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Extension to the case of a magnetic field of Feynman's path-integral upper bound on the ground-state energy: Application to the Fröhlich polaron

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The Feynman inequality $E_G \leq E_{\rm trial}+\lim_{\beta\to\infty}\langle S-S_{\rm trial}\rangle/\beta$ for path integrals provides a powerful upper bound on the ground-state energy E_G of a large variety of systems. $E_{\rm trial}$ is the ground-state energy of some trial system with action $S_{\rm trial}$ for *imaginary* values of the time variable, and S is the action (also expressed in *imaginary time* variables) of the system under study. $\beta = 1/k_BT$, where k_B is the Boltzmann constant and T the temperature. However, the Feynman inequality is not *a priori* justified for a system in a magnetic field, because imaginary terms subsist in the action also after transforming to imaginary time variables. Replacing or extending this inequality when magnetic fields are present has therefore been a long-standing problem. In the present paper we solve this problem. We first derive an inequality, providing an upper bound for the ground-state energy, that is valid even in the case of a nonzero magnetic field,

$$E_G \leq E_{\rm trial} + \langle\infty|\mathcal{T}\{U_{\rm trial}(\infty,-\infty)[V(0)-V_{\rm trial}(0)]\}|-\infty\rangle,$$

for a system with Hamiltonian H_0+V. $\mathcal{T}$ is the time-ordering operator, and $U_{\rm trial}$ is the time evolution operator of a trial system with Hamiltonian $H_0+V_{\rm trial}$ in the interaction representation, with the interactions $V(t)$ and $V_{\rm trial}(t)$ switched on adiabatically. Because of the time ordering, retardation effects are also properly taken into account. The contribution of the magnetic field is included in the unperturbed Hamiltonian H_0. If the time-dependent integrands occurring in the matrix element in the right-hand side of our generalized inequality satisfy certain analyticity conditions in the complex-time plane, this inequality reduces to the Feynman inequality for path integrals. If these analyticity conditions are not satisfied, our generalized inequality may introduce supplementary terms $E^{\rm DB}$ in the right-hand side of the Feynman upper bound,

$$E_G \leq E_{\rm trial} + \lim_{\beta\to\infty}\langle S-S_{\rm trial}\rangle/\beta + E^{\rm DB},$$

because different branch lines or singularities have to be taken into account in the transformation to imaginary time variables. As an important illustration, our generalized inequality is applied to the problem of the Fröhlich polaron in a magnetic field. From the *generalization of the Feynman inequality* derived in the present paper, we determine the conditions to be imposed on the variational parameters in the trial action, such that the Feynman upper bound in its original form remains valid for a polaron in a magnetic field. Some limiting cases are studied analytically to illustrate the relevance of our additional constraints on the variational parameters of the trial system. In the free-particle limit and for a particular value of one of the variational parameters, we explicitly derive the contributions from the branch lines in the complex-time plane which arise if these additional constraints are not satisfied.

I. INTRODUCTION

The Feynman path-integral formulation[1,2] of quantum mechanics provides the following upper bound for the ground-state energy of a system:

$$E_G \leq E_{\rm trial} + \lim_{\beta\to\infty}\frac{\langle S-S_{\rm trial}\rangle_{\rm trial}}{\beta} \tag{1.1}$$

if S *and* $S_{\rm trial}$ *are real.* In (1.1), $E_{\rm trial}$ is the ground-state energy of some "trial" model with action functional $S_{\rm trial}$ for imaginary values of the time variable. S is the action functional of the system under study (also after the substitution $t\to -i\tau\hbar$ in the time integral over the Lagrangian). The path-integral average $\langle\cdots\rangle_{\rm trial}$ is defined with a probability density $\exp(S_{\rm trial})/\int\mathcal{D}x\exp(S_{\rm trial})$:

$$\langle\cdots\rangle_{\rm trial} = \frac{\int\mathcal{D}x(\cdots)\exp(S_{\rm trial})}{\int\mathcal{D}x\exp(S_{\rm trial})}, \tag{1.2}$$

where the denominator is the path integral (for imaginary time variables) of the "trial" model. The condition that S and $S_{\rm trial}$ are real implies the applicability of the Jensen inequality $\langle e^X\rangle \geq e^{\langle X\rangle}$ of probability theory (often called Jensen-Feynman inequality in its path-integral application), which is valid for real random variables X with some normalized probability density.

As an example, it is well known that the Feynman path-integral method with the application of the Jensen-Feynman inequality provides a superior upper bound to the ground-state energy and the free energy of the Fröhlich polaron for arbitrary coupling strength.

But the requirement that the action and the trial action of the system under study are real functions of imaginary time variables is not satisfied for all physical systems. Indeed, for the path integral describing a polaron in a magnetic field, for instance, the condition of a real action functional for imaginary time variables is not fulfilled. Therefore, the Feynman inequality (1.1) could not be applied to the study of a polaron in a magnetic field, and until now the accurate upper bound to the ground-state energy for $\omega_c = 0$ could not be generalized for a nonzero magnetic field.

Despite the lack of a generalization of the Feynman inequality for path integrals to the case of a nonzero magnetic field, Peeters and Devreese[3] (hereafter referred to as PD) developed an approximation scheme for the free energy of a polaron in a magnetic field (for arbitrary coupling, magnetic field, and temperature), based on the *working hypothesis* that the Jensen-Feynman inequality would also be valid for nonzero magnetic field. They used four adjustable parameters: $v_\perp$, $w_\perp$, $v_\parallel$, and $w_\parallel$. A related scheme, with an infinite number of variational parameters, was developed by Saitoh.[4] Although the PD approach happens to reproduce many previously known results in limiting cases for large and small coupling, high and low temperature, and high and low magnetic field, it is *not* based on an extremum principle and therefore it does not *a priori* provide an upper bound for the free energy of a polaron in a magnetic field. Further investigations leading to an extension of the Feynman inequality for path integrals, valid for $\omega_c \neq 0$, are necessary. In the present paper we report such an extension of Feynman's upper bound to the ground-state energy of a polaron in a magnetic field.

The problem tackled in the present paper is not limited to the study of polarons. Feynman and Hibbs[1] already addressed the question of the (non)validity of the Feynman inequality in 1965: *"if the Lagrangian represents a particle in a magnetic field"* ... *"in this case [they] suspect that the [Feynman] inequality (or some simple modification of it) is still valid. However, this has not been proved."*

To the present date, to the best of our knowledge, this problem had not been solved, and the "simple modification" suspected to exist in Ref. 1 had not been given. It is the purpose of the present paper to solve this problem, to provide the extension of the Feynman inequality for the path integral describing a particle in a (static and uniform) magnetic field, and to illustrate its usefulness to study the Fröhlich polaron in a magnetic field: a problem of physical interest.

In what follows, a brief survey is given of previous studies dealing with polarons in a magnetic field and invoking the use of Feynman path integrals in connection with the Feynman inequality.

Although the validity of the Jensen-Feynman inequality for a polaron in a magnetic field had not been proved for $\omega_c \neq 0$, it is known to be valid[5] in the asymptotic limit $\omega_c \to 0$. As a consequence the physical properties of Fröhlich polarons in a sufficiently weak magnetic field—for all coupling α and temperature T—can be analyzed by taking the Feynman path-integral model for zero magnetic field as a starting point. The results of Hellwarth and Platzman[6] for the diamagnetic properties of the Fröhlich polaron also derive their validity from the applicability of the Jensen-Feynman inequality in the asymptotic limit $\omega_c \to 0$. For this weak magnetic-field limit, it is stated in Ref. 5 that the Jensen-Feynman inequality remains valid if the *difference* between the action and the trial action is chosen to be real. PD also satisfy this condition; their results for the free energy of a polaron in the presence of a magnetic field are therefore an upper bound to the exact free energy in the limit $\omega_c \to 0$. Not surprisingly their analytical expressions for the free energy and for the polaron mass in the asymptotic limit $\omega_c \to 0$ indeed agree with the previously known limits for $\alpha \to 0$ and $\alpha \to \infty$.

The difficulty with the Jensen-Feynman inequality for general $\omega_c \neq 0$ can be avoided[7] by first introducing an additional approximation, e.g., based on the Bogolubov inequality,[8,9] which eliminates the imaginary terms in the path integral, so that the Jensen-Feynman inequality can be applied for the resulting (approximate) path integral. Unfortunately, this type of approach leads to a considerable loss of precision, e.g., the coefficient of $\alpha\omega_c$ in the free energy differs by a factor of 2 from the standard perturbative free energy for $\alpha \to 0$ and $\omega_c \to 0$. The resulting approximation is therefore *inadequate*.

Several aspects of the PD approximation, which is—as stated above—based on the working hypothesis that the Jensen-Feynman inequality remains valid for $\omega_c \neq 0$, have been discussed by various authors.

For sufficiently large magnetic fields, it was shown numerically[10] that the PD approximation for the ground-state energy of a polaron in a magnetic field is not an upper bound for the true ground-state energy to first order in the electron-phonon coupling, and even not in the limit $\alpha = 0$ (i.e., for a free particle in a magnetic field). The present authors[11] confirmed this conclusion analytically. Furthermore, it was also suggested in Ref. 10 that the Feynman inequality is valid if applied to a *linearized* polaron model in a magnetic field—as studied and solved by the present authors[11]—and with a *symmetrical* trial action of the PD type. (The linearized polaron model is a mathematical tool without direct physical significance.)

Larsen[12] argued that the application of the PD method to a two-dimensional polaron in a magnetic field does not provide an upper bound for the ground-state energy for $\omega_c \to \infty$ and $\alpha\sqrt{\omega_c} \to \infty$, and for $\omega_c \to \infty$ and $\alpha\sqrt{\omega_c} \to 0$. However, it has been suggested[13,14] that the Larsen approximation does not handle the asymptotic limit of high magnetic fields exactly.

In order to explore the possible regions of validity of the Feynman inequality for $\omega_c \neq 0$, the present authors[11] applied the PD approach to a linearized polaron model in a magnetic field, which they solved exactly. An *analytical* proof was presented that the Feynman inequality is not satisfied *for this model*, if ω_c is sufficiently large.

Also in the asymptotic limit of high magnetic fields, it was argued in Ref. 15 that the Jensen-Feynman inequality does not hold for polarons in two dimensions subjected to a magnetic field.

From the discussion above it follows that the PD treatment is not based on a maximum principle (except in the limit $\omega_c \to 0$) and does not *a priori* provide an upper bound for the free energy of the Fröhlich polaron in a magnetic field.

In the present paper we derive a more general inequality, which remains valid in the case of a nonzero magnetic field, and apply it to the Fröhlich polaron. In other words, we provide the "small modification" suspected to exist by Feynman and Hibbs, which is required to generalize the Feynman inequality, e.g., to a polaron in a nonzero magnetic field.

The formulation and the formalism in the present paper differ from the one used by PD. Contrary to PD, our final expression is now based on a maximum principle and provides an upper bound for the ground-state energy of a polaron in a magnetic field. Our derivation is based on the variational principle of quantum mechanics, applied with ordered operator calculus (i.e., the operator equivalent of the Feynman path integral), in which only the Hermiticity of the Hamiltonian is required. At any stage in the calculation, the corresponding path-integral formulation is readily obtained.

If the following simple but crucial *additional* constraints on the variational parameters $v_\perp$, $w_\perp$, $v_\parallel$, $w_\parallel$ are satisfied,

$$\max(\omega,\omega_c) \leq w_\perp \leq v_\perp, \quad \omega \leq w_\parallel \leq v_\parallel \tag{1.3}$$

(where ω is the frequency of the longitudinal-optical phonons) our upper bound for the ground-state energy of a polaron in a magnetic field reduces formally to the same *functional expression* (1.1) as obtained by PD.

The variational parameters $v_\parallel$, $v_\perp$, $w_\parallel$, and $w_\perp$ are the natural generalizations of the parameters v and w in Feynman's upper bound to the ground-state energy of a polaron without a magnetic field. In the Feynman model, w accounts for the retardation effect due to the elimination of the phonons, and v is the frequency of the coupled harmonic oscillators of the model system, imitating the internal excitations from the interaction with the phonons. The introduction of a magnetic field breaks the spherical symmetry of the polaron Hamiltonian. Therefore, two different sets of variational parameters (for the direction parallel and orthogonal to the magnetic field) constitute a quite natural extension of the Feynman model in the presence of a nonzero magnetic field.

The constraints (1.3) are sufficient conditions for the Feynman inequality in unmodified functional form to remain valid for a polaron in a magnetic field; if these conditions are not satisfied, additional terms E^{DB}—still to be investigated in general—will in principle occur in the right-hand side (rhs) of the Feynman inequality (1.1):

$$E_G \leq E_{\mathrm{trial}} + \lim_{\beta\to\infty} \frac{\langle S - S_{\mathrm{trial}}\rangle}{\beta} + E^{\mathrm{DB}}. \tag{1.4}$$

In the free-particle limit and for $w_\perp = 0$, we evaluate these additional terms explicitly.

II. ORDERED-OPERATOR FORMULATION OF AN UPPER BOUND FOR THE GROUND-STATE ENERGY OF A PARTICLE IN A MAGNETIC FIELD

For a general Hamiltonian of the form

$$H = H_0 + V \tag{2.1}$$

the ground state $|0\rangle$ can be described in the interaction representation, starting from the unperturbed ground state $|-\infty\rangle$ of H_0 at time $t = -\infty$, by adiabatically switching on the interaction:

$$|0\rangle = U(0,-\infty)|-\infty\rangle, \tag{2.2}$$

$$U(t_2,t_1) = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_{t_1}^{t_2} dt\, V(t)\right), \tag{2.3}$$

$$V(t) = \lim_{\epsilon\to 0} e^{-\epsilon|t|} e^{iH_0t/\hbar} V e^{-iH_0t/\hbar}, \tag{2.4}$$

where $\mathcal{T}$ denotes the time-ordering operator. The ground-state energy E_G of H satisfies the variational principle of quantum mechanics with some trial state $|\Psi\rangle$:

$$E_G = \langle 0|H|0\rangle \leq \langle\Psi|H|\Psi\rangle. \tag{2.5}$$

If one chooses a trial state $|\Psi\rangle$ which is the ground state of an exactly solvable model Hamiltonian $H_0 + V_{\mathrm{trial}}$ with ground-state energy E_{trial}, (2.5) can be rewritten as

$$E_G \leq E_{\mathrm{trial}} + \langle\infty|\mathcal{T}\{U_{\mathrm{trial}}(\infty,-\infty)[V(0) - V_{\mathrm{trial}}(0)]\}| - \infty\rangle. \tag{2.6}$$

The time-evolution operator U_{trial} corresponds to the path integral over $\exp(iS_{\mathrm{trial}}/\hbar)$ in the path-integral formulation, with the action S_{trial} expressed in *real* time variables. The generalized inequality (2.6) is therefore intimately connected to the Feynman inequality. However, it is based on the Hermiticity of the Hamiltonians H and H_{trial}, but it does *not* require that the corresponding actions are real functions of the imaginary time variables.

If the matrix element in the rhs of (2.6) satisfies certain analyticity conditions in the complex-time plane, derived below, our generalized inequality (2.6) reduces to the Feynman inequality. We explicitly derive these conditions for a Fröhlich polaron in a magnetic field. However, if these analyticity conditions are not satisfied, the inequality (2.6) remains valid, and in principle introduces additional terms in the rhs of the Feynman inequality (1.1).

For the study of the Fröhlich polaron in a (uniform and homogeneous) magnetic field B, we first consider the more general Hamiltonian:

$$H = H_0 + \mathcal{V}(\mathbf{r}) + \sum_{\mathbf{k}}[W_{\mathbf{k}}(\mathbf{r})a_{\mathbf{k}} + W_{\mathbf{k}}^\dagger(\mathbf{r})a_{\mathbf{k}}^\dagger], \tag{2.7}$$

$$H_0 = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + \sum_{\mathbf{k}} \hbar w a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \tag{2.8}$$

or, in the gauge $\mathbf{A} = (0, Bx, 0)$ with the z axis in the direction of the magnetic field:

$$H_0 = \frac{1}{2m}\left[p_x^2 + (p_y + m\omega_c x)^2 + p_z^2\right] + \sum_{\mathbf{k}} \hbar w a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \tag{2.9}$$

where $\omega_c = |eB|/mc$ is the cyclotron frequency, and $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^\dagger$ are the phonon annihilation and creation operators. Note that the unperturbed Hamiltonian H_0 includes the interaction of the electron with the magnetic field.

With ordered-operator calculus, the phonons can be eliminated in the expectation values. The derivation is given in the Appendix. The procedure is equivalent to Feynman's elimination of the phonons in the path-integral formulation, as, e.g., discussed by Platzman.[16] Denoting

$$\mathbf{r}(t) = e^{iH_0 t/\hbar}\mathbf{r}e^{-iH_0 t/\hbar} \tag{2.10}$$

the interaction term becomes

$$\left\langle 0 \left| \sum_{\mathbf{k}} [W_{\mathbf{k}}(\mathbf{r})a_{\mathbf{k}} + W_{\mathbf{k}}^\dagger(\mathbf{r})a_{\mathbf{k}}^\dagger] \right| 0 \right\rangle = -\frac{i}{2\hbar}\int_{-\infty}^{\infty} dt\, e^{-i\omega|t|-\epsilon|t|} \sum_{\mathbf{k}} \langle\infty|\mathcal{T}[U(\infty,-\infty)W_{\mathbf{k}}(\mathbf{r}(0))W_{\mathbf{k}}^\dagger(\mathbf{r}(t))]|-\infty\rangle. \tag{2.11}$$

The polaron Hamiltonian $H^{\rm pol}$ for a polaron in a magnetic field is a particular case of the Hamiltonian (2.7):

$$H^{\rm pol} = H_0^{\rm pol} + \sum_{\mathbf{k}} (V_k e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}} + V_k^* e^{-i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}^\dagger), \tag{2.12}$$

$$H_0^{\rm pol} = \frac{1}{2m}[p_x^2 + (p_y + m\omega_c x)^2 + p_z^2] + \sum_{\mathbf{k}} \hbar\omega a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \tag{2.13}$$

with the electron-phonon interaction term V_k given by

$$V_k = i\frac{\hbar\omega}{k}\left(\frac{4\pi\alpha}{V}\sqrt{\frac{\hbar}{2m\omega}}\right)^{1/2}, \tag{2.14}$$

where V is the volume of the crystal, and α the dimensionless Fröhlich coupling constant. Note the difference in phonon frequency between H_0 and $H_0^{\rm pol}$.

With $|\Psi^{\rm pol}\rangle$ and $U^{\rm pol}(t_2, t_1)$ denoting the ground state and the time-evolution operator for the polaron, the ground-state energy $E_G^{\rm pol}$ can thus be written as

$$\begin{aligned} E_G^{\rm pol} = {} & \langle\Psi^{\rm pol}(\infty)|\mathcal{T}[U^{\rm pol}(\infty,-\infty)H_0^{\rm pol}(t=0)]|\Psi^{\rm pol}(-\infty)\rangle \\ & -\frac{i}{2\hbar}\sum_{\mathbf{k}}|V_k|^2\int_{-\infty}^{\infty} dt\, e^{-i\omega|t|-\epsilon|t|}\langle\Psi^{\rm pol}(\infty)|\mathcal{T}[U^{\rm pol}(\infty,-\infty)e^{i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}]|\Psi^{\rm pol}(-\infty)\rangle. \end{aligned} \tag{2.15}$$

This means that the polaron ground-state energy is exactly described by the retarded potential (in the interaction representation)

$$V^{\rm pol}(t') = -\frac{i}{2\hbar}\sum_{\mathbf{k}}|V_k^2|\mathcal{T}\int_{-\infty}^{\infty} dt\, e^{-i\omega|t|-\epsilon|t|}e^{i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(t')]}. \tag{2.16}$$

Consider then a model Hamiltonian $H^{\rm lin}$ (which will contain linear electron-phonon interaction terms only, and which will be specified in detail below), with corresponding time evolution operator $U^{\rm lin}(t_2, t_1)$, ground-state energy $E_G^{\rm lin}$, and ground state $|\Psi^{\rm lin}\rangle$. If we impose that $H^{\rm lin}$ has the same unperturbed electronic contribution [Eq. (2.13)] as the polaron Hamiltonian, no ambiguity can arise in the meaning of the time evolution $\mathbf{r}(t)$ of the electron coordinate (2.10) in the interaction representation:

$$\mathbf{r}(t) = e^{iH_0^{\rm pol}t/\hbar}\mathbf{r}e^{-iH_0^{\rm pol}t/\hbar} = e^{iH_0^{\rm lin}t/\hbar}\mathbf{r}e^{-iH_0^{\rm lin}t/\hbar}. \tag{2.17}$$

We then find that an upper bound for the ground-state energy of the polaron in a magnetic field is obtained if $V(0)$ in Eq. (2.6) is replaced by $V^{\rm pol}(0)$:

$$\begin{aligned} E_G^{\rm pol} \le {} & \langle\Psi^{\rm lin}(\infty)|\mathcal{T}[U^{\rm lin}(\infty,-\infty)H_0^{\rm pol}(t=0)]|\Psi^{\rm lin}(-\infty)\rangle \\ & -\frac{i}{2\hbar}\sum_{\mathbf{k}}|V_k|^2\int_{-\infty}^{\infty} dt\, e^{-i\omega|t|-\epsilon|t|}\langle\Psi^{\rm lin}(\infty)|\mathcal{T}[U^{\rm lin}(\infty,-\infty)e^{i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}]|\Psi^{\rm lin}(-\infty)\rangle. \end{aligned} \tag{2.18}$$

Equation (2.6) and its application (2.18) to the polaron in a magnetic field are the core of the present paper. They provide an extension of the Feynman inequality, specified to the case of a polaron in a nonzero magnetic field. Note that Eq. (2.18) involves an integration over *real* time variables, contrary to Feynman's path-integral formulation of the Feynman inequality. In transforming the integrations over real time variables to integrations over imaginary time variables, the domain of analyticity of the integrand must be explored and taken into account. The reason for the difference with the Feynman inequality is that for $\omega_c \neq 0$ branch points and poles can occur in the complex-time plane, related to the intersection of the Landau levels with the continuum; for $\omega_c = 0$ such singularities do not arise.

If the time-dependent integrand in (2.18) satisfies certain analyticity conditions discussed below, (2.18) expressed in terms of Feynman path-integrals, leads to the result that

(a) an upper bound is obtained for the ground-state energy of a polaron in a magnetic field of the same functional form as the one deduced from the Feynman inequality; i.e., if $S^{\rm pol}$ and $S^{\rm lin}$ denote the action functional of the polaron and of the model system at imaginary time β and with the expectation values evaluated with the probability density $\exp(S^{\rm lin})/\int \mathcal{D}x \exp(S^{\rm lin})$ of the model, the Feynman inequality

$$E_G^{\rm pol} \leq E_G^{\rm lin} + \lim_{\beta\to\infty} \frac{\langle S^{\rm pol} - S^{\rm lin}\rangle}{\beta} \tag{2.19}$$

remains valid, but in general only if

(b) supplementary conditions, derived in the present paper, are imposed on the variational parameters in the trial action. These additional constraints arise as a result of the analyticity requirements for the integrand in the right-hand side of the inequality (2.18) when choosing an integration contour in the complex time plane. Contrary to what happens in the case $\omega_c = 0$, the direct substitution $t \longrightarrow -i\hbar\tau$ is no longer allowed for $\omega_c \neq 0$.

(c) If the supplementary conditions mentioned in (b) are not satisfied, it is still possible—at least in principle—to derive an upper bound for the ground-state energy of a polaron in a magnetic field. But its form will in general differ from the Feynman inequality (2.19) because of additional terms appearing in the rhs of (2.19). These terms arise from choosing a Cauchy contour in the complex time plane which circumvents poles and branch lines.

In general it can be stated that (2.19) remains valid for a nonzero magnetic field if the analyticity requirements for the Cauchy integration in the complex-time plane, necessary for our generalization in (2.18), are correctly taken into account. For a specific choice of the trial action (here $S^{\rm lin}$) the analyticity conditions result in constraints on the variational parameters occurring in the trial action.

Note that, if in Eq. (2.18) real times are *directly* substituted by imaginary times ($t \longrightarrow -i\hbar\tau$), exactly the PD approximation for the ground-state energy of a polaron in a magnetic field results. However, as stated above, such a substitution is not legitimate in general, and this is the reason why the PD approximation does not *a priori* provide an upper bound to the ground-state energy of a polaron in a magnetic field.

III. CONSTRUCTION OF A DIAGONALIZABLE LINEARIZED POLARON MODEL

In analogy with Feynman's quadratic trial action $S_{\rm trial}$ in his treatment of the polaron, we require a Hamiltonian $H^{\rm lin}$ for which in the absence of a magnetic field the path-integral formulation and phonon elimination would result in the action $S_{\rm trial}$. Note that a Hamiltonian of the form

$$H^{\rm el} + \hbar w a^\dagger a + [W(\mathbf{r})a + \text{H.c.}]$$

corresponds in the path-integral formulation to the action functional:

$$S^{\rm el} - \int_0^\beta d\tau \int_0^\tau d\sigma\, W(\mathbf{r}(\tau))W^*(\mathbf{r}(\sigma))G_w(\tau-\sigma),$$

where the memory function $G_w(\tau - \sigma)$ is due to the phonon elimination and is given by

$$G_w(u) = \frac{\cosh(\frac{\beta}{2} - u)\hbar w}{\sinh(\frac{\beta}{2})\hbar w}.$$

To account for the spatial asymmetry due to the presence of a magnetic field, it is natural to introduce two independent sets of phonon degrees of freedom, with a different frequency and a different interaction coefficient in the directions parallel or orthogonal to the magnetic field. In so doing one obtains a model which corresponds to the asymmetric trial action proposed by PD. These considerations suggest to introduce the following linearized model Hamiltonian:

$$H^{\rm lin} = H_\perp^{\rm lin} + H_\parallel^{\rm lin}, \tag{3.1}$$

$$H_\perp^{\rm lin} = \frac{1}{2m}\left[p_x^2 + (p_y + m\omega_c x)^2\right] + \frac{2C_\perp}{\hbar w_\perp}\rho^2 + \sum_{\mathbf{k}\in\mathcal{K}_1}\{\hbar w_\perp a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + [i\mathbf{k}\cdot\boldsymbol{\rho}\mathcal{L}_\perp(k)a_{\mathbf{k}} + \text{H.c.}]\}, \tag{3.2}$$

$$H_\parallel^{\rm lin} = \frac{p_z^2}{2m} + \frac{2C_\parallel}{\hbar w_\parallel}z^2 + \sum_{\mathbf{k}\in\mathcal{K}_2}\{\hbar w_\parallel a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + [ik_z z\mathcal{L}_\parallel(k)a_{\mathbf{k}} + \text{H.c.}]\}, \tag{3.3}$$

where $\boldsymbol{\rho}$ is the two-dimensional position vector with components (x, y) in the plane perpendicular to the magnetic field. $\mathcal{K}_1$ and $\mathcal{K}_2$ are two spherical symmetric complementary subsets of the phonon degrees of freedom in wave-vector space. The terms linear in $C_\perp$ and $C_\parallel$ are introduced to ensure the translational invariance[11] of the model if the following conditions are imposed:

$$2C_\perp = \sum_{\mathbf{k}\in\mathcal{K}_1}\frac{k^2}{3}|\mathcal{L}_\perp(k)|^2, \tag{3.4}$$

$$2C_{\parallel} = \sum_{\mathbf{k}\in\mathcal{K}_2} \frac{k^2}{3} |\mathcal{L}_{\parallel}(k)|^2. \tag{3.5}$$

These relations couple the strength of the harmonic interaction in the model with the electron-phonon interaction. Without electron-phonon interaction the electronic part of the unperturbed linear Hamiltonian is identical to the electronic part of the unperturbed polaron Hamiltonian, as required in the previous section.

On the one hand, this linearized model has been studied with Green's-function techniques by Bogolubov and Bogolubov[17] (who take into account the phonon dispersion, but only consider $\omega_c = 0$). On the other hand, the model has been explicitly diagonalized with canonical transformations by the present authors[18] (with dispersionless phonons, and $\omega_c \neq 0$).

The main step in our diagonalization procedure of H^{lin} consists of the introduction of "collective boson annihilation and creation operators," which allow us to replace the phonon bath by a "fictitious particle" as far as its interaction with the electron is concerned:

$$\mathbf{B}_{\perp} \equiv -\frac{1}{\sqrt{2C_{\perp}}} \sum_{\mathbf{k}\in\mathcal{K}_1} \mathbf{k}_{\perp} \mathcal{L}_{\perp}(k) a_{\mathbf{k}}, \tag{3.6}$$

$$B_{\parallel} \equiv -\frac{1}{\sqrt{2C_{\parallel}}} \sum_{\mathbf{k}\in\mathcal{K}_2} k_z \mathcal{L}_{\parallel}(k) a_{\mathbf{k}} \tag{3.7}$$

(and the corresponding creation operators $\mathbf{B}_{\perp}^{\dagger}, B_{\parallel}^{\dagger}$). The introduction of these collective operators in the linear model Hamiltonian allows one to consider the linear interaction of the electron with the phonon bath as a linear interaction with a "fictitious particle." In terms of these collective operators the Hamiltonian of the linear model can be rewritten as

$$H^{\text{lin}} = H_{\perp} + H_{\parallel} + H'', \tag{3.8}$$

$$H_{\perp} = \frac{1}{2m}\left[p_x^2 + (p_y + m\omega_c x)^2\right] + \frac{2C_{\perp}}{\hbar w_{\perp}}\rho^2 + \hbar w_{\perp} \mathbf{B}_{\perp}^{\dagger}\cdot\mathbf{B}_{\perp} - i\sqrt{2C_{\perp}}\boldsymbol{\rho}\cdot(\mathbf{B}_{\perp} - \mathbf{B}_{\perp}^{\dagger}), \tag{3.9}$$

$$H_{\parallel} = \frac{p_z^2}{2m} + \frac{2C_{\parallel}}{\hbar w_{\parallel}} z^2 + \hbar w_{\parallel} B_{\parallel}^{\dagger} B_{\parallel} - i\sqrt{2C_{\parallel}} z (B_{\parallel} - B_{\parallel}^{\dagger}). \tag{3.10}$$

The terms $H_{\perp}$ and $H_{\parallel}$ in the transformed Hamiltonian of the linear model describe an harmonic oscillator subjected to a magnetic field and interacting linearly with a second harmonic oscillator. PD also introduced a "fictitious particle" to imitate the phonon bath. The trial Hamiltonian which they constructed and diagonalized is equivalent to $H_{\perp} + H_{\parallel}$.

H'' accounts for the remaining phonon degrees of freedom after the introduction of the collective operators. The diagonalization of H'' is discussed in detail in Ref. 18, where it is also shown that H'' commutes with both $H_{\perp}$ and $H_{\parallel}$, and that it does not contribute to the equations of motion of the electrons and of the collective operators $\mathbf{B}_{\perp}$ and $B_{\parallel}$. Therefore, H'' can be considered as a constant for the purpose of the present paper. Its relevance is limited to providing the same degrees of freedom in the linear model as in the polaron Hamiltonian.

Assuming that the ground state $|\Psi^{\text{lin}}\rangle$ and the ground-state energy E_G^{lin} of the model Hamiltonian H^{lin} are known, the application of the maximum principle (2.18) requires the evaluation of various matrix elements. Concentrating first on the expectation value of the noninteracting part H_0^{pol} [Eq. (2.13)] of the polaron Hamiltonian, it is useful to express this term in H^{lin}:

$$\begin{aligned} H_0^{\text{pol}} = H^{\text{lin}} &+ \sum_{\mathbf{k}\in\mathcal{K}_1} \hbar(\omega - w_{\perp}) a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \\ &- \left(\frac{2C_{\perp}}{\hbar w_{\perp}}\rho^2 - i\sqrt{2C_{\perp}}\boldsymbol{\rho}\cdot(\mathbf{B}_{\perp} - \mathbf{B}_{\perp}^{\dagger})\right) \\ &+ \sum_{\mathbf{k}\in\mathcal{K}_2} \hbar(\omega - w_{\parallel}) a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \\ &- \left(\frac{2C_{\parallel}}{\hbar w_{\parallel}} z^2 - i\sqrt{2C_{\parallel}} z (B_{\parallel} - B_{\parallel}^{\dagger})\right). \end{aligned} \tag{3.11}$$

If $w_{\perp}$ and $w_{\parallel}$ are chosen to satisfy

$$w_{\perp} \geq \omega, \quad w_{\parallel} \geq \omega \tag{3.12}$$

then obviously the following inequality holds for the expectation value of H_0^{pol} in any state:

$$\begin{aligned} \langle H_0^{\text{pol}} \rangle \leq \langle H^{\text{lin}} \rangle &- \left\langle \frac{2C_{\perp}}{\hbar w_{\perp}}\rho^2 - i\sqrt{2C_{\perp}}\boldsymbol{\rho}\cdot(\mathbf{B}_{\perp} - \mathbf{B}_{\perp}^{\dagger}) \right\rangle \\ &- \left\langle \frac{2C_{\parallel}}{\hbar w_{\parallel}} z^2 - i\sqrt{2C_{\parallel}} z (B_{\parallel} - B_{\parallel}^{\dagger}) \right\rangle. \end{aligned} \tag{3.13}$$

The conditions (3.12) are not very crucial, and could be omitted at the price of evaluating extra terms arising from the expectation values of the phonon number operators. In the actual minimization of the upper bound however, these conditions happen to be satisfied in practice.

Using the maximum principle (2.18), with $U^{\text{lin}}(t_1, t_2)$ the time-evolution operator and $|\Psi^{\text{lin}}(t)\rangle$ the wave function of the linear model at time t, the following upper bound is obtained for the ground-state energy of a polaron in a magnetic field:

$$E_G^{\text{pol}} \leq E^{\text{var}}, \tag{3.14}$$

$$\begin{aligned} E^{\text{var}} = E_G^{\text{lin}} &- \left\langle \Psi^{\text{lin}}(\infty) \middle| \mathcal{T}\left[U^{\text{lin}}(\infty,-\infty)\left(\frac{2C_\perp}{\hbar w_\perp}\rho^2(0) + \frac{2C_\parallel}{\hbar w_\parallel} z^2(0)\right)\right] \middle| \Psi^{\text{lin}}(-\infty)\right\rangle \\ &+ i\sqrt{2C_\perp}\langle \Psi^{\text{lin}}(\infty)|\mathcal{T}\{U^{\text{lin}}(\infty,-\infty)\boldsymbol{\rho}(0)\cdot[\mathbf{B}_\perp(0) - \mathbf{B}_\perp^\dagger(0)]\}|\Psi^{\text{lin}}(-\infty)\rangle \\ &+ i\sqrt{2C_\parallel}\langle \Psi^{\text{lin}}(\infty)|\mathcal{T}\{U^{\text{lin}}(\infty,-\infty)z(0)[B_\parallel(0) - B_\parallel^\dagger(0)]\}|\Psi^{\text{lin}}(-\infty)\rangle \\ &- \frac{i}{2\hbar}\sum_{\mathbf{k}}|V_k|^2\int_{-\infty}^{\infty} dt\, e^{-i\omega|t|-\epsilon|t|}\langle \Psi^{\text{lin}}(\infty)|\mathcal{T}[U^{\text{lin}}(\infty,-\infty)e^{i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}]|\Psi^{\text{lin}}(-\infty)\rangle . \end{aligned} \tag{3.15}$$

The bosons described by the collective annihilation and creation operators $\mathbf{B}_\perp, B_\parallel$ and $\mathbf{B}_\perp^\dagger, B_\parallel^\dagger$ can be eliminated (see the Appendix):

$$\begin{aligned} &i\sqrt{2C_\perp}\langle \Psi^{\text{lin}}(\infty)|\mathcal{T}\{U^{\text{lin}}(\infty,-\infty)\boldsymbol{\rho}(0)\cdot[\mathbf{B}_\perp(0) - \mathbf{B}_\perp^\dagger(0)]\}|\Psi^{\text{lin}}(-\infty)\rangle \\ &\qquad = \frac{i}{2\hbar}2C_\perp\int_{-\infty}^{\infty} dt\, e^{-iw_\perp|t|-\epsilon|t|}\langle \Psi^{\text{lin}}(\infty)|\mathcal{T}\left[U^{\text{lin}}(\infty,-\infty)\boldsymbol{\rho}(0)\cdot\boldsymbol{\rho}(t)\right]|\Psi^{\text{lin}}(-\infty)\rangle , \end{aligned} \tag{3.16}$$

and similarly for the contributions parallel to the magnetic field. The upper bound (3.15) to the ground-state energy of the polaron in a magnetic field then contains matrix elements of electron operators only:

$$\begin{aligned} E^{\text{var}} = E_G^{\text{lin}} &- \left\langle \Psi^{\text{lin}}(0) \middle| \frac{2C_\perp}{\hbar w_\perp}\rho^2(0) + \frac{2C_\parallel}{\hbar w_\parallel}z^2(0) \middle| \Psi^{\text{lin}}(0)\right\rangle \\ &+ \frac{i}{2\hbar}2C_\perp\int_{-\infty}^{\infty} dt\, e^{-iw_\perp|t|-\epsilon|t|}\langle \Psi^{\text{lin}}(\infty)|\mathcal{T}\left[U^{\text{lin}}(\infty,-\infty)\boldsymbol{\rho}(0)\cdot\boldsymbol{\rho}(t)\right]|\Psi^{\text{lin}}(-\infty)\rangle \\ &+ \frac{i}{2\hbar}2C_\parallel\int_{-\infty}^{\infty} dt\, e^{-iw_\parallel|t|-\epsilon|t|}\langle \Psi^{\text{lin}}(\infty)|\mathcal{T}\left[U^{\text{lin}}(\infty,-\infty)z(0)z(t)\right]|\Psi^{\text{lin}}(-\infty)\rangle \\ &- \frac{i}{2\hbar}\sum_{\mathbf{k}}|V_k|^2\int_{-\infty}^{\infty} dt\, e^{-i\omega|t|-\epsilon|t|}\langle \Psi^{\text{lin}}(\infty)|\mathcal{T}[U^{\text{lin}}(\infty,-\infty)e^{i\mathbf{k}\cdot[\mathbf{r}(t)-\mathbf{r}(0)]}]|\Psi^{\text{lin}}(-\infty)\rangle . \end{aligned} \tag{3.17}$$

Because the time-evolution operator U^{lin} corresponds to the path-integral over $\exp(iS^{\text{lin}}/\hbar)$—with S^{lin} the action of the linear model in real time variables—in the path-integral formulation, one immediately recognizes a close similarity between the terms in the rhs of (3.17) and the familiar terms $\left\langle S^{\text{pol}} - S^{\text{lin}}\right\rangle/\beta$ expected from the path-integral treatment.

Equation (3.17) provides our extension of the Feynman upper bound for a polaron in a magnetic field, but it is expressed in *real* time variables. If the time-dependent integrand in (3.17) satisfies the necessary analyticity properties in the complex-time plane to substitute real by imaginary time variables, (3.17) reduces to the Feynman upper bound. This implies that formally the Feynman inequality remains valid under these analyticity constraints.

IV. ALGEBRAIC EXPRESSION FOR THE UPPER BOUND TO THE ENERGY OF A POLARON IN A MAGNETIC FIELD

The explicit evaluation of the matrix elements of the ordered operators in the upper bound (3.17) to the ground-state energy of a polaron in a magnetic field requires the diagonalization of the linear model Hamiltonian (3.8). The diagonalization procedure has been discussed elsewhere[11,18] and is only briefly summarized here.

As mentioned above, the linearized polaron model can be considered as a charged harmonic oscillator in a magnetic field, linearly interacting with a second harmonic oscillator with mass m_2, frequency $w_\perp$, and with position and momentum operators $\boldsymbol{\rho}_2$ and $\mathbf{p}_2$. With the following substitutions:

$$\mathbf{p}_2 = \sqrt{\frac{\hbar m_2 w_\perp}{2}}(\mathbf{B}_\perp + \mathbf{B}_\perp^\dagger), \tag{4.1}$$

$$\boldsymbol{\rho}_2 = i\sqrt{\frac{\hbar}{2m_2 w_\perp}}(\mathbf{B}_\perp - \mathbf{B}_\perp^\dagger), \tag{4.2}$$

$$4C_\perp = \hbar w_\perp \Omega^2, \tag{4.3}$$

the Hamiltonian (3.9) in the plane perpendicular to the magnetic field can indeed be rewritten as

$$\begin{aligned} H_\perp = -\hbar w_\perp + \frac{p_x^2 + (p_y + m\omega_c x)^2}{2m} + \frac{p_2^2}{2m_2} \\ + \tfrac{1}{2}(\Omega\sqrt{m}\rho - w_\perp\sqrt{m_2}\rho_2)^2 . \end{aligned} \tag{4.4}$$

This Hamiltonian can be diagonalized by standard techniques,[3] resulting in the Hamiltonian of three independent harmonic oscillators:

$$H_{\perp} = -\hbar w_{\perp} + \sum_{j=1}^{3} \hbar s_j (b_j^{\dagger} b_j + \tfrac{1}{2}), \tag{4.5}$$

where b_j and $b_j^{\dagger}$ are boson annihilation and creation operators. The eigenfrequencies s_j are the (non-negative) solutions of the equations:

$$s_j(s_j^2 - \Omega^2 - w_{\perp}^2) = (-1)^{j+1}\omega_c(s_j^2 - w_{\perp}^2) \quad \text{for } j = 1,2,3, \tag{4.6}$$

which means that they satisfy the following set of equations:

$$\begin{aligned} &s_1 - s_2 + s_3 = \omega_c, \\ &s_1 s_2 - s_1 s_3 + s_2 s_3 = \Omega^2 + w_{\perp}^2, \\ &s_1 s_2 s_3 = \omega_c w_{\perp}^2. \end{aligned} \tag{4.7}$$

In the process of diagonalization of Eq. (4.4), two canonically conjugate constants of motion Π, Q enter, which satisfy the commutation relation $[P,Q] = \hbar/i$. They are related to the classical orbit center,[19] but do not appear in the Hamiltonian. The explicit transformations of the position and momentum operators into the creation and annihilation operators $b_j^{\dagger}, b_j$ for this diagonalization[18] also involve the expansion coefficients c_j, given by

$$c_j^2 = \frac{\hbar}{2m}\frac{s_j^2 - w_{\perp}^2}{s_j}\frac{1}{3s_j^2 - 2(-1)^{j+1}\omega_c s_j - \Omega^2 - w_{\perp}^2} \tag{4.8}$$

which play an important role in the further treatment.

The adiabatic switching of the interaction in the previous section,

$$\mathcal{L}_{\perp}(k) \longrightarrow \mathcal{L}_{\perp}(k,t) = \mathcal{L}_{\perp}(k)e^{-\epsilon|t|}, \tag{4.9}$$

implies

$$\begin{aligned} &C_{\perp} \longrightarrow C_{\perp}(t) = C_{\perp}e^{-2\epsilon|t|}, \\ &\Omega \longrightarrow \Omega(t) = \Omega e^{-\epsilon|t|}, \end{aligned} \tag{4.10}$$

but this time dependence does not prevent the diagonalization *at any arbitrary time* t. This means that the eigenstates of the linear model can adiabatically be followed at any time, with the eigenfrequencies $s_j(t)$ and the corresponding expansion coefficients $c_j^2(t)$ evolving in time with the replacement of Ω in the equations above by $\Omega(t)$.

In the asymptotic limit $t \to \pm\infty$, i.e., $\Omega(t) \to 0$, the eigenfrequencies s_j and the expansion coefficients c_j are asymptotically given by

$$\begin{aligned} &s_1(t \to \pm\infty) \longrightarrow \omega_c\left(1 + \frac{\Omega^2 e^{-2\epsilon|t|}}{\omega_c^2 - w_{\perp}^2}\right), \\ &s_2(t \to \pm\infty) \longrightarrow w_{\perp}\left(1 + \frac{\Omega^2 e^{-2\epsilon|t|}}{2w_{\perp}(w_{\perp} + \omega_c)}\right), \\ &s_3(t \to \pm\infty) \longrightarrow w_{\perp}\left(1 + \frac{\Omega^2 e^{-2\epsilon|t|}}{2w_{\perp}(w_{\perp} - \omega_c)}\right), \end{aligned} \tag{4.11}$$

$$\begin{aligned} &\frac{2m}{\hbar}c_1^2(t \to \pm\infty) \longrightarrow \frac{1}{\omega_c} + O(\Omega^2 e^{-2\epsilon|t|}), \\ &\frac{2m}{\hbar}c_2^2(t \to \pm\infty) \longrightarrow \frac{\Omega^2 e^{-2\epsilon|t|}}{2w_{\perp}(w_{\perp} + \omega_c)^2}, \\ &\frac{2m}{\hbar}c_3^2(t \to \pm\infty) \longrightarrow \frac{\Omega^2 e^{-2\epsilon|t|}}{2w_{\perp}(w_{\perp} - \omega_c)^2}. \end{aligned} \tag{4.12}$$

The Hamiltonian H_0 without interaction is

$$\begin{aligned} H_0 &= H_{\perp}(t = \pm\infty) \\ &= -\hbar w_{\perp} + \sum_{j=1}^{3} \hbar s_j(\pm\infty)[\tfrac{1}{2} + b_j^{\dagger}(\pm\infty)b_j(\pm\infty)] \end{aligned} \tag{4.13}$$

and the time evolution operator $U_{\perp}(t',t)$ is given by the time-ordered product

$$U_{\perp}(t',t) = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_t^{t'} dt'' V_I(t'')\right), \tag{4.14}$$

$$V_I(t) \equiv e^{iH_0 t/\hbar}\left[H_{\perp}(t) - H_0\right]e^{-iH_0 t/\hbar}. \tag{4.15}$$

If $|N_1, N_2, N_3, Q\rangle_{t;I}$ denotes an eigenstate of the Hamiltonian in the interaction picture at time t, with N_j denoting the number of phonons corresponding to the eigenfrequencies $s_j(t)$, the time evolution operator can be written as

$$U_{\perp}(t',t) = \sum_{N_1,N_2,N_3,Q} \exp\left(-i\int_t^{t'} dt'' E_{N_1,N_2,N_3}(t'')/\hbar\right) |N_1, N_2, N_3, Q\rangle_{t;I}\ {}_{t;I}\langle N_1, N_2, N_3, Q|. \tag{4.16}$$

Starting at time $t = -\infty$ in the unperturbed ground state $|\text{vac}, Q\rangle$, the system will at time t be described by the state

$$|\Psi_I(t)\rangle = \exp\left(-i\int_{-\infty}^{t} dt'' E_{\text{vac}}(t'')/\hbar\right) |\text{vac}, Q\rangle_{t;I}. \tag{4.17}$$

A quantity which is useful for evaluating the expectation values of $\boldsymbol{\rho}(0)\cdot\boldsymbol{\rho}(t)$ and $\exp\{-i\mathbf{k}\cdot[\boldsymbol{\rho}(0) - \boldsymbol{\rho}(t)]\}$ in the upper bound (3.17) for the ground-state energy of the polaron in a magnetic field is

$$\langle\Psi^{\rm lin}(\infty)|\mathcal{T}[U_\perp^{\rm lin}(\infty,-\infty)e^{-i\mathbf{k}'\cdot\boldsymbol{\rho}(t')}e^{i\mathbf{k}\cdot\boldsymbol{\rho}(t)}]|\Psi^{\rm lin}(-\infty)\rangle$$

$$= \sum_{N_1,N_2,N_3,Q'} \exp\left(-i\int_t^{t'} dt'' \sum_{j=1}^{3} N_j s_j(t'')\right) {}_{t';I}\langle {\rm vac}, Q|e^{-i\mathbf{k}'\cdot\boldsymbol{\rho}(t')}|N_1,N_2,N_3,Q'\rangle_{t';I}$$

$$\times {}_{t;I}\langle N_1,N_2,N_3,Q'|e^{i\mathbf{k}\cdot\boldsymbol{\rho}(t)}|{\rm vac},Q\rangle_{t;I}, \tag{4.18}$$

where it is assumed, without loss of generality, that $t' \geq t$.

The remaining matrix elements in the last equation are to be evaluated at given time t' (t), and since the diagonalization of the linear Hamiltonian is known at any time, the evaluation of these matrix elements is straightforward. The transformation laws for the diagonalization[18] allow us to express $i\mathbf{k}\cdot\boldsymbol{\rho}(t)$ in the annihilation and creation operators $b_j(t)$ and $b_j^\dagger(t)$ at time t. Elementary operator calculus then yields

$${}_{t;I}\langle {\rm vac}, Q|e^{-i\mathbf{k}\cdot\boldsymbol{\rho}(t)}|N_1,N_2,N_3,Q\rangle_{t;I} = \langle Q|e^{-i(k_yQ-k_x\Pi/m\omega_c)}|Q'\rangle \prod_{j=1}^{3}\frac{1}{\sqrt{N_j!}}e^{-\frac{1}{2}k_\perp^2c_j^2(t)}\{c_j(t)[-ik_x+(-1)^{j+1}k_y]\}^{N_j}. \tag{4.19}$$

Using this result in Eq. (4.18), the summation over N_1, N_2, N_3, and Q' can be done analytically, giving

$$\langle\Psi^{\rm lin}(\infty)|\mathcal{T}[U_\perp^{\rm lin}(\infty,-\infty)e^{-i\mathbf{k}'\cdot\boldsymbol{\rho}(t')}e^{i\mathbf{k}\cdot\boldsymbol{\rho}(t)}]|\Psi^{\rm lin}(-\infty)\rangle$$

$$= e^{-i\hbar(k_xk_y+k_x'k_y'-2k_yk_x')/2m\omega_c}\langle Q|e^{i(k_y-k_y')Q}e^{-i(k_x-k_x')\Pi/m\omega_c}|Q\rangle$$

$$\times\prod_{j=1}^{3}\exp\{-\tfrac{1}{2}[c_j^2(t)k_\perp^2+c_j^2(t')k_\perp'^2]\}$$

$$\times\prod_{j=1}^{3}\exp\left[[ik_x+(-1)^{j+1}k_y][-ik_x'+(-1)^{j+1}k_y']c_j(t)c_j(t')\exp\left(-i\int_t^{t'}dt''s_j(t'')\right)\right]. \tag{4.20}$$

From this rather general expression, one readily obtains for $\mathbf{k}'=\mathbf{k}$,

$$\langle\Psi^{\rm lin}(\infty)|\mathcal{T}[U_\perp^{\rm lin}(\infty,-\infty)e^{-i\mathbf{k}\cdot\boldsymbol{\rho}(t')}e^{i\mathbf{k}\cdot\boldsymbol{\rho}(t)}]|\Psi^{\rm lin}(-\infty)\rangle$$

$$=\prod_{j=1}^{3}\exp\left\{\frac{-k_\perp^2}{2}\left[c_j^2(t)+c_j^2(t')-2c_j(t)c_j(t')\exp\left(-i\int_t^{t'}dt''s_j(t'')\right)\right]\right\}. \tag{4.21}$$

From the appropriate expansion coefficients in $k_x'k_x$ and $k_y'k_y$, one also obtains from Eq. (4.20):

$$\langle\Psi^{\rm lin}(\infty)|\mathcal{T}\;[U_\perp^{\rm lin}(\infty,-\infty)\boldsymbol{\rho}(t')\cdot\boldsymbol{\rho}(t)]\;|\Psi^{\rm lin}(-\infty)\rangle = 2\sum_{j=1}^{3}c_j(t)c_j(t')\exp\left(-i\int_t^{t'}dt''s_j(t'')\right). \tag{4.22}$$

The contributions in the plane perpendicular to the magnetic field to the upper bound (3.17) for the ground-state energy of the polaron are then fully determined for $t' > t$. The results for $t' < t$ are obtained by interchanging t' and t.

It turns out that the corresponding expressions parallel to the magnetic field can readily be derived by taking the limit $\omega_c \to 0$.

The substitution $t \to -t$ can be used to convert the integration domain $[-\infty, 0]$ into $[0, \infty]$. The following upper bound then results for the ground-state energy of a polaron in a magnetic field:

$$E^{\rm var} = \frac{\hbar}{4}\frac{(v_\parallel - w_\parallel)^2}{v_\parallel} + \frac{\hbar}{2}\sum_{j=1}^{3}s_j - \hbar w_\perp + E_a + E_b, \tag{4.23}$$

$$E_a = \frac{4i}{\hbar}C_\perp\sum_{j=1}^{3}\int_0^\infty dt\, e^{-iw_\perp t-\epsilon t}\left[c_j(t)c_j(0)\exp\left(-i\int_0^t dt''s_j(t'')\right) - c_j^2(0)\right], \tag{4.24}$$

$$E_b = -\frac{i}{\hbar}\sum_{\mathbf{k}}|V_k|^2\int_0^\infty dt\, e^{-i\omega t-\epsilon t}\exp\left\{\frac{-k_\perp^2}{2}\sum_{j=1}^{3}\left[c_j^2(t)+c_j^2(0)-2c_j(t)c_j(0)\exp\left(-i\int_0^t dt'' s_j(t'')\right)\right]\right\}$$
$$\times\exp\left\{\frac{-k_z^2}{2}\left[\lambda^2(t)+\lambda^2(0)-2\lambda(t)\lambda(0)\exp\left(-i\int_0^t dt'' v_\parallel(t'')\right)+\frac{i\hbar}{m}\int_0^t dt''\frac{w_\parallel^2}{v_\parallel^2(t'')}\right]\right\}, \quad (4.25)$$

where

$$\lambda(t) = \sqrt{\frac{\hbar}{2m}\frac{v_\parallel^2(t)-w_\parallel^2}{v_\parallel^3(t)}}, \quad (4.26)$$

$$v_\parallel(t) = \sqrt{w_\parallel^2+\frac{4C_\parallel}{\hbar m w_\parallel}e^{-2\epsilon t}}, \quad (4.27)$$

which implies that $v_\parallel \geq w_\parallel$ since $C_\parallel \geq 0$ because of Eq. (3.5).

Note again that the PD approximation for the ground-state energy of a polaron in a magnetic field is *formally* obtained by taking the limit $\epsilon = 0$, and substituting t by $-i\hbar\tau$ in (4.23). But this limiting process and the direct transition to imaginary times by substitution are not generally valid. The analyticity requirements on the integrand which allow for this substitution are derived in the next section and provide crucial additional constraints on the variational parameters. If these additional constraints are satisfied for acceptable values of the variational parameters, our more general upper bound (4.23) can still be expressed in the same functional form as the Feynman upper bound for a polaron in a magnetic field.

V. INTEGRATION OVER IMAGINARY TIMES

There is little hope to perform the integrations in (4.24) and (4.25) with respect to time analytically, since even for the contributions in the direction parallel to the magnetic field no analytical integration procedure is known. Furthermore, the oscillations in combination with the adiabatic limit $\epsilon \to 0$ are prohibitive for numerical evaluation.

The oscillatory behavior of the integrands in Eqs. (4.24) and (4.25) can possibly be eliminated by integrating over the imaginary time axis. But before closing any contour, one has to examine whether or not the frequencies s_j and the expansion coefficients c_j^2 do introduce poles and/or branch lines as a function of the complex time:

$$z = t + i\tau. \quad (5.1)$$

The frequencies to be integrated are $v_\parallel$ (4.27) and the three solutions s_j of the cubic equation (4.6), which can be rewritten as follows:

$$s_1 - \omega_c = \frac{s_1\Omega^2}{s_1^2 - w_\perp^2}, \quad (5.2)$$

$$s_2 - w_\perp = \frac{s_2\Omega^2}{(s_2+w_\perp)(s_2+\omega_c)}, \quad (5.3)$$

$$s_3 - w_\perp = \frac{s_3\Omega^2}{(s_3+w_\perp)(s_3-\omega_c)}. \quad (5.4)$$

(It is clear that s_1 and s_3 can be interchanged, since both satisfy the same equation. We adopted the convention that s_1 is the solution which coincides with the cyclotron frequency in the limit of zero coupling, and that s_3 equals the variational parameter $w_\perp$ in this limit.)

For real times, it is obvious from (5.2)–(5.4) that (i) s_3 decreases and s_1 increases with increasing Ω^2 if $w_\perp < \omega_c$; (ii) s_1 decreases and s_3 increases with increasing Ω^2 if $w_\perp > \omega_c$; and that in both cases s_2 increases with increasing Ω^2. Hence,

$$w_\perp < \omega_c \Rightarrow s_1 \geq \omega_c, \quad s_2 \geq w_\perp, \quad s_3 \leq w_\perp,$$
$$w_\perp > \omega_c \Rightarrow s_1 \leq \omega_c, \quad s_2 \geq w_\perp, \quad s_3 \geq w_\perp. \quad (5.5)$$

The adiabatic switching of the interaction (4.10) is governed by the time dependence $e^{-2\epsilon t}$, which determines the evolution in time of the frequencies s_j and $v_\parallel$ (4.27). Since these frequencies for $z = t+i\tau$ are multivalued functions of $e^{-2\epsilon z}$ in (4.24) and (4.25), the periodicity π/ϵ of $\Omega^2(z)$ on the imaginary time axis suggests the Riemann surface defined by

$$-\frac{\pi}{2\epsilon} \leq \tau < \frac{\pi}{2\epsilon} \quad (5.6)$$

which includes the real-time axis.

Indeed, for the direction parallel to the magnetic field, branch points in the complex time plane $z = t + i\tau$ arise from $v_\parallel(z)$ if $w_\parallel^2 = -4C_\parallel e^{-2\epsilon z}/\hbar m w_\parallel$. The frequency $v_\parallel(z)$ in the direction parallel to the magnetic field is single valued at the Riemann surface defined above.

In the direction perpendicular to the magnetic field, further analysis is required. Expressing $\Omega^2(z)$ as a function of the complex frequencies $s_1(z)$ and $s_3(z)$,

$$\Omega^2 e^{-2\epsilon z} = \frac{[s_{1,3}(z)-\omega_c][s_{1,3}^2(z)-w_\perp^2]}{s_{1,3}(z)}, \quad (5.7)$$

shows that the real frequencies $s_{1,3} = 0$, $s_{1,3} = \pm w_\perp$, and $s_{1,3} = \omega_c$ are branch points in the complex frequency plane. Depending on the value of the variational parameter $w_\perp$ as compared to ω_c, several possibilities for the branch lines have to be examined according to Eq. (5.5). These possibilities are schematically represented in Fig. 1.

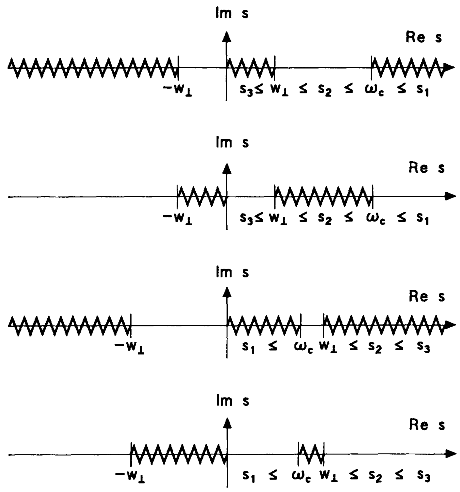

FIG. 1. Possible branch lines in the complex frequency plane for $w_\perp < \omega_c$ and $w_\perp > \omega_c$.

A. $w_\perp < \omega_c$

The branch lines can be chosen on the intervals (i) $[-\infty, -w_\perp]$, $[0, w_\perp]$, and $[\omega_c, \infty]$ or (ii) $[-w_\perp, 0]$ and $[w_\perp, \omega_c]$. In both of these cases at least one of the real frequencies s_1, s_2, or s_3 falls on a branch line, as is clear from the analysis above and from Fig. 1.

B. $w_\perp > \omega_c$

Also in this case two possible sets of branch lines can be chosen: (i) $[-\infty, -w_\perp]$, $[0, \omega_c]$, and $[w_\perp, \infty]$ or (ii) $[-w_\perp, 0]$ and $[\omega_c, w_\perp]$. It is clear from Fig. 1 that only the Riemann surface as defined by the last set of branch lines contains all three real eigenfrequencies s_1, s_2, and s_3.

The analysis of the analyticity of the functions $c_j^2(z)$ [see Eq. (4.8)] does not introduce extra relevant poles or branch lines: elementary algebra reveals that their denominator can only be zero for $s_1 = s_3$ or $s_2 = -s_1$ or $s_2 = -s_3$. These possibilities are already excluded by the condition $w_\perp > \omega_c$.

As a consequence, the analytic continuation in the complex plane of the integrands in the upper bound (4.23)-(4.25) for the ground-state energy of the polaron in a magnetic field is only justified if $w_\perp > \omega_c$. This condition guarantees that the three eigenfrequencies s_j belong to the same Riemann surface.

Under the important condition

$$w_\perp > \omega_c, \tag{5.8}$$

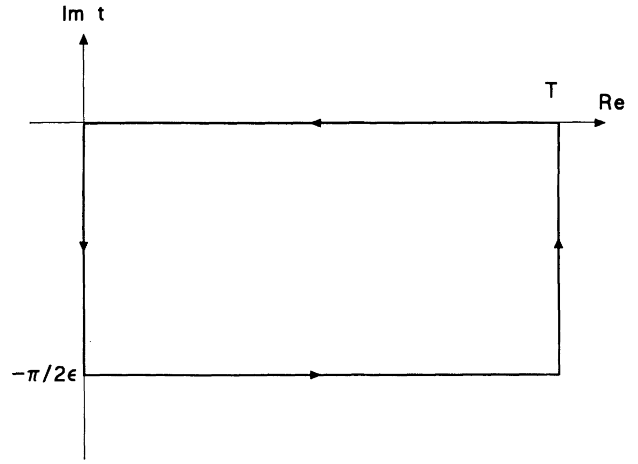

FIG. 2. Contour in the complex time plane with an analytic integrandum for the evaluation of the upper bound to the ground-state energy of a polaron in a magnetic field if $w_\perp > \omega_c$.

a rectangular contour (see Fig. 2) in the complex time plane with vertices 0, $-i\pi/2\epsilon$, $T - i\pi/2\epsilon$, and T, with $T \to \infty$, then encloses a region in which all the functions to be integrated are analytic functions of the complex time variable.

For all the integrations over time, occurring in the expressions (4.24) and (4.25) for the upper bound (4.23) to the energy of the polaron in a magnetic field, the integrals are of the form

$$\int_0^T dt\, F(t) = i \int_0^{-\pi/2\epsilon} d\tau\, F(i\tau) + \int_0^T dt\, F\left(t - \frac{i\pi}{2\epsilon}\right) + i \int_{-\pi/2\epsilon}^0 d\tau\, F(T + i\tau) \tag{5.9}$$

in the limit $T \to \infty$ and subsequently $\epsilon \to 0$. In the limit $T \to \infty$ only the first integral contributes, because for all the cases under consideration $F(\infty + i\tau)$ and $F(t - i\infty)$ are zero, and one obtains

$$E_a = -\frac{4C_\perp}{\hbar} \sum_{j=1}^{3} \int_0^{-\pi/2\epsilon} d\tau\, e^{w_\perp \tau} e^{-i\epsilon\tau} F_j(i\tau), \tag{5.10}$$

$$E_b = \frac{1}{\hbar} \sum_{\mathbf{k}} |V_k|^2 \int_0^{-\pi/2\epsilon} d\tau\, e^{\omega\tau} e^{-i\epsilon\tau} F_{\mathbf{k}}(i\tau), \tag{5.11}$$

with

$$F_j(i\tau) = c_j(i\tau) c_j(0) \exp\left(-i \int_0^{i\tau} dz'' s_j(z'')\right) - c_j^2(0), \tag{5.12}$$

$$F_{\mathbf{k}}(i\tau)=\exp\left\{-\frac{k_\perp^2}{2}\sum_{j=1}^{3}\left[c_j^2(i\tau)+c_j^2(0)-2c_j(i\tau)c_j(0)\exp\left(-i\int_0^{i\tau}dz''s_j(z'')\right)\right]\right\}$$
$$\times\exp\left\{-\frac{k_z^2}{2}\left[\lambda^2(i\tau)+\lambda^2(0)-2\lambda(i\tau)\lambda(0)\exp\left(-i\int_0^{i\tau}dz''v_\parallel(z'')\right)+\frac{i\hbar}{m}\int_0^{i\tau}dz''\frac{w_\parallel^2}{v_\parallel^2(z'')}\right]\right\}. \tag{5.13}$$

Because the frequencies $s_j(z)$ are analytic functions of $z=t+i\tau$ in their integration domain, they can be expanded in a Taylor series in the adiabatic switching parameter ϵ:

$$\exp\left(-i\int_0^{i\tau}dz''s_j(z'')\right)=\exp[s_j(0)\tau+O(\epsilon)] \tag{5.14}$$

and similarly for the expressions in $v_\parallel(i\tau)$, $c_j(i\tau)$, and $\lambda(i\tau)$, giving

$$F_j(i\tau)=c_j^2(0)(e^{s_j(0)\tau}-1)+O(\epsilon), \tag{5.15}$$

$$F_{\mathbf{k}}(i\tau)=\exp\left(-k_\perp^2\sum_{j=1}^{3}c_j^2(0)(1-e^{s_j(0)\tau})\right)$$
$$\times\exp[-k_z^2\lambda^2(0)(1-e^{v_\parallel(0)\tau})]$$
$$\times\exp\left(-k_z^2\frac{\hbar\tau}{2m}\frac{w_\parallel^2}{v_\parallel^2(0)}\right)+O(\epsilon). \tag{5.16}$$

Finally, taking the limit $\epsilon\to 0$, and substituting τ by $-\tau$, the contributions E_a and E_b to the energy expression (4.23) become

$$E_a=-\frac{4C_\perp}{\hbar}\sum_{j=1}^{3}c_j^2\left(\frac{1}{w_\perp}-\frac{1}{w_\perp+s_j}\right)=-\frac{4C_\perp}{\hbar w_\perp}\sum_{j=1}^{3}c_j^2\frac{s_j}{w_\perp+s_j}, \tag{5.17}$$

$$E_b=-\frac{1}{\hbar}\sum_{\mathbf{k}}|V_k|^2\int_0^\infty d\tau\,e^{-\omega\tau}\exp\left(-k_\perp^2\sum_{j=1}^{3}c_j^2(1-e^{-s_j\tau})\right)\exp\left[-\frac{\hbar^2k_z^2}{2m}\left(\frac{w_\parallel^2\tau}{v_\parallel^2}+\frac{v_\parallel^2-w_\parallel^2}{v_\parallel^3}(1-e^{-v_\parallel\tau})\right)\right]. \tag{5.18}$$

To simplify notation, references to the time dependence of the frequencies s_j, $v_\parallel$ and of the expansion coefficients c_j are omitted from here on: all these quantities have to be evaluated at time $t=0$.

For the further algebraic treatment it is useful to express the frequencies s_1 and s_3 in terms of s_2 with the help of (4.7):

$$s_{1,3}=\frac{\omega_c+s_2\pm 2W}{2}, \tag{5.19}$$

$$W\equiv\sqrt{\left(\frac{\omega_c+s_2}{2}\right)^2-\frac{\omega_c w_\perp^2}{s_2}}, \tag{5.20}$$

and similarly

$$c_1^2=\frac{\hbar}{2m\omega_c}\frac{s_3-\omega_c}{s_3-s_1}+\frac{s_3+s_2}{s_3-s_1}c_2^2, \tag{5.21}$$

$$c_3^2=\frac{\hbar}{2m\omega_c}\frac{\omega_c-s_1}{s_3-s_1}-\frac{s_1+s_2}{s_3-s_1}c_2^2. \tag{5.22}$$

The summation term in Eq. (5.17) can, with elementary algebra, be rewritten as

$$\sum_{j=1}^{3}c_j^2\frac{s_j}{w_\perp+s_j}=2\frac{c_2^2s_2^2}{s_2^2-w_\perp^2}. \tag{5.23}$$

Furthermore, in analogy with the direction parallel to the magnetic field, we introduce

$$v_\perp^2=w_\perp^2+\frac{4C_\perp}{\hbar m w_\perp} \tag{5.24}$$

which implies that $v_\perp\geq w_\perp$ since $C_\perp\geq 0$ because of Eq. (3.4), and insert the result (5.17) for E_a in the upper bound Eq. (4.23) for the energy:

$$E^{\text{var}}=\hbar\left(\frac{(v_\parallel-w_\parallel)^2}{4v_\parallel}+\frac{\omega_c}{2}\right)$$
$$+\hbar\left(s_2-w_\perp-\frac{2mc_2^2}{\hbar}s_2^2\frac{v_\perp^2-w_\perp^2}{s_2^2-w_\perp^2}\right)+E_b. \tag{5.25}$$

Introducing

$$D(\tau)=\frac{\hbar\tau}{2m}\frac{w_\parallel^2}{v_\parallel^2}\left(1+\frac{v_\parallel^2-w_\parallel^2}{w_\parallel^2}\frac{1-e^{-v_\parallel\tau}}{v_\parallel\tau}\right), \tag{5.26}$$

$$D_H(\tau)=\sum_{j=1}^{3}c_j^2(1-e^{-s_j\tau}), \tag{5.27}$$

the interaction term E_b can be rewritten as

$$E_b = -\frac{1}{\hbar}\sum_{\mathbf{k}} |V_k|^2 \int_0^\infty d\tau\, e^{-\omega\tau} e^{-k_\perp^2 D_H(\tau)} e^{-k_z^2 D(\tau)}. \tag{5.28}$$

Using the explicit form of V_k for the Fröhlich polaron,

$$V_k = i\frac{\hbar\omega}{k}\left(\frac{4\pi\alpha}{V}\sqrt{\frac{\hbar}{2m\omega}}\right)^{1/2}, \tag{5.29}$$

the summation over the wave vectors can be done analytically:

$$E_b = -\frac{\alpha\hbar\omega}{2\sqrt{\pi}}\sqrt{\frac{\hbar\omega}{2m}}\int_0^\infty d\tau \frac{e^{-\omega\tau}}{\sqrt{D(\tau)}} B\left(\frac{D(\tau)}{D_H(\tau)}\right) \tag{5.30}$$

with

$$B(x) = 2\sqrt{\frac{x}{x-1}}\operatorname{arccosh}(\sqrt{x}) = 2\sqrt{\frac{x}{x-1}}\ln\left(\sqrt{x}+\sqrt{x-1}\right). \tag{5.31}$$

As already mentioned before, the PD (Ref. 3) approximation for the ground-state energy of a polaron in a magnetic field *formally* led to the same functional expression (5.30). However, the derivation of PD was *not* based on a maximum principle, and did not *a priori* provide an upper bound for the ground-state energy.

The main result of the present paper is that the constraints

$$v_\perp \ge w_\perp > \omega_c, \quad w_\perp \ge \omega, \quad v_\parallel \ge w_\parallel \ge \omega \tag{5.32}$$

have to be imposed on the variational parameters to guarantee an upper bound to the exact ground-state energy of a polaron in a magnetic field. These conditions provide the "simple modification" which Feynman and Hibbs[1] suspected to be required for the generalization of the Feynman upper bound to the case of a nonzero magnetic field. If these constraints are not satisfied, additional terms might appear in the rhs of the Feynman inequality (2.19), due to contributions from branch lines and/or poles in the complex-time plane.

The fact that the eigenfrequencies s_j of the linear model system are solutions of a cubic equation, complicates the further analytical treatment of the upper bound E^{var} to the ground-state energy of a polaron in a magnetic field obtained so far. However, s_2 is a monotonic function of $v_\perp$ in the valid region of variation $w_\perp > \omega_c$ and $v_\perp \ge w_\perp$, and one might as well consider s_2 as a variational parameter (satisfying $s_2 \ge w_\perp$) and eliminate $v_\perp$ using the cubic equation (4.6) for s_2:

$$v_\perp^2 = s_2^2 + \omega_c s_2 - \frac{\omega_c w_\perp^2}{s_2} \tag{5.33}$$

giving

$$\frac{2mc_2^2}{\hbar} = \frac{s_2^2 - w_\perp^2}{2s_2^3 + s_2^2\omega_c + w_\perp^2\omega_c}. \tag{5.34}$$

Combining terms, one eventually finds for the energy the more tractable expression

$$E^{\text{var}} = \hbar\frac{\omega_c}{2} + \hbar\frac{(v_\parallel - w_\parallel)^2}{4v_\parallel} + \hbar\frac{(s_2 - w_\perp)^2(s_2^2 - \omega_c w_\perp)}{2s_2^3 + \omega_c s_2^2 + \omega_c w_\perp^2} + E_b, \tag{5.35}$$

where the contribution E_b from the interaction is given in (5.30). Using (5.19)–(5.21), the function $D_H(\tau)$ can also completely be expressed in s_2 and $w_\perp$:

$$D_H(\tau) = \left(\frac{\hbar}{2m\omega_c} + c_2^2\right) T_1(\tau) + c_2^2 T_2(\tau),$$

$$T_1(\tau) = 1 - e^{-(\omega_c+s_2)\tau/2} \times \left(\cosh W\tau + \frac{s_2-\omega_c}{2W}\sinh W\tau\right), \tag{5.36}$$

$$T_2(\tau) = 1 - e^{-s_2\tau} - e^{-(\omega_c+s_2)\tau/2}\frac{s_2+\omega_c}{W}\sinh W\tau,$$

$$W = \sqrt{\left(\frac{\omega_c+s_2}{2}\right)^2 - \frac{\omega_c w_\perp^2}{s_2}}.$$

Note that in the limit $\omega_c = 0$ one immediately recovers the Feynman result for the Fröhlich polaron in the absence of a magnetic field.

VI. ANALYSIS OF SOME LIMITING CASES

The main purpose of the present section is to derive analytical expressions, starting from Eq. (5.35), for our upper bound to the ground-state energy of the Fröhlich polaron in a magnetic field in several limiting cases such as small coupling (i.e., $\alpha \to 0$ and the free-particle limit $\alpha = 0$) combined with $\omega_c \to 0$ or $\omega_c \to \infty$. Some preliminary conclusions will also be drawn for the intermediate coupling regime.

This section emphasizes how the variational upper bound for a polaron in a magnetic field is influenced by the constraints (5.32) established in the present paper. We achieve this by comparing the upper bound (5.35) *including* the additional constraints (5.32) with the approximation of PD, which in pinciple is not an upper bound, but which starts from the same formal expression *without* the constraints.

A. The free-particle limit: Illustration of the general problem

Although the present treatment is rather artificial for the exactly solvable problem of a free particle in a magnetic field, we nevertheless discuss this limit for pedagogical purposes. Since even for a free particle in a magnetic field the Jensen-Feynman inequality does not apply,[10,11] it is instructive to examine how the additional constraints

(5.32) lead to the correct energy in this case. For $\alpha = 0$, the polaron coupling contribution E_b cancels in (5.35) and one has to minimize the following algebraic expression:

$$E^{\mathrm{var}}_{\alpha=0} = \hbar\frac{\omega_c}{2} + \hbar\frac{(s_2 - w_\perp)^2(s_2^2 - \omega_c w_\perp)}{2s_2^3 + \omega_c s_2^2 + \omega_c w_\perp^2}. \quad (6.1)$$

The two constraints $w_\perp \geq \omega$ and $w_\parallel \geq \omega$ are irrelevant for the free-particle limit, because no LO phonons are present. The third constraint $w_\perp > \omega_c$ implies that $s_2 \geq w_\perp$, and hence $s_2^2 \geq \omega_c w_\perp$. This constraint therefore excludes that a minimum can be found below the exact energy, and assures that the minimum of the variational energy for a free particle in a magnetic field is obtained at the exact energy $\hbar\omega_c/2$, with $v_\perp = s_2 = w_\perp$.

However, if one disregards the constraint $w_\perp > \omega_c$ (as in the PD approximation), $s_2^2 - \omega_c w_\perp$ can become negative. The approximation (6.1) for the ground-state energy of a free particle in a magnetic field then shows a (numerically determined) minimum which drops 1.9% below the exact energy $\hbar\omega_c/2$. Indeed, for $w_\perp < \omega_c$ the expression (6.1) does not provide an upper bound to the ground-state energy: extra terms can appear in the rhs of (6.1) due to possible branch lines in the complex-time plane.

Example of the generalization of the Feynman inequality for $\omega_c \neq 0$ if the additional constraints are not satisfied

The relevance of the contributions to the upper bound for the ground-state energy, due to the occurrence of branch lines in the complex-time plane for $w_\perp \leq \omega_c$ is clearly illustrated in the limit $w_\perp = 0$. In this case, i.e., if our additional constraints are not satisfied, the contribution E_a [Eq. (4.24)] is zero, because $C_\perp = 0$ for $w_\perp = 0$ from Eq. (4.3). Furthermore, the eigenfrequencies s_j of the model system can readily be calculated from Eq. (4.6):

$$s_1|_{w_\perp=0} = \tfrac{1}{2}(\sqrt{\omega_c^2 + 4\Omega^2} + \omega_c), \quad (6.2)$$

$$s_2|_{w_\perp=0} = \tfrac{1}{2}(\sqrt{\omega_c^2 + 4\Omega^2} - \omega_c), \quad (6.3)$$

$$s_3|_{w_\perp=0} = 0. \quad (6.4)$$

For $w_\perp = 0$, the upper bound (4.23) to the ground-state energy, evaluated from our fundamental inequality (2.18) with integrations along the real-time axis, becomes in the free-particle limit

$$E^{\mathrm{var}}_{\alpha=0,w_\perp=0} = \frac{\hbar}{2}\sqrt{\omega_c^2 + 4\Omega^2}. \quad (6.5)$$

This expression is different from the limit $w_\perp = 0$ in Eq. (6.1). [It should be recalled that (6.1) was obtained under the condition that our additional constraints are satisfied, which is not the case for the limit $w_\perp = 0$ considered here.]

In this limit $\alpha = 0$ and $w_\perp = 0$, we obtained in the upper bound for the ground-state energy the following contribution E^{DB}, which is different from zero because of the existence of different branch lines in the complex-time plane:

$$E^{\mathrm{DB}}_{\alpha=0,w_\perp=0} = \frac{\hbar\Omega^2}{\sqrt{\omega_c^2 + 4\Omega^2}}. \quad (6.6)$$

Note that the upper bound (6.5) to the ground-state energy of a free particle in a magnetic field, valid if our additional constraints are not satisfied, reaches its minimum for $\Omega = 0$ at the exact ground-state energy $\hbar\omega_c/2$.

B. The polaron weak-coupling limit

The free-particle result suggests that both $s_2 - w_\perp$ and $v_\perp - w_\perp$ are of order α. To second order in $s_2 - w_\perp$, the upper bound (5.35) to the energy of the polaron in a magnetic field becomes

$$\begin{aligned} E^{\mathrm{var}}_{\alpha\to 0} = {} & \hbar\frac{\omega_c}{2} + \hbar\frac{(v_\parallel - w_\parallel)^2}{4v_\parallel} \\ & + \hbar\frac{(w_\perp - \omega_c)}{2w_\perp(w_\perp + \omega_c)}(s_2 - w_\perp)^2 \\ & + E_b + O((s_2 - w_\perp)^3). \end{aligned} \quad (6.7)$$

Because of the constraint $w_\perp > \omega_c$, E_b in Eq. (5.30) is the only term that can be negative. E_b is proportional to the polaron coupling strength α, and its evaluation to second order therefore only requires expansions of E_b to first order in $s_2 - w_\perp$.

The condition $w_\perp > \omega_c$ is again important to allow for the expansion of W [see (5.36)]:

$$W = \tfrac{1}{2}(w_\perp - \omega_c)\left(1 + (s_2 - w_\perp)\frac{w_\perp + 3\omega_c}{(w_\perp - \omega_c)^2} + \dots\right). \quad (6.8)$$

Furthermore, using the expansion

$$\frac{2mc_2^2}{\hbar} = \frac{s_2 - w_\perp}{w_\perp(w_\perp + \omega_c)} + \cdots, \quad (6.9)$$

the following expression is obtained for $D_H(\tau)$:

$$D_H(\tau) = D_H^{(0)}(\tau) + \frac{s_2 - w_\perp}{w_\perp} D_H^{(1)}(\tau) + \cdots, \quad (6.10)$$

$$D_H^{(0)}(\tau) = \frac{\hbar\tau}{2m}\frac{1 - e^{-\omega_c\tau}}{\omega_c\tau}, \quad (6.11)$$

$$\begin{aligned} D_H^{(1)}(\tau) = \frac{\hbar\tau}{2m}\Bigg(& 1 - e^{-\omega_c\tau} \\ & + \frac{w_\perp + \omega_c}{w_\perp - \omega_c} e^{-\omega_c\tau}\phi[(w_\perp - \omega_c)\tau] \\ & + \frac{\omega_c\phi(\omega_c\tau) + w_\perp\phi(w_\perp\tau)}{w_\perp + \omega_c}\Bigg) \end{aligned} \quad (6.12)$$

with

$$\phi(x) \equiv \frac{1 - x - e^{-x}}{x}. \quad (6.13)$$

A similar expansion with respect to $v_\| - w_\|$ gives, for the parallel direction,

$$D(\tau) = D^{(0)}(\tau) + \frac{v_\| - w_\|}{w_\|} D^{(1)}(\tau), \tag{6.14}$$

$$D^{(0)}(\tau) = \frac{\hbar\tau}{2m}, \tag{6.15}$$

$$D^{(1)}(\tau) = \frac{\hbar\tau}{2m} 2\phi(w_\|\tau), \tag{6.16}$$

with the following result for E_b to second order in the polaron coupling:

$$E_b = -\alpha\hbar\omega\mathcal{E}^{(0,0)} - \alpha\hbar\omega\frac{s_2 - w_\perp}{w_\perp}\mathcal{E}_\perp^{(1)} - \alpha\hbar\omega\frac{v_\| - w_\|}{w_\|}\mathcal{E}_\|^{(1)} + \cdots, \tag{6.17}$$

$$\mathcal{E}^{(0,0)} = \frac{1}{2\sqrt{\pi}}\sqrt{\frac{\hbar\omega}{2m}}\int_0^\infty d\tau\, e^{-\omega\tau}\frac{1}{\sqrt{D^{(0)}(\tau)}} B\left(\frac{D^{(0)}(\tau)}{D_H^{(0)}(\tau)}\right), \tag{6.18}$$

$$\mathcal{E}_\perp^{(1)} = \frac{1}{2\sqrt{\pi}}\sqrt{\frac{\hbar\omega}{2m}}\int_0^\infty d\tau\, e^{-\omega\tau} D_H^{(1)}(\tau)\frac{d}{dD_H^{(0)}(\tau)}\left[\frac{1}{\sqrt{D^{(0)}(\tau)}} B\left(\frac{D^{(0)}(\tau)}{D_H^{(0)}(\tau)}\right)\right], \tag{6.19}$$

$$\mathcal{E}_\|^{(1)} = \frac{1}{2\sqrt{\pi}}\sqrt{\frac{\hbar\omega}{2m}}\int_0^\infty d\tau\, e^{-\omega\tau} D^{(1)}(\tau)\frac{d}{dD^{(0)}(\tau)}\left[\frac{1}{\sqrt{D^{(0)}(\tau)}} B\left(\frac{D^{(0)}(\tau)}{D_H^{(0)}(\tau)}\right)\right]. \tag{6.20}$$

Minimizing $E^{\text{var}}_{\alpha\to 0}$ (6.7) with respect to $s_2 - w_\perp$ and $v_\| - w_\|$ leads to

$$s_2 - w_\perp = \alpha\omega\mathcal{E}_\perp^{(1)} + O(\alpha^2), \tag{6.21}$$

$$v_\| - w_\| = 2\alpha\omega\mathcal{E}_\|^{(1)} + O(\alpha^2), \tag{6.22}$$

$$\frac{1}{\hbar\omega}E^{\text{var}}_{\alpha\to 0} = \frac{\omega_c}{2\omega} - \alpha\mathcal{E}^{(0,0)} - \frac{\omega}{2w_\perp}\frac{w_\perp + \omega_c}{w_\perp - \omega_c}(\alpha\mathcal{E}_\perp^{(1)})^2 - \frac{\omega}{w_\|}(\alpha\mathcal{E}_\|^{(1)})^2 + O(\alpha^3). \tag{6.23}$$

For general ω_c this expression for the interaction term E_b in the energy seems intractable analytically, even to first order in the polaron coupling strength. Therefore, we restrict the further analytical treatment to the limits of high and low magnetic fields.

1. $\omega_c \to 0$ in the polaron weak-coupling limit

For sufficiently low magnetic field, the expansion of $D_H^{(0)}(\tau)$ and $D_H^{(1)}(\tau)$ [Eqs. (6.11) and (6.12)] to first order in ω_c gives

$$D_H^{(0)}(\tau)_{\omega_c\to 0} = \frac{\hbar\tau}{2m}(1 - \tfrac{1}{2}\omega_c\tau), \tag{6.24}$$

$$D_H^{(1)}(\tau)_{\omega_c\to 0} = 2\frac{\hbar\tau}{2m}\left[\phi(w_\perp\tau) + \omega_c\tau\left(1 + \frac{\phi(w_\perp\tau)}{w_\perp\tau}\right)\right]. \tag{6.25}$$

Therefore, $D^{(0)}(\tau)/D_H^{(0)}(\tau) = 1 + \omega_c\tau/2 + \cdots$ in this limit. Using the expansion (for $x \geq 1$):

$$B(x)_{x\to 1} = 2[\,1 + \tfrac{1}{3}(x-1) - \tfrac{2}{15}(x-1)^2 + \tfrac{8}{105}(x-1)^3 + \cdots] \quad \text{for } x \geq 1 \tag{6.26}$$

the energy corrections to first order in ω_c become

$$\begin{aligned} \mathcal{E}^{(0,0)}_{\omega_c\to 0} &= \frac{1}{2\sqrt{\pi}}\sqrt{\omega}\int_0^\infty d\tau\frac{e^{-\omega\tau}}{\sqrt{\tau}}2(1 + \tfrac{1}{6}\omega_c\tau + \cdots) = 1 + \frac{1}{12}\frac{\omega_c}{\omega} + \cdots, \\ \mathcal{E}^{(1)}_{\perp,\omega_c\to 0} &= \frac{1}{2\sqrt{\pi}}\sqrt{\omega}\int_0^\infty d\tau\frac{e^{-\omega\tau}}{\sqrt{\tau}}\frac{-4}{3}\left[\phi(w_\perp\tau) + \omega_c\tau\left(\tfrac{7}{5}\phi(w_\perp\tau) + 1 + \frac{\phi(w_\perp\tau)}{w_\perp\tau}\right) + \cdots\right], \\ \mathcal{E}^{(1)}_{\|,\omega_c\to 0} &= \frac{1}{2\sqrt{\pi}}\sqrt{\omega}\int_0^\infty d\tau\frac{e^{-\omega\tau}}{\sqrt{\tau}}\frac{-2}{3}\phi(w_\|\tau)\left(1 - \tfrac{13}{10}\omega_c\tau + \cdots\right). \end{aligned} \tag{6.27}$$

Neglecting the terms proportional to ω_c in $\mathcal{E}_\perp^{(1)}$ and $\mathcal{E}_\|^{(1)}$ introduces an error of order $\alpha^2\omega_c$ in the energy, because $\mathcal{E}_\perp^{(1)}$ and $\mathcal{E}_\|^{(1)}$ provide the contributions of order α^2 to the energy of a polaron in a magnetic field [see Eq. (6.23)]. Using

$$\int_0^\infty d\tau\frac{e^{-\omega\tau}}{\sqrt{\tau}}\phi(u\tau) = -\sqrt{\frac{\pi}{\omega}}\frac{(\sqrt{u+\omega} - \sqrt{\omega})^2}{u} \tag{6.28}$$

one easily derives

$$\mathcal{E}^{(1)}_{\perp,\omega_c\to 0} = \frac{2}{3w_\perp}(\sqrt{w_\perp+\omega}-\sqrt{\omega})^2 + O(\omega_c), \tag{6.29}$$

$$\mathcal{E}^{(1)}_{\perp,\omega_c\to 0} = \frac{1}{3w_\parallel}(\sqrt{w_\parallel+\omega}-\sqrt{\omega})^2 + O(\omega_c). \tag{6.30}$$

Inserting these results in Eq. (6.23) one finds for $\omega_c \to 0$:

$$\frac{1}{\hbar\omega}E^{\text{var}}_{\substack{\alpha\to 0\\ \omega_c\to 0}} = \frac{\omega_c}{2\omega} - \alpha\left(1+\frac{1}{12}\frac{\omega_c}{\omega}\right) - \frac{\alpha^2\omega}{9}\left(2\frac{(\sqrt{w_\perp+\omega}-\sqrt{\omega})^4}{w_\perp^3} + \frac{(\sqrt{w_\parallel+\omega}-\sqrt{\omega})^4}{w_\parallel^3}\right) + O(\alpha^3) + O(\alpha^2\omega_c) \tag{6.31}$$

which is minimal for $w_\perp = w_\parallel = 3\omega$, giving

$$\frac{1}{\hbar\omega}E^{\text{var}}_{\substack{\alpha\to 0\\ \omega_c\to 0}} = \frac{\omega_c}{2\omega} - \alpha - \frac{\alpha^2}{81} - \frac{\alpha}{12}\frac{\omega_c}{\omega} + O(\alpha^3) + O(\alpha^2\omega_c). \tag{6.32}$$

The same expansion was found by PD. For $\omega_c = 0$ the expected Feynman result to second order in α is obtained.

Since $w_\perp$ and $w_\parallel$ turn out to be of order 3ω for low magnetic fields, the constraints $w_\perp > \omega_c$, $w_\perp \geq \omega$, and $w_\parallel \geq \omega$ are automatically fulfilled for $\alpha \to 0$ and $\omega_c \to 0$. As is now clear from the conditions derived in the present paper, the PD result for the energy of a polaron in a magnetic field happens to constitute an upper bound if $\alpha \to 0$ and $\omega_c \to 0$, and in this limiting case the PD conjecture happens to be valid. For the higher-order terms in ω_c we therefore refer to Peeters and Devreese.[3]

2. $\omega_c \to \infty$ in the polaron weak-coupling limit

The first-order correction in the electron-phonon coupling constant α to the upper bound for the ground-state energy of a polaron in a magnetic field is for general ω_c determined by

$$\mathcal{E}^{(0,0)} = \frac{\omega}{2\pi}\int_0^\infty d\tau \frac{e^{-\omega\tau}}{\sqrt{\tau}} B\left(\frac{\omega_c\tau}{1-e^{-\omega_c\tau}}\right). \tag{6.33}$$

Because $B(u)$ behaves as $2\ln(2\sqrt{u})$ for $u\to\infty$, the substitution $u = \omega_c\tau$ reveals that the integral is divergent for $\omega_c \to \infty$. However, this limiting behavior of the function B for large $\omega_c\tau$ can be added and substracted in the integrand, so that the divergent term is extracted from the integral:

$$\mathcal{E}^{(0,0)} = \frac{\omega}{2\pi}\int_0^\infty d\tau \frac{e^{-\omega\tau}}{\sqrt{\tau}}\left[B\left(\frac{\omega_c\tau}{1-e^{-\omega_c\tau}}\right) - 2\ln(2\sqrt{\omega_c\tau})\right] + \tfrac{1}{2}[\ln(\omega_c/\omega) - \mathcal{C}], \tag{6.34}$$

where $\mathcal{C}$ is Euler's constant. For large $\omega_c\tau$ the term in the square brackets is of order $1/\omega_c\tau$, and the remaining integral converges. With the substitution $u = \omega_c\tau$, one obtains

$$\mathcal{E}^{(0,0)} = \tfrac{1}{2}[\ln(\omega_c/\omega) - \mathcal{C}] + \frac{\omega}{2\pi}\frac{1}{\sqrt{\omega_c}}\int_0^\infty du \frac{e^{-u\omega/\omega_c}}{\sqrt{u}} \times \left[B\left(\frac{u}{1-e^{-u}}\right) - 2\ln(2\sqrt{u})\right]. \tag{6.35}$$

The expansion of the integral in powers of ω/ω_c leads to

$$\mathcal{E}^{(0,0)} = \tfrac{1}{2}[\ln(\omega_c/\omega) - \mathcal{C}] + O(\sqrt{\omega/\omega_c}) \tag{6.36}$$

in agreement with previous variational results[20–22] and to be compared with the PD expression:

$$\mathcal{E}^{(0,0)}_{\text{PD}} = \frac{1}{2}\left(\ln(\omega_c/\omega) - \mathcal{C} + \frac{\ln(\omega_c/\omega)}{\sqrt{\omega_c/\omega}}\right) + O(\sqrt{\omega/\omega_c}). \tag{6.37}$$

The additional term in $\mathcal{E}^{(0,0)}$ found by PD introduces a supplementary (negative) contribution

$$-\frac{\alpha\hbar\omega}{2}\frac{\ln(\omega_c/\omega)}{\sqrt{\omega_c/\omega}}$$

to the energy to first order in α in the asymptotic limit $\omega_c \to \infty$, which is removed by the inclusion of our additional constraints.

C. Intermediate coupling strength for polarons

For intermediate and large polaron coupling strength, the evaluation of the variational upper bound Eq. (5.35) and its minimization have to be performed numerically. However, because the formal expression which we obtained happens to be the same as the one obtained by PD—which was not variational—we are now in a position to analyze the implications of the additional constraints of the present paper on the basis of the PD numerical results.

Without imposing a restriction on the values of $w_\perp$, PD found two minima in E^{var} as a function of $w_\perp$ for a wide range of values of α and ω_c. This is typically illustrated in Fig. 6 of Ref. 3, where for $\alpha = 5$ the position of the global minimum in the approximation to the energy as a function of $w_\perp$ discontinuously switches from the first to the second minimum with increasing ω_c. For $\alpha = 5$, this transition occurs at $\omega_c = 2.76\omega$. From the parameter values explicitly given in the figure caption by PD , one readily checks that the constraints $v_\parallel \geq w_\parallel \geq \omega$ and $v_\perp \geq w_\perp$ are indeed fulfilled. But the additional condition $w_\perp > \omega_c$, found in the present paper, is not satisfied for the minimum at the lower values of $(w_\perp/v_\perp)^2$ in Fig. 6 of Ref. 3. The "first-order phase transition" suggested by PD, at present has no variational justification, and needs further investigation.

VII. CONCLUDING REMARKS

The extension of the Feynman upper bound for the ground-state energy to the case of nonzero magnetic fields is certainly not justified in general without modification. The free-particle limit of the PD approximation for the polaron in a magnetic field provides an unambiguous counterexample.

In the present paper we have derived the "minor modification" which is required to generalize the Feynman inequality to the case of a nonzero magnetic field. We derived a generalized inequality, which provides an upper bound to the ground-state energy valid also for $\omega_c \neq 0$, and determined the conditions under which our maximum principle reduces to the Feynman inequality. Our treatment is based on the Rayleigh-Ritz variational principle of quantum mechanics, expressed in ordered operators. At any stage of the derivation, the correspondence with the Feynman path-integral formulation is established in real time variables.

The resulting upper bound which we derive for the ground-state energy of a particle in a magnetic field is formally very similar to the one which would follow from the application of the Feynman inequality as valid for $\omega_c = 0$, with the crucial difference that our generalized inequality is expressed in *real* time variables.

If the substitution $t = -i\hbar\tau$ to imaginary times would be allowed in the upper bound for the ground-state energy of a particle in a nonzero magnetic field, the same formal upper bound for the ground-state energy as from the Feynman inequality would still result. This means that the Feynman inequality can still be applied in the case of a nonzero magnetic field under the condition, however, derived in the present paper, that the analyticity of the propagator in the complex time plane allows for the substitution of real by imaginary time variables. If this substitution is not allowed, in principle, additional terms will appear in the rhs of the Feynman inequality (1.1). These supplementary terms can be the subject of further analysis.

The usefulness of our extension (2.6) of the Feynman inequality, as presented in the present paper, is illustrated in (2.18) by applying it to the problem of the Fröhlich polaron in a magnetic field. With the same trial system as in the PD approximation, our analyticity requirement amounts to the condition that the variational parameters of the trial system satisfy the constraints

$$\max(\omega,\omega_c) \leq w_\perp \leq v_\perp, \quad \omega \leq w_\parallel \leq v_\parallel,$$

where ω is the LO phonon frequency.

The implications of these additional constraints, derived here, were examined analytically in the weak-coupling limit. For $\omega_c \rightarrow 0$ we showed that the PD results are variational, as expected, because minimization of the upper bound automatically happens to fulfill the additional constraints introduced here. But both in the free-particle limit and in the limit $\omega_c \rightarrow \infty$, the additional constraints are not automatically fulfilled.

For the free particle in a magnetic field the PD approximation leads to an energy minimum below the exact ground-state energy, which is eliminated if our additional constraints are satisfied, and an upper bound is found with its minimum at the exact ground-state energy if these constraints are taken into account.

In this free-particle limit, we derived here the contribution $E^{\rm DB}$ to the upper bound for the ground-state energy from the presence of different branch lines in the complex time plane for the case $w_\perp = 0$. We also showed how the Feynman inequality is generalized if the additional constraints are not satisfied, and that this generalization also leads to the exact ground-state energy $\hbar\omega_c/2$.

Furthermore, the possibility of the "first-order phase transition" suggested in the PD approximation, does not follow from our generalized inequality which reduces to the Feynman inequality if the additional constraints are included.

Note added in proof. Without retardation, e.g., for a particle in a Coulomb potential subjected to a magnetic field, our inequality (2.6) implies the validity of the Feynman upper bound without modifications. The possibility of branch lines in the complex time plane is a direct consequence of retardation effects, and its implications as well as the rigorous mathematical justification of the transition from Eq. (2.15) to (2.18) deserve further study.

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APPENDIX: PHONON ELIMINATION FOR LINEAR PHONON INTERACTIONS

In this appendix we summarize the boson elimination technique for linearly interacting bosons in the time-ordered operator formalism,[23] used several times in the present paper. The procedure is equivalent to Feynman's elimination of the phonons in the path-integral formulation, as, e.g., exposed by Platzman.[16] The elimination is performed on the following Hamiltonian:

$$H = H_0 + \mathcal{V}(\mathbf{r},t) + \sum_{\mathbf{k}}[W_{\mathbf{k}}(\mathbf{r},t)a_{\mathbf{k}} + W_{\mathbf{k}}^\dagger(\mathbf{r},t)a_{\mathbf{k}}^\dagger], \tag{A1}$$

where $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^\dagger$ are phonon annihilation and creation operators. H_0 is the Hamiltonian of an electron in a magnetic field and of a bath of free phonons with frequency w:

$$H_0 = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + \sum_{\mathbf{k}} \hbar w a_{\mathbf{k}}^\dagger a_{\mathbf{k}}. \tag{A2}$$

Both the polaron Hamiltonian and the Hamiltonian of the linear model are of this form.

In the interaction representation the time evolution operator is given by

$$U(t_2,t_1) = \mathcal{T}\exp\left(-\frac{i}{\hbar}\int_{t_1}^{t_2} dt\, V(t)\right), \tag{A3}$$

where $\mathcal{T}$ denotes the time-ordering operator, and $V(t)$ is the interaction term in the Hamiltonian, written in the interaction representation:

$$V(t) = e^{iH_0t/\hbar}\Big(\mathcal{V}(\mathbf{r},t) + \sum_{\mathbf{k}}[\,W_{\mathbf{k}}(\mathbf{r},t)a_{\mathbf{k}} + W_{\mathbf{k}}^\dagger(\mathbf{r},t)a_{\mathbf{k}}^\dagger]\Big)e^{-iH_0t/\hbar}. \tag{A4}$$

Introducing

$$\mathbf{r}(t) \equiv e^{iH_0t/\hbar}\mathbf{r}e^{-iH_0t/\hbar} \tag{A5}$$

and filling out the time evolution of the phonon operators in the interaction picture explicitly, the time evolution operator becomes

$$U(t_2,t_1) = \mathcal{T}\exp\frac{-i}{\hbar}\int_{t_1}^{t_2} dt\left(\mathcal{V}(\mathbf{r}(t),t) + \sum_{\mathbf{k}}[W_{\mathbf{k}}(\mathbf{r}(t),t)a_{\mathbf{k}}e^{-iwt} + W_{\mathbf{k}}^\dagger(\mathbf{r}(t),t)a_{\mathbf{k}}^\dagger e^{iwt}]\right). \tag{A6}$$

Using Feynman's ordered operator calculus,[23] the time evolution operator can be disentangled with all the creation operators for the phonons to the left of all the annihilation operators:

$$U(t_2,t_1) = \mathcal{A}(t_2,t_1)\mathcal{U}(t_2,t_1), \tag{A7}$$

$$\mathcal{A}(t_2,t_1) = \mathcal{T}\exp -\frac{i}{\hbar}\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger \int_{t_1}^{t_2} dt W_{\mathbf{k}}^\dagger(\mathbf{r}(t),t)e^{iwt}, \tag{A8}$$

$$\mathcal{U}(t_2,t_1) = \mathcal{T}\exp -\frac{i}{\hbar}\int_{t_1}^{t_2} dt\left(\widetilde{\mathcal{V}}(\mathbf{r}(t),t) + \sum_{\mathbf{k}}\widetilde{W}_{\mathbf{k}}(\mathbf{r}(t),t)\widetilde{a}_{\mathbf{k}}(t)e^{-iwt}\right), \tag{A9}$$

where the tilde on the operators indicates the time evolution introduced by the disentangling

$$\widetilde{O}(t) \equiv \mathcal{A}^{-1}(t,t_1)O\mathcal{A}(t,t_1). \tag{A10}$$

If an operator $f(t)$ commutes with the boson operators a and $a^\dagger$, elementary operator algebra yields

$$\left[\mathcal{T}\exp\left(a^\dagger\int_{t_1}^{t_N} dt f(t)\right)\right]^{-1} a\left[\mathcal{T}\exp\left(a^\dagger\int_{t_1}^{t_N} dt f(t)\right)\right] = a + \int_{t_1}^{t_N} dt\left[\mathcal{T}\exp\left(a^\dagger\int_{t_1}^{t} dt' f(t')\right)\right]^{-1} \times f(t)\left[\mathcal{T}\exp\left(a^\dagger\int_{t_1}^{t} dt' f(t')\right)\right]. \tag{A11}$$

With $f(t)$ replaced by $-\frac{i}{\hbar}W_{\mathbf{k}}^\dagger(\mathbf{r}(t),t)e^{iwt}$, one then obtains

$$\widetilde{a}_{\mathbf{k}}(t) = a_{\mathbf{k}} - \frac{i}{\hbar}\int_{t_1}^{t} dt'\widetilde{W}_{\mathbf{k}}^\dagger(\mathbf{r}(t'),t')e^{iwt'}, \tag{A12}$$

giving for the disentangled time evolution operator,

$$\mathcal{U}(t_2,t_1) = \mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{t_1}^{t_2} dt\left(\widetilde{\mathcal{V}}(\mathbf{r}(t),t) - \frac{i}{\hbar}\sum_{\mathbf{k}}\widetilde{W}_{\mathbf{k}}(\mathbf{r}(t),t)\int_{t_1}^{t} dt'\widetilde{W}_{\mathbf{k}}^\dagger(\mathbf{r}(t'),t')e^{-iw(t-t')} + \sum_{\mathbf{k}}\widetilde{W}_{\mathbf{k}}(\mathbf{r}(t),t)a_{\mathbf{k}}e^{-iwt}\right)\right]. \tag{A13}$$

If the system is in the phonon ground state of H_0 at $t = -\infty$, i.e., if $|-\infty\rangle$ is a vacuum state for the phonons, the annihilation operators in the exponent of the previous expression do not contribute to the time evolution of this state and can be omitted:

$$\mathcal{U}(t_2,-\infty)|-\infty\rangle = \mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{-\infty}^{t_2} dt\left(\widetilde{\mathcal{V}}(\mathbf{r}(t),t) - \frac{1}{\hbar^2}\int_{-\infty}^{t_2} dt\int_{-\infty}^{t} dt' e^{-iw(t-t')} \times \sum_{\mathbf{k}} \widetilde{W}_{\mathbf{k}}(\mathbf{r}(t),t)\widetilde{W}_{\mathbf{k}}^{\dagger}(\mathbf{r}(t'),t')\right)\right]|-\infty\rangle . \quad \text{(A14)}$$

The full time evolution operator $U(t_2,t_1)$ [see Eq. (A7)] acts on the ground state and introduces many phonon states with evolving time, but if the interactions are switched on adiabatically the system eventually is again in the ground state at $t=\infty$. The creation operators acting to the left in $U(t_2,t_1)$ leave $\langle\infty|$ invariant in $\langle\infty|U(\infty,-\infty)|-\infty\rangle$, and all the tildes on the operators can therefore be omitted:

$$\langle\infty|U(\infty,-\infty)|-\infty\rangle = \left\langle\infty\left|\mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\left(\mathcal{V}(\mathbf{r}(t),t) - \frac{1}{\hbar^2}\int_{-\infty}^{\infty} dt\int_{-\infty}^{t} dt' e^{-iw(t-t')}\sum_{\mathbf{k}} W_{\mathbf{k}}(\mathbf{r}(t),t)W_{\mathbf{k}}^{\dagger}(\mathbf{r}(t'),t')\right)\right]\right|-\infty\right\rangle . \quad \text{(A15)}$$

Both in the polaron problem and in the linear model under consideration here, $W_{\mathbf{k}}^{\dagger}$ is the complex conjugate of $W_{\mathbf{k}}$. Therefore, interchanging the positions of $W_{\mathbf{k}}$ and $W_{\mathbf{k}}^{\dagger}$ is equivalent to replacing $\mathbf{k}$ by $-\mathbf{k}$. The asymmetry in the double time integral can then be eliminated by the introduction of a factor of $\frac{1}{2}$ and integrating both time variables to ∞:

$$\langle\infty|U(\infty,-\infty)|-\infty\rangle = \left\langle\infty\left|\mathcal{T}\exp\left[-\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\left(\mathcal{V}(\mathbf{r}(t),t) - \frac{1}{2\hbar^2}\int_{-\infty}^{\infty} dt\int_{-\infty}^{\infty} dt' e^{-iw|t-t'|}\sum_{\mathbf{k}} W_{\mathbf{k}}(\mathbf{r}(t),t)W_{\mathbf{k}}^{\dagger}(\mathbf{r}(t'),t')\right)\right]\right|-\infty\right\rangle . \quad \text{(A16)}$$

This result allows to calculate the expectation value

$$\sum_{\mathbf{k}}\langle 0|W_{\mathbf{k}}(\mathbf{r})a_{\mathbf{k}} + W_{\mathbf{k}}^{\dagger}(\mathbf{r})a_{\mathbf{k}}^{\dagger}|0\rangle$$

which is repeatedly needed in the present paper. Using

$$(Wa+W^{\dagger}a^{\dagger}) = i\hbar\frac{\partial}{\partial\lambda}e^{\frac{-i\lambda}{\hbar}(Wa+W^{\dagger}a^{\dagger})}\Big|_{\lambda=0} \quad \text{(A17)}$$

and

$$\sum_{\mathbf{k}}\langle 0|W_{\mathbf{k}}(\mathbf{r})a_{\mathbf{k}} + W_{\mathbf{k}}^{\dagger}(\mathbf{r})a_{\mathbf{k}}^{\dagger}|0\rangle = \sum_{\mathbf{k}}\langle\infty|U(\infty,0)[W_{\mathbf{k}}(\mathbf{r})a_{\mathbf{k}} + W_{\mathbf{k}}^{\dagger}(\mathbf{r})a_{\mathbf{k}}^{\dagger}]U(0,-\infty)|-\infty\rangle \quad \text{(A18)}$$

the required expectation value can be obtained by replacing $W_{\mathbf{k}}(\mathbf{r}(t),t)$ in the time evolution operator by $[1+\lambda\delta(t)]W_{\mathbf{k}}(\mathbf{r}(t),t)$, taking the derivative with respect to λ, and putting $\lambda=0$. The final result is

$$\left\langle 0\left|\sum_{\mathbf{k}}[W_{\mathbf{k}}(\mathbf{r})a_{\mathbf{k}} + W_{\mathbf{k}}^{\dagger}(\mathbf{r})a_{\mathbf{k}}^{\dagger}]\right|0\right\rangle = -\frac{i}{2\hbar}\int_{-\infty}^{\infty} dt\, e^{-iw|t|}\sum_{\mathbf{k}}\langle\infty|\mathcal{T}[U(\infty,-\infty)W_{\mathbf{k}}(\mathbf{r}(0),0)W_{\mathbf{k}}^{\dagger}(\mathbf{r}(t),t)]|-\infty\rangle \quad \text{(A19)}$$

which is the basic relation[23,16] for several phonon eliminations in this paper.

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[1]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965), p. 308.
[2]R. P. Feynman, Phys. Rev. **97**, 660 (1955); *Statistical Mechanics: A Set of Lectures* (Benjamin, New York, 1972).
[3]F. M. Peeters and J. T. Devreese, Phys. Rev. B **25**, 7281

(1982); **25**, 7302 (1982).
[4]M. Saitoh, J. Phys. Soc. Jpn. **50**, 2295 (1981).
[5]J. T. Marshall and M. S. Chawla, Phys. Rev. B **2**, 4283 (1970).
[6]R. W. Hellwarth and P. M. Platzman, Phys. Rev. **128**, 1599 (1962).
[7]V. I. Sheka, L. S. Khazan, and E. V. Mozdor, Fiz. Tverd. Tela (Leningrad) **18**, 3240 (1976) [Sov. Phys. Solid State **18**, 1890 (1976)].
[8]I. A. Kvasnikov, Akad. Nauk SSSR **110**, 755 (1956).
[9]D. Ruelle, *Statistical Mechanics: Rigorous Results* (Benjamin, New York, 1969).
[10]S. N. Gorskhov, A. V. Zabrodin, C. Rodriguez, and V. K. Fedyanin, Teor. Mat. Fiz. **62**, 304 (1985).
[11]J. T. Devreese and F. Brosens, in *Path Summation: Achievements and Goals*, edited by S. Lundqvist, A. Ranfagni, V. Sa-yakanit, and L. S. Schulman (World Scientific, Singapore, 1988), pp. 74–91; Phys. Status Solidi B **145**, 517 (1988); *Proceedings of the Third International Conference on Path-Integrals from meV to MeV, Bangkok*, edited by V. Sa-yakanit *et al.* (World Scientific, Singapore, 1989), pp. 300–308.
[12]D. M. Larsen, Phys. Rev. B **32**, 2657 (1985).
[13]M. Batthacharya, A. Chatterjee, and T. K. Mitra, Phys. Lett. A **134**, 391 (1989).
[14]J. T. Devreese and F. Brosens, Solid State Commun. **77**, 583 (1991).
[15]K. M. Broderix, N. Heldt, and H. Leschke, Z. Phys. B **66**, 507 (1987).
[16]P. M. Platzman, in *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Oliver and Boyd, London, 1963), p. 123.
[17]N. N. Bogolubov and N. N. Bogolubov, Jr., *Some Aspects of Polaron Theory* (World Scientific, Singapore, 1988).
[18]J. T. Devreese, F. Brosens, and R. Evrard, in *Selected Topics of Statistical Mechanics*, edited by A. A. Logunov, N. N. Bogolubov, Jr., V. G. Kadyshevsky, and A. S. Shumovsky (World Scientific, Singapore, 1990).
[19]J. T. Devreese, E. P. Kartheuser, R. Evrard, and A. Baldereschi, Phys. Status Solidi B **59**, 629 (1973); J. T. Devreese, in *Polarons in Ionic Crystals and Polar Semiconductors*, edited by J. T. Devreese (North-Holland, Amsterdam, 1972), p. 83.
[20]D. M. Larsen, Phys. Rev. **135**, A419 (1964).
[21]R. Evrard, E. Kartheuser, and J. T. Devreese, Phys. Status Solidi **41**, 431 (1970).
[22]Y. Lépine and D. Matz, Can. J. Phys. **54**, 1979 (1976).
[23]R. P. Feynman, Phys. Rev. **84**, 108 (1951).