp}}\left[17+\frac{3}{\sqrt{1+v_{\perp}}}\right]-\frac{40}{v_{\perp}^{2}}(\sqrt{1+v_{\perp}}-1)\right], \tag{69b}$$

$$\epsilon_{\perp}^{\beta}=\frac{1}{10v_{\perp}}\left[1-\frac{2}{v_{\perp}}\left[1-\frac{1}{\sqrt{1+v_{\perp}}}\right]\right], \tag{69c}$$

and

$$\epsilon_{||}=\alpha\left[\epsilon_{||}^{0}+\epsilon_{||}^{c}\omega_c+\epsilon_{||}^{\beta}\frac{1}{\beta}+\cdots\right] \tag{70}$$

with

$$\epsilon_{||}^{0}=\frac{2}{3v_{||}}\left[1-\frac{2}{v_{||}}(\sqrt{1+v_{||}}-1\right], \tag{71a}$$

$$\epsilon_{||}^{c}=\frac{1}{10v_{||}}\left[1-\frac{2}{v_{||}}\left[1-\frac{1}{\sqrt{1+v_{||}}}\right]\right], \tag{71b}$$

$$\epsilon_{||}^{\beta}=\frac{1}{30v_{||}}\left[-1+\frac{1}{v_{||}}\left[62+\frac{18}{\sqrt{1+v_{||}}}\right]-\frac{160}{v_{||}}(\sqrt{1+v_{||}}-1)\right]. \tag{71c}$$

Still, there are two variational parameters $v_{\perp}$ and $v_{||}$ present in Eqs. (69a)–(69c) and (71a)–(71c). Because the magnetic field and temperature dependence of the variational parameters were, to lowest order in ω_c and $1/\beta$, taken into account by $w_{\perp}$ and $w_{||}$ [see Eq. (61)], $v_{\perp}$ and $v_{||}$ may be chosen in such a way that they minimize the free energy at zero temperature and zero magnetic field, and thus $v=v_{\perp}=v_{||}$. Feynman found in Ref. 15 the value $v=3$. Note that in Ref. 15 one considered w instead of v and found $w=3$, but in the small coupling limit one also has $v=w+O(\alpha)$. Inserting $v_{\perp}=v_{||}=3$ into Eqs. (69a)–(69c) and (71a)–(71c) gives $\epsilon_{\perp}^{0}=\epsilon_{||}^{0}=\frac{2}{27}$, $\epsilon_{\perp}^{c}=\frac{13}{405}$, $\epsilon_{\perp}^{\beta}=\epsilon_{||}^{c}=\frac{1}{45}$, and $\epsilon_{||}^{\beta}=\frac{22}{405}$.

Using Eqs. (61), (68), and (70) we obtain for the masses of the Feynman polaron, to first order in α, ω_c, and $1/\beta$,

$$M_{\perp}=1+\alpha\left[\frac{4}{27}+\frac{26}{405}\omega_c+\frac{2}{45}\frac{1}{\beta}\right] \tag{72a}$$

and

$$M_{||}=1+\alpha\left[\frac{4}{27}+\frac{2}{45}\omega_c+\frac{44}{405}\frac{1}{\beta}\right]. \tag{72b}$$

The zero-temperature and zero magnetic field limit gives $M_{\perp}=M_{||}=1+\alpha\frac{4}{27}+O(\alpha^2)$; it is identical to the result as obtained by Feynman in Ref. 15 (see also Ref. 40) and close to the correct perturbation theory result[41] for the polaron mass $1+\alpha/6+O(\alpha^2)$. Note that $M_{\perp}$, as function of the magnetic field, increases faster than $M_{||}$ (namely $\frac{26}{405}\approx 0.064$ and $\frac{2}{45}\approx 0.044$). The temperature dependence of $M_{\perp}$ and $M_{||}$ is different. This is not surprising because Eqs. (72a) and (72b) were derived with the condition $1/\beta \ll \omega_c \ll 1$, which means that the zero magnetic field limit for finite temperature does not apply.

The α^2 correction term to the free energy F_{as} [see Eq. (65)] is given by (to first order in ω_c and $1/\beta$ and for $v=v_{\perp}=v_{||}=3$)

$$-\frac{\alpha^2}{81}\left[1-\frac{\omega_c}{9}+\frac{4}{9}\frac{1}{\beta}\right]. \tag{73}$$

The first term, $-\alpha^2/81$, has been given in Ref. 15 and can be compared to the exact result $-0.01592\alpha^2$ as obtained from fourth-order perturbation theory.[42] Note that in second order of the coupling the magnetic field contributes positively to the free energy.

It has been argued by several authors that from the ground-state energy of a polaron in a weak magnetic field one can define an effective polaron (magnetic[43]) mass m_H. Namely, the term linear in the magnetic field is of the form $\omega_c/2m_H$. If we combine Eqs. (65), (66), (67), and (73) we find for the term linear in the magnetic field the expression

$$\frac{\omega_c}{2}\left[1-\tfrac{1}{6}\alpha+\tfrac{2}{729}\alpha^2+O(\alpha^3)\right]$$

from which we obtain the polaron magnetic mass

$$m_H=1+\tfrac{1}{6}\alpha+\tfrac{73}{2916}\alpha^2+O(\alpha^3). \tag{74}$$

This result was already obtained by Marshall and Chawla.[16] Note that Eq. (74) agrees very well with Feynman's[15] polaron mass,

$$m_F=1+\tfrac{1}{6}\alpha+\tfrac{72}{2916}\alpha^2+O(\alpha^3)\ . \tag{75}$$

The coefficients of the α^2 term differ only by 1.4% ($\frac{72}{2916}=0.02469$ while $\frac{73}{2916}=0.02503$).

b. $\omega_c \gg 1$

In the limit of large magnetic fields we shall calculate the polaron free energy to first order in α. It is not easy to calculate the masses of the Feynman polaron $M_\perp$ and $M_\parallel$ to first order in α because in the limit $\omega_c \gg 1$ it turns out that, e.g., $v_\perp$ and $w_\perp$ increase with the magnetic field, but of course, such that $v_\perp/w_\perp=1+O(\alpha)$ (this conclusion is based on numerical work which will be presented in paper II). This makes it very difficult to perform an analytic calculation of $M_\perp$ and $M_\parallel$ to first order in α, or of the free energy to second order in α.

For large magnetic fields $D_H(u)\sim 1/\omega_c$, and thus the integrand of Eq. (55) may be expanded in $D_H(u)/D(u)\ll 1$. Furthermore, setting $\epsilon_\perp=\epsilon_\parallel=0$ is possible because we are only interested in the first-order correction in α. For low temperature ($\beta\gg 1$ and thus $\beta\gg 1/\omega_c\gg 1$) Eq. (55) has the asymptotic form

$$F_I=\frac{\alpha}{2}\left[(\ln\omega_c-c)\left[1+\frac{1}{4\beta}+\frac{9}{32\beta^2}+\cdots\right]+\frac{\ln\omega_c}{\sqrt{\omega_c}}+\frac{1}{\sqrt{\omega_c}}[\ln 2+\zeta(\tfrac{3}{2})]+\cdots\right] \tag{76}$$

with $c\approx 0.5772$ the constant of Euler and $\zeta(x)$ the zeta function. In the zero-temperature limit several authors[3,5,12] have found the dominant term, $-\alpha\ln\sqrt{\omega_c}$. For high temperature ($\beta\ll 1$) such that $\omega_c\gg 1/\beta\gg 1$, Eq. (55) becomes

$$F_I=\frac{\alpha}{2}\left[\frac{\pi}{\beta}\right]^{1/2}\left[\left[1+\frac{\beta^2}{48}+\cdots\right]\ln\left[\frac{\beta\omega_c}{4}\right]-\frac{\beta^2}{16}+\frac{2}{\sqrt{\pi}}\left[1-\frac{3}{4\beta\omega_c}-\frac{15}{32\beta^2\omega_c^2}+\cdots\right]\frac{\ln 2\omega_c}{\sqrt{\beta\omega_c}}+\frac{\zeta(\frac{3}{2})}{\sqrt{\pi}}\frac{1}{\sqrt{\beta\omega_c}}+\cdots\right], \tag{77}$$

The appearance of the term $\alpha/\sqrt{\beta}$ is typical for the high-temperature limit. However, for large magnetic fields this term is changed with a factor $\ln\omega_c$, which is typical for the large magnetic field limit [see Eq. (77)]. Recently, Saitoh[18] obtained the same asymptotic expansions as given by Eqs. (76) and (77), but in Ref. 18 only the coefficients of the $\ln\omega_c$ term and the ω_c-independent term were calculated.

2. $\beta\omega_c \ll 1$

Note that in this limit the electron free energy [Eq. (63)] has the expansion

$$F_e=\frac{3}{2\beta}\ln(2\pi\beta)+\frac{\beta\omega_c^2}{24}+O(\beta^3\omega_c^4)\ . \tag{78}$$

For $\alpha\ll 1$ and $\beta\omega_c\ll 1$ the difference between $D_H(u)$ and $D(u)$ is of the order $\epsilon_\perp$, $\epsilon_\parallel$, and $\beta^3\omega_c^2$. Thus we may use $H(u)/D(u)\ll 1$ to evaluate Eq. (55). In the following we study the low- and high-temperature limit separately.

a. $\beta\gg 1$

This is the small magnetic field and low- (but nonzero) temperature limit such that $\omega_c\ll 1/\beta\ll 1$. The first-order correction in α to the polaron free energy is $-F_{I,0}$, with

$$F_{I,0}=\alpha\left[\left[1+\frac{1}{4\beta}+\frac{9}{32\beta^2}+\cdots\right]+\frac{\beta\omega_c^2}{72}\left[1-\frac{3}{4\beta}-\frac{15}{32\beta^2}+\cdots\right]+\cdots\right]. \tag{79}$$

The zero magnetic field term is equal to the result obtained in Ref. 44. Note that in the case $\omega_c\ll 1/\beta\ll 1$ the polaron free energy has no linear term in the magnetic field. This is manifestly different with the case $1/\beta\ll\omega_c\ll 1$ [see Eq. (67)], where such a linear term is present.

The magnetic field correction term to the polaron free energy is [see Eqs. (78) and (79)]

$$\frac{\beta\omega_c^2}{24}\left[1-\frac{\alpha}{3}+O(\alpha^2)\right]. \tag{80}$$

Hellwarth and Platzman[14] then defined a polaron magnetic mass, m_H, by arguing that Eq. (80) is the magnetic field correction to the free energy of a particle with mass

$$\frac{m_H}{m}=\frac{1}{[1-\frac{1}{3}\alpha+O(\alpha^2)]^2}=1+\tfrac{1}{6}\alpha+O(\alpha^2),$$

which, to first order in α, is the correct expression for the polaron mass.

For the parameter $\epsilon_{||}$ we found the expression

$$\epsilon_{||}=\alpha\left[\epsilon_{||}^0+\epsilon_{||}^\beta\frac{1}{\beta}+\cdots\right] \tag{81}$$

with ϵ^0 given by Eq. (71a) and

$$\epsilon_{||}^\beta=\frac{1}{6v_{||}}\left[1+\frac{2}{v_{||}}\left[5+\frac{3}{\sqrt{1+v_{||}}}\right]-\frac{32}{v_{||}}(\sqrt{1+v_{||}}-1)\right]. \tag{82}$$

The magnetic field correction to $\epsilon_{||}$ is unimportant. Similarly as before we take $v_{||}=3$ and find $\epsilon_{||}^0=\frac{2}{27}$ and $\epsilon_{||}^\beta=\frac{8}{81}$. The magnetic-field-independent term of $\epsilon_\perp$ is identical to Eq. (81), as expected. The magnetic field corrections to $\epsilon_\perp$ are of secondary importance; they are of the order of $\beta^2\omega_c^2$.

The α^2 correction to the free energy is given by [see Eq. (65)]

$$-\alpha^2\left[\frac{1}{81}+\frac{4}{729}\frac{1}{\beta}+\cdots\right]. \tag{83}$$

The first term, $-\alpha^2/81$, is identical to the first term of Eq. (73).

The mass of the isotropic Feynman polaron becomes

$$M=1+\alpha\left[\frac{4}{27}+\frac{16}{81}\frac{1}{\beta}+O\left[\frac{1}{\beta^2}\right]\right], \tag{84}$$

which is identical to the result of Ref. 40. Recently, Saitoh[44] defined the polaron mass as the inverse of the ratio of the acceleration rate to a fictitiously applied force and found

$$m^*=1+\alpha\left[\frac{1}{6}-\frac{1}{8\beta}+O\left[\frac{1}{\beta^2}\right]\right].$$

Note that such a definition results in a different temperature behavior of the polaron mass. The temperature dependence of Ref. 44 is hard to understand because it is generally believed[25,40,45,46] that the polaron mass has to increase with temperature if $\beta\gg1$. Such an increase is attributed[25,40,45] to the nonparabolicity of the polaron energy spectrum.[47–49]

b. $\beta\ll1$

The first-order correction in the electron-phonon coupling of the free energy is obtained from Eq. (55) which, in the high-temperature limit, has the series expansion

$$-F_I=-\alpha\left[\frac{\pi}{\beta}\right]^{1/2}\left[1+\frac{\beta^2}{48}+\frac{\beta^2\omega_c^2}{288}+\cdots\right]. \tag{85}$$

For zero magnetic field, Saitoh[44] has studied the same high-temperature limit.[50]

The analytic calculation of the α^2 term is difficult and will not be given. The reason is that at high temperature the parameters $v_\perp$, $v_{||}$, $w_\perp$, and $w_{||}$ increase with increasing temperature. This is confirmed by a numerical variational calculation of the free energy (see, e.g., Ref. 45 and paper II). Note that for high magnetic fields we found a similar increase of the variational parameters.

B. Strong electron-phonon coupling ($\alpha\gg1$)

In the following we assume that $\beta v\gg1$. For the limit of strong electron-phonon coupling one has $v_{||}\sim\alpha^2$, which implies that the temperature range is not severely restricted, namely $\beta\gg1/\alpha^2$.

1. $\omega_c/v\ll1$

In the small magnetic field case the anisotropy between the effective electron-phonon coupling parallel and perpendicular to the magnetic field will be small. It is of secondary importance. Because we are only interested in the dominant terms in the free energy we may take $v=v_\perp=v_{||}$ and $w=w_\perp=w_{||}$. Therefore the free energy will be indicated by F_{sy} (see Sec. IV).

The present small magnetic field limit (meaning small relative to the electron-phonon strength) implies that we may use $H(u)/D(u)\ll1$ in the evaluation of the integral appearing in F_I [see Eq. (55)]. However, to obtain an explicit expression for the variational parameter v it is necessary to make further restrictions on the range of α, β, and ω_c. From now on we assume $\beta\gg1$.

a. $\beta\omega_c(w^2/v^2) \gg 1$

This limit contains the zero-temperature case. Summing up all the restrictions, we are in the situation such that $1 \ll v^2/w^2 \ll \beta\omega_c \ll \beta v$ and with $\beta \gg 1$. The dominant contributions to the free energy are found to be (we took $w=1$, see, e.g., Ref. 15)

$$F_{sy}=\frac{3}{2\beta}\ln(2\pi\beta)-\frac{1}{\beta}\ln\left[\frac{\beta\omega_c}{2}\right]-\frac{1}{\beta}\ln v+\tfrac{3}{4}v-\tfrac{3}{2}-\alpha\left[\frac{v}{\pi}\right]^{1/2}\left[1+\frac{1}{v}\left[2\ln 2-\frac{1}{2}+\frac{1}{3\beta}\right]\right]$$
$$+\frac{\omega_c}{v^2}\left[1-\frac{1}{3\sqrt{\pi}}\frac{\alpha}{\sqrt{v}}+\cdots\right]+\frac{3}{16}\frac{\omega_c^2}{v}\left[1-\frac{2}{9\sqrt{\pi}}\frac{\alpha}{\sqrt{v}}+\cdots\right]+\cdots . \tag{86a}$$

Minimizing F_{sy} to v results in

$$v=\frac{4\alpha^2}{9\pi}-(4\ln 2-1)+\frac{2}{\beta}+\frac{\omega_c}{2}\frac{1}{(4\alpha^2/9\pi)^2}+\frac{\omega_c^2}{4}\frac{1}{(4\alpha^2/9\pi)}, \tag{86b}$$

which, in the limit $\beta\to\infty$ and $\omega_c\to 0$, reduces to the expression already obtained by Feynman.[15,51] From Eq. (86b) the mass of the (isotropic) Feynman polaron is easily obtained:

$$M=\frac{16\alpha^4}{81\pi^2}-\frac{8\alpha^2}{9\pi}(4\ln 2-1)+\frac{16\alpha^2}{9\pi}\frac{1}{\beta}+\frac{\omega_c}{4\alpha^2/9\pi}+\frac{\omega_c^2}{2} . \tag{87}$$

The leading term, $16\alpha^4/81\pi^2$, was already obtained in Ref. 13. Note that for small magnetic fields and low temperatures the polaron mass (87) enhances with increasing magnetic field strength and increasing temperature. We found the same quantitative behavior in the case of small electron-phonon coupling.

Inserting the value $v=4\alpha^2/9\pi$ into Eq. (86a) gives the following expression for the polaron free energy:

$$F_{sy}=F_p+F_\alpha+F_c \tag{88}$$

with

$$F_p=\frac{3}{2\beta}\ln\left[\frac{2\pi\beta}{16\alpha^4/81\pi^2}\right]-\frac{1}{\beta}\ln\left[\frac{\beta\omega_c/2}{16\alpha^4/81\pi^2}\right], \tag{89a}$$

$$F_\alpha=-\frac{\alpha^2}{3\pi}-3(\ln 2+\tfrac{1}{4}), \tag{89b}$$

$$F_c=\frac{\omega_c}{2}\frac{1}{16\alpha^4/81\pi^2}+\frac{\omega_c^2}{8}\frac{1}{(16\alpha^4/81\pi^2)^{1/2}} . \tag{89c}$$

The first term F_p is the free energy of a particle, with mass $16\alpha^4/81\pi^2$ (which is the polaron mass), which interacts with a magnetic field. F_α is the well-known[15,51] self-energy in the strong-coupling limit. The magnetic-field-dependent term F_c contains a linear term in ω_c which is the zero-point energy of a particle, with mass $16\alpha^4/81\pi^2$, in a magnetic field. This term does not appear in Ref. 12. The ω_c^2 term represents a diamagnetic shift; it is equal to the diamagnetic shift found in Ref. 12.

b. $\beta\omega_c(w^2/v^2) \ll 1$

The zero magnetic field limit is contained in this case. The free energy becomes

$$F_{sy}=\frac{3}{2\beta}\ln(2\pi\beta)-\frac{3}{\beta}\ln v+\tfrac{3}{4}v-\tfrac{3}{2}-\alpha\left[\frac{v}{\pi}\right]^{1/2}\left[1+\frac{1}{v}\left[2\ln 2-\frac{1}{2}+\frac{1}{\beta}\right]\right]$$
$$+\frac{3}{16}\frac{\omega_c^2}{v}\left[1-\frac{2}{9\sqrt{\pi}}\frac{\alpha}{\sqrt{v}}+\frac{2}{3}\frac{\beta}{v^3}+\cdots\right]+\cdots \tag{90a}$$

A minimalization of this expression with respect to v results in the following value for the variational parameter:

$$v=\frac{4\alpha^2}{9\pi}-(4\ln 2-1)+\frac{6}{\beta}+\frac{\omega_c^2}{4}\frac{1}{4\alpha^2/9\pi}\left[1+\frac{4}{3}\frac{\beta}{(4\alpha^2/9\pi)^3}\right] \tag{90b}$$

from which we obtain the mass of the Feynman polaron

$$M=\frac{16\alpha^4}{81\pi^2}-\frac{8\alpha^2}{9\pi}(4\ln 2-1)+\frac{48\alpha^2}{9\pi}\frac{1}{\beta}+\frac{\omega_c^2}{2}\left[1+\frac{4}{3}\left[\frac{9\pi}{4\alpha^2}\right]^3\beta\right]. \quad (91)$$

Note that Eqs. (87) and (91) coincide if $\beta\to\infty$ and $\omega_c\to 0$, as should be the case.

Because the polaron is a quasiparticle, there are different possibilities for the definition of the polaron mass. Recently, in the absence of a magnetic field, Saitoh[44] defined the polaron mass as the acceleration rate against a fictitiously applied force. In the considered limits he found $16\alpha^4/81\pi^2 - 128\alpha^4/243\pi^3\beta$. Note that with increasing temperature the polaron mass decreases. In another article[17] Saitoh presented still another definition for the polaron mass, which was based on the zero magnetic field diamagnetic susceptibility. Such a definition resulted in the asymptotic expression $16\alpha^4/81\pi^2-512\alpha^{10}/19683\pi^2\beta$. This expression also gives a decreasing polaron mass with increasing temperature, but the coefficient of the temperature-dependent term differs considerably with that of Ref. 44.

Inserting $v=4\alpha^2/9\pi$ into Eq. (90a) gives the following value for the free energy:

$$F_{\rm sy}=F_p'+F_\alpha+F_{\omega_c}' \quad (92)$$

with

$$F_p'=\frac{3}{2\beta}\ln\left[\frac{2}{16\alpha^4/81\pi^2}\right]+\frac{\beta\omega_c^2}{24}\frac{1}{(16\alpha^4/81\pi^2)^2}, \quad (93a)$$

$$F_{\omega_c}'=\frac{\omega_c^2}{8}\frac{1}{(16\alpha^4/81\pi^2)^{1/2}}\times\left[1+\frac{2\beta}{3}\frac{1}{(16\alpha^4/81\pi^2)^{3/2}}\right] \quad (93b)$$

and F_α is given by Eq. (89b). F_p' is the free energy of a particle with mass $16\alpha^4/9\pi$ in the limit $\beta\omega_c/(16\alpha^4/9\pi)\ll 1$. The diamagnetic shift is, apart from the temperature correction, identical to that of Eq. (89c).

2. $\omega_c/v_{||}^2\gg 1$

This is the large magnetic field limit, because for $\alpha\gg 1$ one has $v_{||}/w_{||}\gg 1$ (remember that for $\alpha\gg 1$ we may take $w_{||}=1$). In the beginning of Sec. V B on the strong electron-phonon coupling we assumed that $\beta v_{||}\gg 1$, which in the present case also implies that $\beta\omega_c\gg 1$. For large magnetic fields one has $v_\perp<v_{||}$ (cf. the case for $\alpha\ll 1$ and $\omega_c\gg 1$), which implies that $\omega_c/v_\perp^2\gg 1$. The above-mentioned conditions $\beta v_{||}\gg 1$, $\beta\omega_c\gg 1$, $\omega_c/v_{||}^2\gg 1$, $\omega_c/v_\perp^2\gg 1$, $v_{||}\gg 1$ allow us to calculate the asymptotic expansion of the free energy

$$F_{\rm as}=\frac{3}{2\beta}\ln(2\pi\beta)+\frac{\omega_c}{2}-\frac{1}{\beta}\ln v_{||}+\frac{v_{||}}{4}-\frac{\alpha}{2}\left[\frac{v_{||}}{\pi}\right]^{1/2}\ln\frac{4\omega_c}{v_{||}}. \quad (94a)$$

Minimizing this expression to the variational parameter $v_{||}$ results in

$$v_{||}=\frac{\alpha^2}{\pi}\ln^2\left[\frac{4\pi\omega_c}{\alpha^2e^2}\right]+\frac{8}{\beta} \quad (94b)$$

from which we obtain the polaron mass parallel to the magnetic field

$$M_{||}=\frac{\alpha^4}{\pi^2}\ln^4\left[\frac{4\pi\omega_c}{\alpha^2e^2}\right]+\frac{16\alpha^2}{\pi\beta}\ln^2\left[\frac{4\pi\omega_c}{\alpha^2e^2}\right]. \quad (95)$$

The free energy becomes

$$F_{\rm as}=F_e-\frac{\alpha^2}{4\pi}\ln^2\left[\frac{4\pi\omega_c}{\alpha^2e^2}\right], \quad (96)$$

where

$$F_e=\frac{3}{2\beta}\ln(2\pi\beta)+\frac{\omega_c}{2}$$

is the free energy of a free electron in a magnetic field in the limit $\omega_c\gg 1$. Again, $M_{||}$ increases if the lattice temperature increases.

Saitoh[17] also studied the present asymptotic limit and found a polaron mass that decreases with increasing temperature. Furthermore, the dominant electron-phonon contribution to $M_{||}$ and $F_{\rm as}$ differs slightly with ours, namely, in Eqs. (95) and (96) we must take powers of the term $\ln(4\pi\omega_c/\alpha^2e^2)$, which in Ref. 17 is replaced by $\ln(2\pi\omega_c/\alpha^2e^2)$.

Two remarks are in order. First, the dominant contribution to the free energy resulting from the electron-phonon interaction comes entirely from

the interaction of the electron with the phonons along the magnetic field. This is apparent from Eq. (94a), where only the parameter $v_{||}$ enters into the dominant term of F_{as}. The effective electron-phonon interaction perpendicular to the magnetic field, as simulated by $v_{\perp}$, enters only in terms which are of order $1/\omega_c$. If we want to determine $v_{\perp}$, it will be necessary to calculate F_{as} at least to order $1/\omega_c$. However, Eq. (96) already suggests that $M_{\perp}=1+O(1/\omega_c)$. Indeed, the free energy F_{as} [Eq. (96)] results from a free electron in a magnetic field plus a correction due to the electron-phonon interaction along the field. Thus perpendicular to the field the effective coupling between the electron and the phonons is at least of order $1/\omega_c$. In paper II we will show numerically that indeed $M_{\perp}\rightarrow 1$ in the limit $\omega_c\rightarrow\infty$. Second, the electron self-energy, which is proportional to $\alpha^2\ln^2\omega_c$, can be understood as follows. For small α the electron self-energy which is proportional to α, for $\omega_c=0$ becomes proportional to $\alpha\ln\omega_c$ for $\omega_c\gg 1$. In the large-α limit the electron self-energy is proportional to α^2 for $\omega_c=0$, while it is proportional to $(\alpha\ln\omega_c)^2$ for $\omega_c\gg 1$. Thus as far as the magnetic field is concerned, for $\omega_c\gg 1$, its influence on the electron self-energy can approximately be taken into account by replacing the electron-phonon coupling constant α by $\alpha\ln\omega_c$ in the limit $\omega_c\gg 1$.

VI. CONCLUSION

In the present paper an approximate expression for the free energy of a polaron in an uniform magnetic field was obtained for arbitrary values of temperature, electron-phonon coupling strength, and magnetic field strength. This result was derived in the spirit of Feynman's polaron theory,[15] where we generalized the trial action to account for the anisotropy in the effective electron-phonon interaction. We reobtained most of the existing polaron theories as special cases.

Saitoh[17,18] (see also Ref. 14) considered a general quadratic action to simulate the electron motion. The resulting approximation to the free energy contains an infinite number of variational parameters, while in the present approach only four parameters have to be determined variationally. However, in Refs. 17 and 18 no numerical results were presented. In spite of the much larger effort needed in performing the variational calculation, we do not expect that such an approach will give a substantial improvement to the present result. This is suggested by the numerical work of Adamowski *et al.*,[53] who considered the zero magnetic field limit of such an approach. In Ref. 53 an improvement to the Feynman result[15,54] was obtained which, for all values of the electron-phonon coupling strength, was smaller than 1%.

In paper II several thermodynamic quantities are calculated numerically, i.e., we present figures for the magnetization, the susceptibility, the internal energy, the entropy, and the specific heat. A detailed numerical comparison between different theories will be presented.

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APPENDIX

We present intuitive arguments in favor of the validity of the Feynman inequality in the case when a magnetic field is present. Feynman showed[13,19,20] in the case of zero magnetic field that his approximate calculation of the free energy provides an upper bound to the exact free energy,

$$F\leq F_{ph}+F_m-\frac{1}{\beta}\langle S-S_m\rangle_m \tag{A1}$$

with S the action of the polaron after the elimination of the phonon variables and F is the corresponding exact free energy. F_{ph} is the free energy of the phonons, F_m is the free energy corresponding with the trial action S_m, and $\langle\ \rangle_m$ is an average with weight function $\exp(S_m)$. Note that Feynman considers the free energy F shifted with the constant contribution F_{ph}. Inequality (A1) provides a variational principle to determine the parameters in the trial action S_m. The proof of (A1) is based on the fact that S and S_m are real. For nonzero magnetic field strength the actions S and S_m contain an imaginary term, which implies that the original proof of Feynman's variational principle no longer holds. Although a strict mathematical proof is lacking, we have intuitive reasons for assuming that the Feynman variational principle [Eq. (A1)] is still valid in the present situation. The motivation for this originates from the Bogolyubov inequality[21]

$$F \leq F_0 + \langle H - H_0 \rangle_0 . \quad \text{(A2)}$$

H and H_0 are Hermitian Hamiltonians with corresponding free energies F and F_0. The equilibrium average with the Hamiltonian H_0 is indicated by $\langle\ \rangle_0$. Inequality (A2) can be obtained from inequality (A1), and vice versa,[22] if the actions S and S_m are derivable from some Hermitian Hamiltonians H and H_0. Now note that even if a magnetic field is applied, inequality (A2) still holds as long as the Hamiltonians H and H_0 are Hermitian. Thus inequality (A1) must also be valid, although S and S_m are complex quantities. This indicates that the condition for S and S_m to be real, which was needed in the proof of (A1), is too restrictive.

The above comparison between the Feynman inequality [Eq. (A1)] and the Bogolyubov inequality [Eq. (A2)] is instructive for our problem. In the present situation the actions S and S_m are obtained from Hermitian Hamiltonians, respectively, H and H_0, after the elimination of the phonon variables. This implies that S and S_m are nonlocal in time or that S and S_m cannot be expressed directly in terms of Hermitian Hamiltonians that are local in time. This prevents us from using directly the above-mentioned link between Eq. (A1) and Eq. (A2).

In summary, we have the following arguments at our disposal for the justification of the use of inequality (A1) in the problem under study. First, the reason why the Feynman inequality could not be proved in a strict mathematical sense is the appearance of spurious imaginary terms that disappear after the path integral has been evaluated. Indeed, it turns out that all calculated quantities are real, although the weight function in the path integral, $\exp(S_m)$, is complex. Second, it will turn out that our results are consistent with the assumption that Eq. (A1) is valid for the present situation. For example, in Sec. V all the existing limiting values for the polaron ground-state energy that have been proved to be upper bounds to the exact ground-state energy (see, e.g., Ref. 12) are reobtained with the present approach. To conclude the above discussion, we accept that Eq. (A1) is valid if the actions S and S_m can be obtained, in one way or another (e.g., after the elimination of some variables), from Hermitian Hamiltonians H and H_0. The last condition is satisfied in the present case. Note that in Ref. 19 (p. 308) Feynman already made the conjecture that inequality (A1) should be valid if a magnetic field is present. Feynman's argumentation was based on the comparison between the zero-temperature limit of Eq. (A1) and the Rayleigh-Ritz variational method, while our argumentation relies on the comparison between Eq. (A1) and the Bogolyubov inequality [Eq. (A2)].

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[1] An ideal polaron gas is defined as a gas consisting of non-interacting polarons. In the dilute regime the study of such a system is equivalent to the study of one polaron. In the following all thermodynamic quantities will be calculated for one polaron in such a gas.

[2] The polaron mass in the present paper (and in next paper, paper II) is defined as the mass of the Feynman polaron model.

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[50]It should be noted that the coefficient of the β^2 term in Ref. 44 has to be $\frac{1}{48}$ instead of $\frac{5}{48}$.
[51]In Ref. 52 it was found recently that the $2\ln 2$ term appearing in the free energy [Eq. (86a)], the variational parameter [Eq. (86b)] and in the polaron mass [Eq. (87)] should be replaced by $2\ln 2+C$ (with C Euler's constant). But in Ref. 52 the appearance of the constant C originates from a wrong asymptotic expansion. Namely, the formula just above Eq. (18) in Ref. 52 should have the expansion $A\sim\alpha\sqrt{\Omega/\pi}[1+(2\ln 2)/\Omega+\Theta(1/\Omega^2)]$ instead of $A\sim\alpha\sqrt{\Omega/\pi}[1+(2\ln 2+C)/\Omega+\Theta(1/\Omega^2)]$.
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