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Internal consistency of the path-integral calculation of the mass of the Fröhlich polaron

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Feynman's formula for the effective mass of the Fröhlich polaron is rederived from the formalism of projected partition functions. The mass is calculated as inverse of the diffusion coefficient of the polaron trajectory in imaginary time. It is shown that correlation between the electron and phonon boundary conditions in imaginary time is necessary for consistent derivation of the Feynman result.

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I. INTRODUCTION

Fifty years ago Feynman published his seminal paper[1] on the Fröhlich polaron, in which he combined path integration and an action variational principle to obtain the polaron energy and effective mass. Subsequently, Feynman's method was generalized by many authors,[2–5] for a comprehensive review see, for example, Refs. 6–8. When the exact polaron energy and mass were calculated by Fourier quantum Monte Carlo[9,10] and diagrammatic quantum Monte Carlo[11,12] methods, Feynman's polaron energy was found to be remarkably accurate deviating from the exact value by less than 0.5% for all couplings. In contrast, Feynman's mass formula[1,13] overestimated the exact mass by as much as 50% leaving room for possible improvements. Generalizations of the original calculation[2,3,14,15] produced either no or very small, less than 1%, numerical correction to the mass. (In some instances, the correction was of the wrong sign.[3,14]) Thus the generalizations did not improve the agreement between the analytical and numerical masses. The much larger error in the mass was not regarded as something unexpected. It was known since Feynman's paper that the mass did not satisfy a variational principle, and therefore the accuracy of the approximate treatment was expected to be somewhat uncontrolled.

In Feynman's method,[1,16,17] phonon variables are integrated out analytically resulting in a self-interacting retarded one-electron action. Phonon integration is performed under periodic boundary conditions in imaginary time. Periodic boundary conditions are also assumed for the electron trajectory. Both conditions are perfectly appropriate for the energy calculation, since the ground-state energy is obtained from a full thermodynamic partition function. However, later, in the mass calculation the electron trajectory is broken and its $\tau=0$ and $\tau=\beta$ ends are displaced relative to each other. The effective mass is inferred from variation of the polaron energy with real space separation of the two ends of the trajectory. In Feynman's approach, the retarded polaron action is *not* corrected for this displacement. In other words, the action resulted from phonon integration for a periodic electron trajectory is carried over to an open electron trajectory.

In a parallel research on the Holstein polaron[18–20] it was realized that the boundary conditions for the phonon and electron variables must be synchronized for consistent calculation of the polaron mass. That is, they are either both periodic or both open. And when they are both open they are correlated. The correlation follows because the electron and phonons are coupled in one system and share a common integral of motion, the polaron momentum. Accurate account of the correlation results in a polaron action different from the periodic phonon action derived by Feynman. Thus the question arises of whether this difference is significant enough to yield a correction to the Feynman mass formula. Such a correction might account for the deviation from the Monte Carlo mass.

This question is investigated in the present paper. It is shown that proper boundary conditions in imaginary time do *not* produce a numerical correction to the Feynman result. However, the original mass calculation is found to be internally inconsistent. The terms in the polaron action that are small in the energy calculation (and rightly neglected by Feynman) are not small in the mass calculation and cannot be neglected. But if the boundary conditions are properly taken into account, those terms are small in both calculations. Thus the correlation between the electron and phonon boundary conditions restores the consistency of the mass calculation and leads to the correct final formula.

II. EFFECTIVE MASS FROM SHIFTED BOUNDARY CONDITIONS

The polaron mass can be calculated as the inverse diffusion coefficient of an open-ended polaron path in imaginary time. This section contains a derivation of this relation. The derivation is general and valid for any nonrelativistic composite particle. The momentum $\hbar\mathbf{K}$ of a translation invariant system is a constant of motion. In the polaron case, this is the sum of an electron momentum and momenta of all excited optical phonons. One defines the *projected partition function* as a Gibbs sum restricted to states with the same $\mathbf{K}$:

$$Z_{\mathbf{K}}=\sum_{n}\langle n|e^{-\beta H}|n\rangle\cdot\delta_{\mathbf{K}\mathbf{K}_n}. \tag{1}$$

Here $|n\rangle$ are eigenstates of the Hamiltonian H, $\hbar\mathbf{K}_n$ is the momentum of state $|n\rangle$, and $\beta=(k_BT)^{-1}$ is inverse temperature. The system is assumed to occupy a finite volume V, and the wave vector is quantized to a discrete set of values $\mathbf{K}_n$. To transform $Z_{\mathbf{K}}$, introduce real-space configurations $|Q\rangle$ which are direct products of all the degrees of freedom in the system. For the Fröhlich polaron, $|Q\rangle=|\mathbf{r}\rangle\Pi_{\mathbf{r}'}|\mathbf{P}(\mathbf{r}')\rangle$, where $\mathbf{r}$ is the electron position and $\mathbf{P}(\mathbf{r}')$ is the polarization at point $\mathbf{r}'$. The states Q form a complete orthogonal basis $I = \int dQ|Q\rangle\langle Q|$ and $\langle Q_1|Q_2\rangle = \delta(Q_1 - Q_2)$, where the unity operator and the delta function are also direct products between different degrees of freedom. Inserting two unity operators in Eq. (1) the partition function is rewritten as follows:

$$Z_{\mathbf{K}} = \int dQ_1 dQ_2 \langle Q_2|e^{-\beta H}|Q_1\rangle \cdot W_{\mathbf{K}}, \tag{2}$$

$$W_{\mathbf{K}} = \sum_n \langle Q_1|n\rangle\langle n|Q_2\rangle \delta_{\mathbf{K}\mathbf{K}_n} = \langle Q_1|\mathbf{K}\rangle\langle \mathbf{K}|Q_2\rangle. \tag{3}$$

The meaning of the last expression is that both configurations Q_1 and Q_2 have to be projected on the same wave vector $\mathbf{K}$. To perform projection consider a parallel shift of configuration Q by a three-dimensional vector $\mathbf{R}$. The resulting state will be denoted as $|Q+\mathbf{R}\rangle$. (Note that summation is only symbolic here.) An arbitrary configuration Q generates a family of states $|\mathbf{K}_Q\rangle = V^{-1}\int d\mathbf{R} e^{-i\mathbf{K}\cdot\mathbf{R}}|Q+\mathbf{R}\rangle$. Inversely, $|Q+\mathbf{R}\rangle = \Sigma_{\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{R}}|\mathbf{K}_Q\rangle$. In $W_{\mathbf{K}}$ only the respective components $|\mathbf{K}_{Q_1}\rangle$ and $|\mathbf{K}_{Q_2}\rangle$ of $|Q_1\rangle$ and $|Q_2\rangle$ survive projection on $\mathbf{K}$. As a result, one obtains

$$\begin{aligned} W_{\mathbf{K}} &= \langle \mathbf{K}_{Q_1}|\mathbf{K}_{Q_2}\rangle \\ &= \frac{1}{V^2}\int d\mathbf{R}_1 d\mathbf{R}_2 \langle Q_1 + \mathbf{R}_1|Q_2 + \mathbf{R}_2\rangle e^{i\mathbf{K}(\mathbf{R}_1 - \mathbf{R}_2)} \\ &= \frac{1}{V}\int d(\Delta\mathbf{r}) e^{i\mathbf{K}\Delta\mathbf{r}} \langle Q_1 + \Delta\mathbf{r}|Q_2\rangle \\ &= \frac{1}{V}\int d(\Delta\mathbf{r}) e^{i\mathbf{K}\Delta\mathbf{r}} \cdot \delta[(Q_1 + \Delta\mathbf{r}) - Q_2], \end{aligned} \tag{4}$$

where $\Delta\mathbf{r} = \mathbf{R}_1 - \mathbf{R}_2$. The resulting delta function ensures that a many body configuration Q_2 is identical to a configuration Q_1 shifted by $\Delta\mathbf{r}$. Substitution in Eq. (2) and integration over Q_2 yield

$$Z_{\mathbf{K}} = \frac{1}{V}\int d(\Delta\mathbf{r}) e^{i\mathbf{K}\Delta\mathbf{r}} \int dQ \langle Q + \Delta\mathbf{r}|e^{-\beta H}|Q\rangle. \tag{5}$$

The matrix element under the dQ integral is the density matrix operator taken between an arbitrary real-space configuration Q and the *same* configuration shifted by $\Delta\mathbf{r}$. Since Q is a many body state all particles shift in parallel. In the polaron system the electron coordinate $\mathbf{r}$ and polarization profile $\mathbf{P}(\mathbf{r}')$ shift together. Equation (5) suggests defining the *shift partition function*

$$Z_{\Delta\mathbf{r}} = \int dQ \langle Q + \Delta\mathbf{r}|e^{-\beta H}|Q\rangle, \tag{6}$$

which is characterized by the shift vector $\Delta\mathbf{r}$. The zero-shift partition function, $Z_{\Delta\mathbf{r}=0}$, coincides with the usual thermodynamic partition function. Equation (5) states that the projected partition function and the shift partition function satisfy a Fourier-type relation

$$Z_{\mathbf{K}} = \frac{1}{V}\int d(\Delta\mathbf{r}) e^{i\mathbf{K}\Delta\mathbf{r}} \cdot Z_{\Delta\mathbf{r}}. \tag{7}$$

This relation is valid at any temperature T. In the low-temperature limit, $Z_{\mathbf{K}}$ is dominated by the lowest energy eigenvalue with given wave vector, which allows derivation of a useful formula for the effective mass. At small $\mathbf{K}$, the energy is approximated by $E_{\mathbf{K}} = E_G + \hbar^2\mathbf{K}^2/2m^*$, and the projected partition function $Z_{\mathbf{K}} \to e^{-\beta E_{\mathbf{K}}}$ as $T \to 0$. Expanding Eq. (7) to the second order in $\mathbf{K}$ one obtains

$$e^{-\beta E_G}\left(1 - \frac{\beta\hbar^2\mathbf{K}^2}{2m^*}\right) = \frac{1}{V}\int d(\Delta\mathbf{r})\left[1 + i(\mathbf{K}\Delta\mathbf{r}) - \frac{(\mathbf{K}\Delta\mathbf{r})^2}{2}\right] Z_{\Delta\mathbf{r}}. \tag{8}$$

On the right, the linear term in $\mathbf{K}$ vanishes after integration by inversion symmetry: $Z_{-\Delta\mathbf{r}} = Z_{\Delta\mathbf{r}}$. The rest is transformed as

$$\frac{\beta\hbar^2\mathbf{K}^2}{m^*} = \frac{\int d(\Delta\mathbf{r})(\mathbf{K}\Delta\mathbf{r})^2 Z_{\Delta\mathbf{r}}}{\int d(\Delta\mathbf{r}) Z_{\Delta\mathbf{r}}} \equiv \langle(\mathbf{K}\Delta\mathbf{r})^2\rangle_{\text{shift}}. \tag{9}$$

The definition of $Z_{\Delta\mathbf{r}}$, Eq. (6), implies that the ratio of two integrals in the last expression is the mean value of $(\mathbf{K}\Delta\mathbf{r})^2$ evaluated with shifted boundary conditions in imaginary time. The latter means the initial (at imaginary time $=0$) and final (at imaginary time $=\beta$) configurations are the same, see Eq. (6), but they can be shifted relative to each other by a three dimensional vector $\Delta\mathbf{r}$. This shift vector is arbitrary. Averaging under shifted boundary conditions is understood hereafter as averaging over $\Delta\mathbf{r}$, with the weight given by $Z_{\Delta\mathbf{r}}$. Upon expansion of the square in Eq. (9), the mixed terms average to zero by symmetry, $\langle(\Delta r_i)(\Delta r_j)\rangle_{\text{shift}} = 0$, while the diagonal terms are equal, $\langle(\Delta r_i)^2\rangle_{\text{shift}} = 1/3\langle(\Delta\mathbf{r})^2\rangle_{\text{shift}}$. That results in

$$\frac{1}{m^*} = \frac{1}{3\beta\hbar^2}\frac{\int d(\Delta\mathbf{r})(\Delta\mathbf{r})^2 Z_{\Delta\mathbf{r}}}{\int d(\Delta\mathbf{r}) Z_{\Delta\mathbf{r}}} = \frac{\langle(\Delta\mathbf{r})^2\rangle_{\text{shift}}}{3\beta\hbar^2}. \tag{10}$$

This equation allows an elegant interpretation of the effective mass in terms of *imaginary time diffusion*. Since the shift vector is not fixed, the system evolution from the initial to the final configuration can be regarded as diffusion during time $t = \hbar\beta$. In normal three-dimensional diffusion, the mean squared displacement is proportional to the time interval, $\langle(\Delta\mathbf{r})^2\rangle = 6Dt$, where D is the diffusion coefficient. Thus Eq. (10) is rewritten as

$$\frac{1}{m^*} = \frac{2D}{\hbar}. \tag{11}$$

Note, that Eq. (10) can also be regarded as a fluctuation-dissipation relation. The effective mass characterizes dynamical response, while the mean squared displacement is an equilibrium property.

Equation (10) is especially useful in understanding mass enhancement of composite particles such as the polaron. Interaction with various fields (e.g., phonons) increases the statistical weight of trajectories with small $\langle(\Delta\mathbf{r})^2\rangle$ thereby slowing down the diffusion and increasing the particle's mass. Thus the mass enhancement is conveniently visualized as the increased "stiffness" of the trajectories. Equation (10) or its analogues were used in Monte Carlo calculations of the effective masses of polarons,[9,10,18–20] bipolarons,[21] and defects in superfluid helium.[22]

III. POLARON ACTION

The results of the previous section have important implications for the Fröhlich polaron. As soon as the two ends of the electron path are allowed to shift relative from each other to obtain the mass, the polarization profile must shift accordingly. Thus phonon integration has to be performed under more general boundary conditions in imaginary time than periodic. In general, this should modify the polaron action. The modified polaron action is calculated in this section.

A starting point is the polaron action as formulated by Fröhlich[23] and Schultz:[16]

$$\begin{aligned} S[\mathbf{r}(\tau);\mathbf{P}(\mathbf{r}',\tau)] = &-\int_0^\beta d\tau \frac{m\dot{\mathbf{r}}^2}{2\hbar^2} \\ &+ |e|\int_0^\beta d\tau \int d\mathbf{r}'\left(\nabla_{\mathbf{r}'}\frac{1}{|\mathbf{r}'-\mathbf{r}|}\right)\mathbf{P}(\mathbf{r}') \\ &- \frac{\mu}{2}\int_0^\beta d\tau \int d\mathbf{r}'\left[\frac{\dot{\mathbf{P}}^2(\mathbf{r}')}{\hbar^2} + \Omega^2\mathbf{P}^2(\mathbf{r}')\right], \end{aligned} \tag{12}$$

$$\mu = \frac{4\pi}{\Omega^2}\,\frac{\varepsilon_0\varepsilon_\infty}{\varepsilon_0-\varepsilon_\infty}. \tag{13}$$

Here Ω is the optical phonon frequency, ε_0 and ε_∞ are the static and high-frequency electric permittivities of the crystal, $|e|$ is the unit charge, and m is the band mass of the electron. $\mathbf{r}(\tau)$ is the imaginary-time electron trajectory. $\mathbf{P}(\mathbf{r}',\tau)$ is the imaginary-time polarization trajectory. A dot above a variable denotes partial derivative with respect to imaginary time τ. The action is supplemented by shifted boundary conditions

$$\mathbf{r}(\beta) = \mathbf{r}(0) + \Delta\mathbf{r}, \tag{14}$$

$$\mathbf{P}(\mathbf{r}',\beta) = \mathbf{P}(\mathbf{r}'-\Delta\mathbf{r},0), \tag{15}$$

where $\Delta\mathbf{r}$ is an arbitrary three-dimensional vector. Except for the boundary conditions phonon integration proceeds along the lines outlined by Schultz.[16] The polarization field is expanded in a Fourier series with real amplitudes A and B:

$$\mathbf{P}(\mathbf{r}',\tau) = \sqrt{\frac{2}{V}}\sum_{(q_x>0)}\frac{\mathbf{q}}{|\mathbf{q}|}[A_{\mathbf{q}}(\tau)\cos\mathbf{q}\cdot\mathbf{r}' + B_{\mathbf{q}}(\tau)\sin\mathbf{q}\cdot\mathbf{r}']. \tag{16}$$

Note that the sum over $\mathbf{q}$ extends only over half of momentum space, which is indicated by "$(q_x>0)$." The Fourier-transformed polaron action (12) and boundary condition (15) become

$$\begin{aligned} S[\mathbf{r}(\tau);A_{\mathbf{q}}(\tau),B_{\mathbf{q}}(\tau)] \\ = &-\int_0^\beta d\tau\frac{m\dot{\mathbf{r}}^2}{2\hbar^2} \\ &+ \sum_{(q_x>0)}\int_0^\beta d\tau\Bigg\{-\frac{\mu}{2\hbar^2}\left[\dot{A}_{\mathbf{q}}^2+\dot{B}_{\mathbf{q}}^2\right] \\ &- \frac{\mu\Omega^2}{2}[A_{\mathbf{q}}^2+B_{\mathbf{q}}^2] \\ &+ \frac{4\pi|e|}{|\mathbf{q}|}\sqrt{\frac{2}{V}}[A_{\mathbf{q}}(\tau)\sin\mathbf{q}\cdot\mathbf{r}(\tau) - B_{\mathbf{q}}(\tau)\cos\mathbf{q}\cdot\mathbf{r}(\tau)]\Bigg\}, \end{aligned} \tag{17}$$

$$A_{\mathbf{q}}(\beta)\cos\mathbf{q}\Delta\mathbf{r} + B_{\mathbf{q}}(\beta)\sin\mathbf{q}\Delta\mathbf{r} = A_{\mathbf{q}}(0), \tag{18}$$

$$-A_{\mathbf{q}}(\beta)\sin\mathbf{q}\Delta\mathbf{r} + B_{\mathbf{q}}(\beta)\cos\mathbf{q}\Delta\mathbf{r} = B_{\mathbf{q}}(0). \tag{19}$$

Since action (17) is diagonal in amplitudes A and B, path integration can be performed for each component independently. Using the standard methods[1,16,17] one obtains in the low-temperature limit $e^{\hbar\Omega\beta}\gg 1$:

$$S[\mathbf{r}(\tau);A_{\mathbf{q}}(0),A_{\mathbf{q}}(\beta),B_{\mathbf{q}}(0),B_{\mathbf{q}}(\beta)] = -\int_0^\beta d\tau\frac{m\dot{\mathbf{r}}^2}{2\hbar^2} + \sum_{(q_x>0)}S_{\mathbf{q}}, \tag{20}$$

$$\begin{aligned} S_{\mathbf{q}} = &-\frac{\mu}{2\hbar^2}\hbar\Omega[A_{\mathbf{q}}^2(0)+A_{\mathbf{q}}^2(\beta)+B_{\mathbf{q}}^2(0)+B_{\mathbf{q}}^2(\beta)] \\ &+ \frac{\hbar^2}{2\mu}\frac{(4\pi|e|)^2}{q^2}\frac{2}{V}\int_0^\beta\int_0^\beta d\tau' d\tau'' G(\tau',\tau'') \\ &\times\cos\mathbf{q}[\mathbf{r}(\tau')-\mathbf{r}(\tau'')] \\ &+ \frac{(4\pi|e|)}{q}\sqrt{\frac{2}{V}}\int_0^\beta d\tau\{e^{-\hbar\Omega\tau}[A_{\mathbf{q}}(0)\sin\mathbf{q}\cdot\mathbf{r}(\tau) \\ &- B_{\mathbf{q}}(0)\cos\mathbf{q}\cdot\mathbf{r}(\tau)] + e^{-\hbar\Omega(\beta-\tau)}[A_{\mathbf{q}}(\beta)\sin\mathbf{q}\cdot\mathbf{r}(\tau) \\ &- B_{\mathbf{q}}(\beta)\cos\mathbf{q}\cdot\mathbf{r}(\tau)]\}, \end{aligned} \tag{21}$$

$$\begin{aligned} G(\tau',\tau'') \\ = \frac{1}{\hbar\Omega\sinh\hbar\Omega\beta}\begin{cases}\sinh\hbar\Omega\tau'\,\sinh\hbar\Omega(\beta-\tau''), & \tau'<\tau'', \\ \sinh\hbar\Omega(\beta-\tau')\sinh\hbar\Omega\tau'', & \tau'>\tau''.\end{cases} \end{aligned} \tag{22}$$

The action is still a functional of two end polarizations, at $\tau=0$ and $\tau=\beta$. However, those are related by the conditions (18) and (19). Final integration over the end variables leads, after straightforward algebra, to

$$S_{\Delta\mathbf{r}}[\mathbf{r}(\tau)] = -\int_0^\beta d\tau \frac{m\dot{\mathbf{r}}^2}{2\hbar^2} + \frac{\alpha}{2\sqrt{2}}\left(\frac{\hbar^5\Omega^3}{m}\right)^{1/2}\int_0^\beta\int_0^\beta d\tau' d\tau''\left\{\frac{e^{-\hbar\Omega|\tau'-\tau''|}}{|\mathbf{r}(\tau')-\mathbf{r}(\tau'')|} + \frac{e^{-\hbar\Omega(\beta-|\tau'-\tau''|)}}{|[\mathbf{r}(\tau')-\mathbf{r}(\tau'')]\mathrm{sgn}(\tau'-\tau'')-\Delta\mathbf{r}|}\right\}, \tag{23}$$

$$\alpha = \frac{|e|^2}{2\hbar\Omega}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right)\sqrt{\frac{2m\Omega}{\hbar}}, \tag{24}$$

where α is the Fröhlich coupling constant. $\Delta\mathbf{r}$ in the denominator of the last term in Eq. (23) is a direct consequence of the shifted boundary conditions for the polarization field. It is convenient to perform a linear transformation $\mathbf{r}(\tau)=\mathbf{r}'(\tau)+(\tau/\beta)\Delta\mathbf{r}$, which transforms path integration to periodic boundary conditions. The resulting action is

$$\bar{S}_{\Delta\mathbf{r}}[\mathbf{r}(\tau)] = -\frac{m}{2\hbar^2}\frac{(\Delta\mathbf{r})^2}{\beta} - \int_0^\beta d\tau \frac{m\dot{\mathbf{r}}^2}{2\hbar^2} + \frac{\alpha}{2\sqrt{2}}\left(\frac{\hbar^5\Omega^3}{m}\right)^{1/2}\int_0^\beta\int_0^\beta d\tau' d\tau''\left\{\frac{e^{-\hbar\Omega|\tau'-\tau''|}}{\left|\mathbf{r}(\tau')-\mathbf{r}(\tau'')+\frac{\tau'-\tau''}{\beta}\Delta\mathbf{r}\right|} + \frac{e^{-\hbar\Omega(\beta-|\tau'-\tau''|)}}{\left|[\mathbf{r}(\tau')-\mathbf{r}(\tau'')]\mathrm{sgn}(\tau'-\tau'')-\frac{\beta-|\tau'-\tau''|}{\beta}\Delta\mathbf{r}\right|}\right\}. \tag{25}$$

The bar over S indicates that the action is a functional of a path periodic in imaginary time. The full shift partition function (6) is given by

$$Z_{\Delta\mathbf{r}} = Z_{\mathrm{ph}}\int_{(\mathbf{r},0)}^{(\mathbf{r},\beta)} \mathcal{D}\mathbf{r}\, e^{\bar{S}_{\Delta\mathbf{r}}[\mathbf{r}(\tau)]}, \tag{26}$$

where $\mathcal{D}\mathbf{r}$ is path integration over electron coordinates. Z_{ph} is the partition function of a free polarization field. This is a multiplicative constant that cancels out in the mass calculation, see Eq. (10).

The polaron mass originates from explicit dependence of action (25) on the shift vector $\Delta\mathbf{r}$. The first term corresponds to the bare electron mass. Phonon-induced mass enhancement comes from the double integral. The two integrands have similar functional dependence on $\mathbf{r}(\tau)$, but make different contributions to the action. The first integrand exponentially decays away from the diagonal $\tau'=\tau''$. Since the odd powers of $\Delta\mathbf{r}$ vanish in path integration, the first fraction's contribution is $O(\beta)+O[(\Delta\mathbf{r})^2\beta^{-1}]+O[(\Delta\mathbf{r})^4\beta^{-3}]+\cdots$. The first term of this expansion adds to the polaron energy, while the second one adds to the mass.

Consider the second fraction in the double integral (25), which is the main focus of the present study. The exponential numerator limits integration to finite intervals around the points $(0,\beta)$ and $(\beta,0)$. In the denominator, the combination $(\beta-|\tau'-\tau''|)=O(1)$. Therefore the second fraction's contribution to the action is $O(1)+O[(\Delta\mathbf{r})^2\beta^{-2}]+O[(\Delta\mathbf{r})^4\beta^{-4}]+\cdots$. In the $\beta\to\infty$ limit, each term in this expansion is small in comparison with the corresponding term from the previous series with the same power of $\Delta\mathbf{r}$. Thus the *entire* second fraction can be omitted in favor of the first one.

Here comes the critical observation. Such a nice term-by-term domination of the first fraction over the second one takes place *only* as a result of the shifted boundary conditions for the polarization. Indeed, without the latter the combination in the denominator of the second fraction in Eq. (25) would have been $(|\tau'-\tau''|/\beta)\Delta\mathbf{r}=O(\Delta\mathbf{r})$ instead of $[(\beta-|\tau'-\tau''|)/\beta]\Delta\mathbf{r}=O[(\Delta\mathbf{r})\beta^{-1}]$. As a result, the second expansion would have been $O(1)+O[(\Delta\mathbf{r})^2]+O[(\Delta\mathbf{r})^4]+\cdots$. The first term is still small compared to the corresponding term from the first fraction, which leads to the correct polaron energy. However, the $(\Delta\mathbf{r})^2$ term now dominates its counterpart from the first fraction, which totally confuses calculation of the effective mass. Thus the neglect of the shifted boundary conditions in phonon integration results in a serious internal inconsistency in the mass calculation. Apparently, Feynman avoided this difficulty by omitting the second fraction in Eq. (23) from the outset. Had he retained the full form of the phonon propagator, including the second part $e^{-\hbar\Omega(\beta-|\tau'-\tau''|)}$, he would have faced the problem outlined here.

The analysis presented in this section enables to safely neglect the second fraction in Eq. (25). However, it will still be included in the forthcoming mass calculation in order to illustrate further the above argument.

IV. POLARON MASS

The polaron action (25) is real. Therefore the shifted partition function satisfies the Jensen-Feynman inequality

$$\int_{\mathbf{r}_0}^{\mathbf{r}_0}\mathcal{D}\mathbf{r}\cdot e^{\bar{S}_{\Delta\mathbf{r}}[\mathbf{r}(\tau)]} \geqslant e^{\langle \bar{S}_{\Delta\mathbf{r}}[\mathbf{r}(\tau)] - \bar{S}^0_{\Delta\mathbf{r}}[\mathbf{r}(\tau)]\rangle_0}\int_{\mathbf{r}_0}^{\mathbf{r}_0}\mathcal{D}\mathbf{r}\cdot e^{\bar{S}^0_{\Delta\mathbf{r}}[\mathbf{r}(\tau)]}, \tag{27}$$

where $\langle\cdots\rangle_0$ denotes averaging with the trial action $\bar{S}_0$. Feynman's trial model consists of two particles with masses m

and M, which are elastically coupled with a spring constant κ. Note that if the first particle's mass is different from the electron mass m, the difference $\langle \bar{S}-\bar{S}_0\rangle_0$ diverges. The second particle's mass M and κ are variational parameters. It is customary to replace them with two parameters $w=\hbar\sqrt{\kappa/M}$ and $v=w\sqrt{1+M/m}$ which both have units of energy. Calculation of the right-hand side of Eq. (27) is tedious, but proceeds along essentially the same lines as the original Feynman calculation. Therefore the intermediate steps are not presented here. An important note concerns the $\Delta\mathbf{r}$ dependence of the trial action. It is fully represented by the term $-[(m+M)/2\hbar^2][(\Delta\mathbf{r})^2/\beta]$, reflecting the fact that the total mass of the trial model is $m+M$. As a result of the calculation, inequality (27) takes the form

$$Z_{\Delta\mathbf{r}} \geqslant Z_{\mathrm{ph}}\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}\exp\left\{-\beta E_F + O(1) - \frac{m_F}{2\hbar^2}\frac{(\Delta\mathbf{r})^2}{\beta} + O\left[(\Delta\mathbf{r})^4\beta^{-3}\right] + \cdots\right\}, \tag{28}$$

$$E_F = \frac{3}{4}\frac{(v-w)^2}{v} - \frac{\alpha}{2\sqrt{\pi}}(\hbar\Omega)^{3/2}\frac{1}{\beta}\int_0^\beta\int_0^\beta d\tau' d\tau'' \frac{e^{-\hbar\Omega|\tau'-\tau''|} + e^{-\hbar\Omega(\beta-|\tau'-\tau''|)}}{[\Phi(\tau',\tau'')]^{1/2}}, \tag{29}$$

$$m_F = m\left\{1 + \frac{\alpha}{6\sqrt{\pi}}(\hbar\Omega)^{3/2}\frac{1}{\beta}\int_0^\beta\int_0^\beta d\tau' d\tau'' \times \frac{|\tau'-\tau''|^2 e^{-\hbar\Omega|\tau'-\tau''|} + (\beta-|\tau'-\tau''|)^2 e^{-\hbar\Omega(\beta-|\tau'-\tau''|)}}{[\Phi(\tau',\tau'')]^{3/2}}\right\}, \tag{30}$$

$$\Phi(\tau',\tau'') = \frac{1}{1+\dfrac{M}{m}}\left\{|\tau'-\tau''| - \frac{(\tau'-\tau'')^2}{\beta}\right\} + \frac{1}{v\left(1+\dfrac{m}{M}\right)} \times\left\{1 - \frac{1}{2}e^{-2v\tau'} - \frac{1}{2}e^{-2v(\beta-\tau')} - \frac{1}{2}e^{-2v\tau''} - \frac{1}{2}e^{-2v(\beta-\tau'')} + e^{-v(\tau'+\tau'')} + e^{-v[2\beta-(\tau'+\tau'')]} - e^{-v|\tau'-\tau''|}\right\}. \tag{31}$$

E_F and m_F stand for the Feynman energy and Feynman mass, respectively. These definitions are understood as functional dependencies only, the optimal values of parameters v and w are yet to be determined. Both E_F and m_F contain terms that originate from the last fraction in the action (25). The critical question is about the order of their contribution in the low-temperature limit $\beta\to\infty$. In Eq. (29) the two double integrals are $O(\beta)$ and $O(1)$, respectively. The second one can therefore be omitted. The same is true about the two double integrals in Eq. (30). In the second one, the integration region is limited to where the combination $(\beta-|\tau'-\tau''|)\leqslant(\hbar\Omega)^{-1}=O(1)$. Since the pre-exponential factor is exactly the same combination squared, it is $O(1)$ throughout the essential integration region. As a result, the entire second double integral is $O(1)$. Therefore it can be omitted in favor of the first integral, which is $O(\beta)$. Now recall that the pre-exponential factor $(\beta-|\tau'-\tau''|)^2$ derives from the shifted boundary conditions of the phonon integration. Without the latter, the pre-exponential factor would have been $|\tau'-\tau''|^2$, that is the same as in the first integral. Therefore, it would have been $O(\beta^2)$ in the essential integration region. That would have resulted in the second integral being $O(\beta^2)$ and its contribution to the mass $O(\beta)$, which, of course, makes no sense. Thus the shifted boundary conditions in phonon integration are essential for the correct form of the pre-exponential factor and, in the end, for the consistency of the entire mass calculation. Once the second integrals in Eqs. (29) and (30) are safely omitted, the first ones can be transformed according to the relation

$$\int_0^\beta\int_0^\beta d\tau' d\tau'' g(|\tau'-\tau''|) \approx 2\beta\int_0^\beta d\tau g(\tau), \tag{32}$$

which is valid for any function g in the limit $\beta\to\infty$. The Feynman energy and mass assume their final forms

$$E_F = \frac{3}{4}\frac{(v-w)^2}{v} - \frac{\alpha}{\sqrt{\pi}}(\hbar\Omega)^{3/2}\int_0^\infty d\tau \frac{e^{-\hbar\Omega\tau}}{[F(\tau)]^{1/2}}, \tag{33}$$

$$m_F = m\left\{1 + \frac{\alpha}{3\sqrt{\pi}}(\hbar\Omega)^{3/2}\int_0^\infty d\tau \frac{\tau^2 e^{-\hbar\Omega\tau}}{[F(\tau)]^{3/2}}\right\}, \tag{34}$$

$$F(\tau) = \frac{w^2}{v^2}\tau + \frac{v^2-w^2}{v^3}(1-e^{-v\tau}). \tag{35}$$

The last step is choosing optimal values of v and w. The standard approach has always been to minimize E_F first and then substitute the obtained values into the expression for m_F. However, the variational theorem (28) is valid for any $\Delta\mathbf{r}$ and not for just the zero shift vector. The question therefore is whether the other terms in the polaron action change the optimal values of the variational parameters. Let v_0 and w_0 minimize function $E_F(v,w)$ defined by Eq. (33). As such, they satisfy the equations $\partial E_F/\partial v=0$ and $\partial E_F/\partial w=0$ and a necessary concavity condition. With other terms included, one has to minimize $E_F+\mathrm{const}/\beta+(m_F/2\hbar^2)(\Delta\mathbf{r}/\beta)^2+\cdots$. Note that the second and third terms are of the same order $O(\beta^{-1})$. Minimization yields $v=v_0+\delta v$, and $w=w_0+\delta w$, where δv, $\delta w=O(\beta^{-1})$. Some parts of the corrections δv and δw depend explicitly on $\Delta\mathbf{r}$. However, the *minimum energy itself* receives a correction that is only quadratic in δv and δw. The leading $\Delta\mathbf{r}$ correction to the minimal polaron action is $O[(\Delta\mathbf{r}/\beta)^2]$, which does not affect the effective mass term $-(m_F/2\hbar^2)(\Delta\mathbf{r})^2/\beta$ in the $\beta\to\infty$ limit. To conclude, the polaron mass is still determined by the original Feynman procedure: minimize the energy (33) first, and then use the optimal parameters to calculate the mass from Eq. (34).

V. SUMMARY

In this paper, calculation of the Fröhlich polaron effective mass has been analyzed for robustness to boundary conditions in imaginary time. It has been shown that a consistent mass calculation must involve a correlation between the boundary conditions of the electron and phonon coordinates. The $\tau=\beta$ end points of all paths have to be shifted by the same vector $\Delta\mathbf{r}$ relative to their $\tau=0$ end points. Then the effective mass is found as inverse diffusion coefficient of the many body path, see Eq. (11), where $\Delta\mathbf{r}$ is used as a diffusion distance and $\beta\to\infty$ as a diffusion time. This conclusion is not limited to the polaron system but is valid for any composite nonrelativistic quantum particle.

It has also been shown that the correlation between the electron and phonon boundary conditions is critical for the consistency of the polaron mass calculation. It results in the correct form of a prefactor in the intermediate expression for mass, Eq. (30), which allows dropping the second double integral altogether. In the original Feynman calculation, the second double integral was omitted from the beginning, i.e., during the energy calculation, and therefore did not cause any problems in the mass calculation. Such an approach was internally inconsistent. It has been shown here that the consistency is restored via correct treatment of the shifted boundary conditions.

Finally, it has been shown that all the above considerations do not change the numerical values of the polaron effective mass obtained in Refs. 1 and 13. The optimal values of the variational parameters are still determined by minimization of the ground-state energy (33) alone. The effective mass then follows from expression (34) evaluated at the optimal values of v and w.

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