Functional-integral approach to the polaron mass

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Making use of functional-integration techniques, we calculate the formal free energy of a polaron in the subspace of fixed total momentum **Q**. Utilizing this result, we prove an analytical expression for the polaron mass. We include numerical results of variational and Monte Carlo types. As a by-product, we comment on the position of the continuum edge of the polaronic energy spectrum for fixed **Q**.

I. INTRODUCTION AND STATEMENT OF THE PROBLEM

The standard polaron model is defined by Fröhlich's Hamiltonian $\tilde{H}$. Introducing energy and length units $\hbar\omega$ and $\sqrt{\hbar/m\omega}$, where $\omega>0$ is an arbitrary frequency and m the electron band mass, $\tilde{H}$ reads as follows:

$$\frac{1}{\hbar\omega}\tilde{H} := \frac{\mathbf{p}^2}{2}+\sum_{\mathbf{k}}\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\frac{1}{\sqrt{V}}\sum_{\mathbf{k}}(g_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{q}}a_{\mathbf{k}}+\text{H.c.}) \; . \tag{1}$$

On the right-hand side of Eq. (1), all quantities are dimensionless. In particular, $\mathbf{p}$ and $\mathbf{q}$ are the momentum and position operators of the electron, whereas $\mathbf{k}$, $\omega_{\mathbf{k}}$, $a_{\mathbf{k}}$, and $a_{\mathbf{k}}^{\dagger}$ are the wave-vector, dispersion, annihilation, and creation operators of a phonon. Finally, $g_{\mathbf{k}}$ is the electron-phonon coupling and V the quantization volume. To complete our list of notation, we introduce the electron-phonon coupling constant α as

$$g_{\mathbf{k}} =: \sqrt{\alpha}\tilde{g}_{\mathbf{k}} \; . \tag{2}$$

Throughout this paper we assume $\omega_{\mathbf{k}}>0$ and inversion symmetry of $g_{\mathbf{k}}$ and $\omega_{\mathbf{k}}$.

The spectral properties of $\tilde{H}$ can conveniently be derived from the diagonal element of the reduced density matrix ρ, defined as

$$\rho(\alpha,\beta) := \mathrm{tr}_{\mathrm{ph}}\langle \mathbf{r} \mid e^{-\beta\tilde{H}} \mid \mathbf{r}\rangle \; . \tag{3}$$

In (3), $\mathrm{tr}_{\mathrm{ph}}$ indicates the trace operation with respect to phonons, β is a formal inverse temperature ($\beta\hbar\omega>0$), and $\mid \mathbf{r}\rangle$ an eigenstate of the position operator $\mathbf{q}$ with eigenvalue $\mathbf{r}$. As $\tilde{H}$ is translationally invariant, ρ does not depend on $\mathbf{r}$.

In a first step, we perform a Lee-Low-Pines transformation[1] within ρ. Considering the unitary transformation

$$U := \exp\left[i\mathbf{q}\cdot\sum_{\mathbf{k}}\mathbf{k}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\right] , \tag{4}$$

one has (because of familiar trace properties)

$$\rho(\alpha,\beta)=\mathrm{tr}_{\mathrm{ph}}\langle \mathbf{r} \mid Ue^{-\beta\tilde{H}}U^{-1} \mid \mathbf{r}\rangle \; . \tag{5}$$

On the other hand, it is easily verified that

$$Ue^{-\beta\tilde{H}}U^{-1}=e^{-\beta H} , \tag{6}$$

where

$$\frac{1}{\hbar\omega}H := \frac{1}{2}\left[\mathbf{p}-\sum_{\mathbf{k}}\mathbf{k}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\right]^2+\sum_{\mathbf{k}}\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} +\frac{1}{\sqrt{V}}\sum_{\mathbf{k}}(g_{\mathbf{k}}a_{\mathbf{k}}+\text{H.c.}) \; . \tag{7}$$

It is obvious that H commutes with $\mathbf{p}$; in fact, $\mathbf{p}$ is the unitary transform of the total momentum $\mathbf{P}$, that is, $\mathbf{p}=U\mathbf{P}U^{-1}$. Therefore, we conclude from (5)–(7) that $\rho(\alpha,\beta)$ admits a momentum decomposition as follows:

$$\rho(\alpha,\beta)=\frac{1}{(2\pi)^3}\int d^3Q\,\mathrm{tr}_{\mathrm{ph}}e^{-\beta H_{\mathbf{Q}}} =: \frac{1}{(2\pi)^3}\int d^3Q\,\rho(\alpha,\beta,\mathbf{Q}) \; . \tag{8}$$

$H_{\mathbf{Q}}$ differs from H in (7) only insofar as $\mathbf{p}$ has to be replaced by its possible eigenvalue $\mathbf{Q}$.

The partition function $\rho(\alpha,\beta,\mathbf{Q})$ is the central quantity of this paper. In Sec. II, we shall prove a functional-integral representation for $\rho(\alpha,\beta,\mathbf{Q})$. This will extensively be used in Sec. III, where we discuss the free energy $F(\alpha,\beta,\mathbf{Q})$, corresponding to $\rho(\alpha,\beta,\mathbf{Q})$:

$$\rho(\alpha,\beta,\mathbf{Q}) =: \exp[-\beta F(\alpha,\beta,\mathbf{Q})] \; . \tag{9}$$

In particular, we derive a new, analytical result for the polaron mass $m_p(\alpha)$, defined by means of the ground-state energy $E_0(\alpha,\mathbf{Q})$:

$$\frac{m}{m_p(\alpha)} := \frac{1}{3\hbar\omega}\Delta_{\mathbf{Q}}E_0(\alpha,\mathbf{Q})\mid_{\mathbf{Q}=0} \; . \tag{10}$$

Moreover, we present an intuitive argument for the position of the continuum edge of the spectrum of $H_{\mathbf{Q}}$. We close Sec. III with numerical results for the polaron mass. These are of variational and (for the first time) Monte Carlo type. Finally, Sec. IV contains a comparison with previous work.

II. FUNCTIONAL-INTEGRAL REPRESENTATION OF $\rho(\alpha,\beta,\mathbf{Q})$

Starting from $H_{\mathbf{Q}}$ in Eq. (8), one may write

$$\frac{1}{\hbar\omega}H_{\mathbf{Q}}=\mathbf{A}^2+h\ , \tag{11}$$

where

$$\mathbf{A}:=\frac{1}{\sqrt{2}}\left[\mathbf{Q}-\sum_{\mathbf{k}}\mathbf{k}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}\right]\ , \tag{12}$$

$$h:=\sum_{\mathbf{k}}\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\frac{1}{\sqrt{V}}\sum_{\mathbf{k}}(g_{\mathbf{k}}a_{\mathbf{k}}+\text{H.c.})\ . \tag{13}$$

Therefore we find from (8):

$$\rho(\alpha,\beta,\mathbf{Q})=\text{tr}_{\text{ph}}\left[e^{-Bh}T_{\tau}\exp\left[-\int_0^B d\tau\,\mathbf{A}^2(\tau)\right]\right]\ . \tag{14}$$

In (14), we defined

$$B:=\beta\hbar\omega,\quad \mathbf{A}(\tau):=e^{\tau h}\mathbf{A}e^{-\tau h}\ . \tag{15}$$

T_{τ} is a τ-ordering operator. At a first glance, it seems difficult to evaluate the trace in Eq. (14), as $\mathbf{A}^2(\tau)$ is of fourth order in the phonon operators. The decisive idea to overcome this problem is to linearize the exponent $\mathbf{A}^2(\tau)$ by means of the so-called Hubbard-Stratonovich trick (for a review see Mühlschlegel[2]). Introducing an auxiliary field $\mathbf{x}(\tau)$, one has

$$\rho(\alpha,\beta,\mathbf{Q})=\int D^3x\,\exp\left[-\int_0^B d\tau\,\mathbf{x}^2(\tau)\right]\text{tr}_{\text{ph}}\left[e^{-Bh}T_{\tau}\exp\left[-2i\int_0^B d\tau\,\mathbf{x}(\tau)\cdot\mathbf{A}(\tau)\right]\right]\ . \tag{16}$$

In (16), $\int D^3x$ indicates functional integration over the auxiliary field (again, see Ref. 2). We mention that such a procedure was earlier proposed by Kochetov, Kuleshov, and Smondyrev[3] and Grote.[4]

The remaining exponents are bilinear in $a_{\mathbf{k}},a_{\mathbf{k}}^{\dagger}$; consequently, the trace operation can be done by standard methods. As for a detailed calculation, see Schultz.[5] One arrives at

$$\rho(\alpha,\beta,\mathbf{Q})=\int D^3x\prod_{\mathbf{k}}(1-e^{-f_{\mathbf{k}}[B,\mathbf{x}]})^{-1}\exp\left[-\int_0^B d\tau[\mathbf{x}^2(\tau)+\sqrt{2}i\mathbf{x}(\tau)\cdot\mathbf{Q}]-\tilde{\phi}[\mathbf{x}]\right]\ , \tag{17}$$

where

$$f_{\mathbf{k}}[B,\mathbf{x}]:=\omega_{\mathbf{k}}B-\sqrt{2}i\mathbf{k}\cdot\int_0^B d\tau\,\mathbf{x}(\tau)\ , \tag{18}$$

$$\tilde{\phi}[\mathbf{x}]:=-\frac{1}{V}\sum_{\mathbf{k}}|g_{\mathbf{k}}|^2\int_0^B\int_0^B d\tau\,d\tau'\exp(-f_{\mathbf{k}}[\tau,\mathbf{x}]+f_{\mathbf{k}}[\tau',\mathbf{x}])\{\Theta(\tau-\tau')+(\exp f_{\mathbf{k}}[B,\mathbf{x}]-1)^{-1}\}\ . \tag{19}$$

It is important that we can establish a link between functional integrals of the type of (16) and (17) and functional integrals of Wiener-Feynman type. Formally,[6] this is done by two successive substitutions. Firstly, let

$$\mathbf{x}(\tau)=:\frac{1}{\sqrt{2}}\dot{\mathbf{y}}(\tau),\quad \mathbf{y}(0)=\mathbf{0},\quad \mathbf{y}(B)=\mathbf{R}\ . \tag{20}$$

Secondly, put

$$\mathbf{y}(\tau)=:\mathbf{z}(\tau)+\frac{\tau}{B}\mathbf{R},\quad \mathbf{z}(0)=\mathbf{z}(B)=\mathbf{0}\ . \tag{21}$$

Then we arrive at

$$\rho(\alpha,\beta,\mathbf{Q})=\int d^3R\frac{\cos(\mathbf{Q}\cdot\mathbf{R})\exp(-R^2/2B)}{\prod_{\mathbf{k}}[1-\exp(-\omega_{\mathbf{k}}B+i\mathbf{k}\cdot\mathbf{R})]}\int\delta^3z\,\exp\left[-\int_0^B d\tau\tfrac{1}{2}\dot{\mathbf{z}}^2(\tau)-\phi[\mathbf{z}]\right]\ , \tag{22}$$

where now

$$\phi[\mathbf{z}]:=-\frac{1}{V}\sum_{\mathbf{k}}|g_{\mathbf{k}}|^2\int_0^B\int_0^B d\tau\,d\tau'\exp\left[-\left[\omega_{\mathbf{k}}-\frac{i\mathbf{k}\cdot\mathbf{R}}{B}\right](\tau-\tau')+i\mathbf{k}\cdot[\mathbf{z}(\tau)-\mathbf{z}(\tau')]\right]$$

$$\times\{\Theta(\tau-\tau')-[\exp(\omega_{\mathbf{k}}B-i\mathbf{k}\cdot\mathbf{R})-1]^{-1}\}\ . \tag{23}$$

Equations (22) and (23) represent the central result of this paper. Two things should be realized: in (22), $\int\delta^3z$ indicates familiar Wiener integration over real, closed paths with starting and ending point $\mathbf{0}$, and integration of (22) with respect to $\mathbf{Q}$ yields a term $\delta(\mathbf{R})$; thereby we recover Feynman's[7] well-known result for $\rho(\alpha,\beta)$ that is the non-momentum-decomposed density matrix.

III. RESULTS

To begin with, we prove the inequalities

$$F(\alpha,\beta,\mathbf{Q}\neq\mathbf{0})>F(\alpha,\beta,\mathbf{0}),\quad E_0(\alpha,\mathbf{Q}\neq\mathbf{0})\geq E_0(\alpha,\mathbf{0})\ , \tag{24}$$

the latter being a consequence of the former. We note that it would be highly desirable to have

$E_0(\alpha,\mathbf{Q}\neq\mathbf{0})>E_0(\alpha,\mathbf{0})$, thereby excluding the possibility of symmetry breaking in systems described by a Hamiltonian $H_{\mathbf{Q}}$. In fact, for short-range couplings $g_{\mathbf{k}}$, Spohn[8] proved this result by showing that

$$\lim_{\beta\to\infty}\frac{1}{(2\pi)^3}\int d^3Q\,Q^2\rho(\alpha,\beta,\mathbf{Q})/\rho(\alpha,\beta)=0\ . \tag{25}$$

Using (22) and (23), we can directly recover this equation.

The proof of (24) is simple. Inspection of (22) shows that $\rho(\alpha,\beta,\mathbf{Q})$ may be written as

$$\rho(\alpha,\beta,\mathbf{Q})=\int d^3R\,\cos(\mathbf{Q}\cdot\mathbf{R})f(\alpha,\beta,\mathbf{R})\ , \tag{26}$$

where $f(\alpha,\beta,\mathbf{R})$ is strictly positive for every finite value of $\mathbf{R}$ (recall that $\omega_{\mathbf{k}}$ and $g_{\mathbf{k}}$ have inversion symmetry). Consequently, we find

$$\rho(\alpha,\beta,\mathbf{Q}\neq\mathbf{0})<\rho(\alpha,\beta,\mathbf{0})\ , \tag{27}$$

which proves (24) because of Eq. (9).

We are now going to discuss an interesting property of the exact eigenvalues of $H_{\mathbf{Q}}$, which shows up in the limit $V\to\infty$. In view of Eq. (22), let us define

$$\bar{\rho}(\alpha,\beta,\mathbf{Q}):=\int d^3R\,\cos(\mathbf{Q}\cdot\mathbf{R})\exp\left[-\frac{R^2}{2B}\right]\times\int\delta^3z\,\exp\left[-\int_0^B d\tau\tfrac{1}{2}\dot{\mathbf{z}}^2(\tau)-\phi[\mathbf{z}]\right]\ . \tag{28}$$

Because of $\omega_{\mathbf{k}}>0$, we derive, from (22),

$$\rho(\alpha,\beta,\mathbf{Q})=\bar{\rho}(\alpha,\beta,\mathbf{Q})+\sum_{\mathbf{k}}e^{-B\omega_{\mathbf{k}}}\bar{\rho}(\alpha,\beta,\mathbf{Q}-\mathbf{k})+O(e^{-2\bar{\omega}B})\ , \tag{29}$$

where $\bar{\omega}$ denotes the minimum of $\omega_{\mathbf{k}}$.

For $\alpha=0$, (29) is readily interpreted. Because of

$$\bar{\rho}(0,\beta,\mathbf{Q})=\exp\left[-\frac{Q^2}{2}B\right] \tag{30}$$

we may state the following: the first term on the right-hand side of (29) contains the one-particle, zero-phonon contribution to the partition function, and the second term contains the one-particle, one-phonon contributions (notice that the total momentum is fixed as $\mathbf{Q}$). With respect to the eigenvalues of $(\hbar\omega)^{-1}H_{\mathbf{Q}}$, this term-by-term analysis leads us to two (in this case trivial) conclusions: (1) for sufficiently small $\mathbf{Q}$ the ground-state energy is $Q^2/2$ and determined by the first term, and (2) if $Q^2/2$ is an eigenvalue, the same holds true for $\omega_{\mathbf{k}}+(\mathbf{Q}-\mathbf{k})^2/2$, the latter originating from the second term.

For $\alpha>0$, things are far more complicated. To begin with, we notice that Eq. (27) is also valid for $\bar{\rho}(\alpha,\beta,\mathbf{Q})$. In addition, $\bar{\rho}(\alpha,\beta,\mathbf{Q})$ is a continuous function of $\mathbf{Q}$. Combining these properties and choosing $|\mathbf{Q}|$ sufficiently small, we deduce from (29) for the ground-state energy:

$$E_0(\alpha,\mathbf{Q})=-\lim_{\beta\to\infty}\frac{1}{\beta}\ln\bar{\rho}(\alpha,\beta,\mathbf{Q})\ . \tag{31}$$

This is the generalization of conclusion (1) above.

For finite values of V, the corresponding generalization of conclusion (2) cannot hold. Representing $\phi[z]$ from Eq. (23) as a power series in $\exp(-B\omega_{\mathbf{k}})$ and inserting this series into Eq. (28), one realizes that $\bar{\rho}(\alpha,\beta,\mathbf{Q})$ is also a power series in $\exp(-B\omega_{\mathbf{k}})$. Consequently, the first term in Eq. (29) generates contributions of order $\exp(-B\omega_{\mathbf{k}})$, which add to the second term. One should notice, however, that all these additional contributions are of order $1/V$ as compared to those which are already present; in the limit $V\to\infty$, they will vanish. We conclude for $V\to\infty$ that if $E_0(\alpha,Q)$ is an eigenvalue of $H_{\mathbf{Q}}$, the same holds true for $\hbar\omega\omega_{\mathbf{k}}+E_0(\alpha,\mathbf{Q}-\mathbf{k})$. This, indeed, is the generalization of conclusion (2). We add, as a comment, that our intuitive argument can be rigorously justified within a totally different variational approach (see a forthcoming publication of Löwen[9]).

If one takes this for granted, one may prove an important result for the position of the continuum edge $E_c(\alpha,\mathbf{Q})$ of the spectrum of $H_{\mathbf{Q}}$. As $\hbar\omega\omega_k+E_0(\alpha,\mathbf{Q}-\mathbf{k})$ is an eigenvalue in the continuous part of the spectrum (for $V\to\infty$, $\mathbf{k}$ is a continuous variable), we have

$$E_c(\alpha,\mathbf{Q})\le\inf_{\mathbf{k}}[\hbar\omega\omega_{\mathbf{k}}+E_0(\alpha,\mathbf{Q}-\mathbf{k})]\ . \tag{32}$$

On the other hand, Fröhlich[10] proved that the right-hand side of (32) is a *lower* bound for $E_c(\alpha,\mathbf{Q})$. Concerning the connection between Fröhlich's functional-analytical work and polaron problems, we refer to a recent paper of one of us (H.L.),[11] who obtained an analogous result for magnetopolarons.

Combining both inequalities, we find

$$E_c(\alpha,\mathbf{Q})=\inf_{\mathbf{k}}[\hbar\omega\omega_{\mathbf{k}}+E_0(\alpha,\mathbf{Q}-\mathbf{k})]\ . \tag{33}$$

As an application, we consider "standard" optical polarons with constant dispersion ω. Then, because of $\omega_{\mathbf{k}}\equiv1$ and (24),

$$E_c(\alpha,\mathbf{Q})=\hbar\omega+E_0(\alpha,\mathbf{0})\ . \tag{34}$$

Notice that $E_c(\alpha,\mathbf{Q})$ no longer depends on $\mathbf{Q}$.

We close this section with a compilation of our numerical results. All of those are valid for the quoted standard case

$$\omega_{\mathbf{k}}=1,\quad g_{\mathbf{k}}=-i(2\sqrt{2}\pi\alpha)^{1/2}/k\ . \tag{35}$$

In a first part, we turn to variational bounds for $\rho(\alpha,\beta,\mathbf{Q})$ and the ground-state energy. An introductory comment is necessary: Because of the factor $\cos(\mathbf{Q}\cdot\mathbf{R})$ appearing in (22), Jensen's inequality (providing the basis for variational calculations) cannot be applied for arbitrary Q. For $Q=0$, however, the integrand is strictly positive and Jensen's inequality holds. Therefore a quadratic trial action yields an upper bound on $F(\alpha,\beta,\mathbf{Q})$, at least for $Q=0$. Because of the continuity of all quantities in Q, this remains an upper bound for sufficiently small Q.

We used as a variational trial action a general quadratic, but translationally invariant functional of $\mathbf{z}$, namely

$$\phi_0[\mathbf{z}] := \int_0^B \int_0^B d\tau\, d\tau' f(\tau-\tau')\mathbf{z}(\tau)\cdot\mathbf{z}(\tau') , \quad (36)$$

where $f(\tau-\tau')=f(\tau'-\tau)$ can be assumed and

$$\int_0^B d\tau\, f(\tau-\tau')=0 \quad (37)$$

must hold to guarantee translational invariance. The application of Jensen's inequality is now straightforward (though lengthy) and was extensively discussed for $\rho(\alpha,\beta)$ by Adamowski, Leschke, and one of the present authors (B.G.) in Ref. 12. All steps of the calculation can easily be transferred to the present case; only one additional integration, originating from the $\mathbf{R}$ integration in Eq. (22), has to be done. One finds

$$\frac{1}{\hbar\omega}E_0(\alpha,\mathbf{Q}) \le \frac{3}{2\pi}\int_0^\infty d\mu \left[\ln\left[1+\frac{F(\mu)}{\mu^2}\right] - \frac{F(\mu)}{\mu^2+F(\mu)} \right] - \frac{\alpha}{\sqrt{2}}\int_0^\infty d\tau \frac{e^{-\tau}}{\Delta(\tau)} + \left[1+\frac{\pi\alpha}{6\sqrt{2}}\int_0^\infty d\tau \frac{\tau^2 e^{-\tau}}{\Delta^3(\tau)}\right]^{-1}\frac{Q^2}{2} , \quad (38)$$

where $F(\mu)$ is the Fourier transform of $f(\tau)$ (in the limit $B\to\infty$) and

$$\Delta^2(\tau) := \int_0^\infty d\mu \frac{1-\cos(\mu\tau)}{\mu^2+F(\mu)} . \quad (39)$$

Obviously (38) constitutes an upper bound on $E_0(\alpha,\mathbf{Q})$, which contains an adjustable function $F(\mu)$. This may be used to minimize the bound. Having in mind that we should keep Q small, we can put $Q=0$ for the minimization procedure, thereby admitting an error of order Q^4. In any case we find

$$\frac{m_p(\alpha)}{m} = 1+\frac{\pi\alpha}{6\sqrt{2}}\int_0^\infty d\tau \frac{\tau^2 e^{-\tau}}{\Delta^3(\tau)} , \quad (40)$$

where on the right-hand side the minimizing function $F(\mu)$ has to be inserted. This function was calculated in Ref. 12. Actual results for m_p/m can be found in the table.

We add as a remark that (40) is a generalization of Feynman's formula (see Ref. 7). Interestingly enough, the small-α and large-α behavior of (40) can be discussed analytically, if one uses the corresponding function $F(\mu)$ from Ref. 12. We find

$$\lim_{\alpha\to 0}\frac{1}{\alpha}\left[\frac{m_p(\alpha)}{m}-1\right] = \frac{1}{6} , \quad (41)$$

$$\lim_{\alpha\to\infty}\frac{1}{\alpha^4}\left[\frac{m_p(\alpha)}{m}\right] = \frac{16}{81\pi^2} = 0.020\,01\ldots . \quad (42)$$

The same results can be derived from Feynman's formula.[13] One should notice that the right-hand side of (42) is approximately 10% smaller than the exact value (see Sec. IV).

Finally, we turn to Monte Carlo results for the polaron mass. Viewed from a more principal standpoint, it is a challenging task to evaluate Eq. (10) directly, utilizing Eq. (22). To do so, let us define a generalized (temperature-dependent) polaron mass by

$$\frac{m}{m_p(\alpha,\beta)} := \frac{1}{3\hbar\omega}\Delta_{\mathbf{Q}}F(\alpha,\beta,\mathbf{Q})\Big|_{\mathbf{Q}=0} = -\frac{1}{3B}\Delta_{\mathbf{Q}}\ln\rho(\alpha,\beta,\mathbf{Q})\Big|_{\mathbf{Q}=0} . \quad (43)$$

First of all, we remark that $m_p(\alpha,\beta)$ is analytic in α and β. For $\beta\to\infty$, this was proven by Spohn.[8] For $0<\beta<\infty$, two of us (B.G. and H.L.) have published[14] an estimation procedure for functional integrals, which can be directly transferred to $F(\alpha,\beta,\mathbf{Q})$. As a consequence, $F(\alpha,\beta,\mathbf{Q})$ and $m_p(\alpha,\beta)$ are analytical functions in all parameters. Obviously, $m_p(\alpha)$ can be found from $m_p(\alpha,\beta)$, if we let $\beta\to\infty$. Inserting Eq. (22) on the right-hand side of (43) and making use of the abbreviations we introduced in Eq. (26), we arrive at

$$\frac{m}{m_p(\alpha,\beta)} = \frac{1}{3B}\int d^3R\, R^2 f(\alpha,\beta,\mathbf{R}) \Big/ \int d^3R\, f(\alpha,\beta,\mathbf{R}) . \quad (44)$$

Remembering that $f(\alpha,\beta,\mathbf{R})$ is positive, one realizes that m/m_p is represented as an expectation value. In Ref. 15, Becker and two of the present authors (B.G. and H.S.) evaluated this type of expression in connection with Monte Carlo calculations for $\rho(\alpha,\beta)$. The present case differs from the previous one only insofar as one additional integration has to be done. Again, we can profitably make use of previous work and proceed as in the quoted paper. A collection of results can be found in Table I: We add as information that the statistical error of the calculation is rapidly increasing with increasing α. For $\alpha=3$, the error is on a 4% scale. At the moment, reasonable accuracy is only guaranteed for $\alpha\le 3$. Within these limits, we find good agreement with the variational data.

IV. COMPARISON WITH PREVIOUS WORK

There exists an enormous amount of literature on the subject of the "polaron mass." We restrict our comparison to those publications where m_p is defined as in Eq. (10). In doing so, we exclude, e.g., mass definitions via response to an external field. Even then there is no chance to be complete. We hope, however, to be representative.

A large group of publications is concerned with a direct perturbational or variational treatment of the Hamiltonian $H_{\mathbf{Q}}$. We mentioned Lee, Low, and Pines[1] and add Haga,[16] Höhler,[17] Gross,[18] Krivoglaz and Pekar,[19] Röseler,[20] and Larsen.[21] Larsen's work is the most involved; his results for the polaron mass are given in Table I. We find excellent agreement for small α, but growing discrepancies for $\alpha>2$. We recall that the same

TABLE I. Comparison of various results for the polaron mass. "Variational" and "Monte Carlo" correspond to Eqs. (40) and (44) in this paper; the data of Larsen, and Schultz and Feynman can be found in Refs. 21 and 23.

	m_p/m			
α	Variational	Monte Carlo	Larsen	Schultz-Feynman
0.1	1.017	1.017	1.017	1.017
0.5	1.090	1.087	1.089	1.090
1.0	1.196	1.187	1.191	1.196
2.0	1.476	1.448	1.434	1.472
3.0	1.900	1.832	1.723	1.889
4.0	2.606		2.038	2.579
5.0	3.940		2.354	3.887

holds true for the variational bounds on the ground-state energy, which were compared in Ref. 12: In the intermediate- and strong-coupling regime, the functional-integral bounds are systematically lower than all others, leading to the conclusion that this method is more adequate.

It is well known that many authors used functional-integral methods before us in polaron-physics. Besides Feynman's[7] pioneering work we quote Osaka,[22] Schultz,[23] Abe and Okamoto,[24] Kochetov, Kuleshov, and Smondyrev,[25] Sayakanit,[26] and Arisawa and Saitoh.[27] For comparison, we have added the data of Schultz in Table I; he uses Feynman's formula. Of particular interest are the recent papers of Spohn[8,28] on the mass of an optical polaron. They provide an excellent review of the mathematical background and clarify the strong-coupling behavior of the mass. Using scaling arguments, he finds that

$$\lim_{\alpha\to\infty} \frac{1}{\alpha^4}\left[\frac{m_p(\alpha)}{m}\right] = \frac{4\sqrt{2}\pi}{3}\int d^3r\,|\psi(\mathbf{r})|^4\,, \quad (45)$$

where $\psi(\mathbf{r})$ is the minimizing solution of Pekar's variational problem (again, see Ref. 8). It is well known that this problem was extensively studied by Miyake,[29] who found a numerical solution leading to

$$\lim_{\alpha\to\infty} \frac{1}{\alpha^4}\left[\frac{m_p(\alpha)}{m}\right] = 0.022\,70\ldots\,. \quad (46)$$

In conclusion, we may confirm Schulman's[30] statement: "what makes the polaron special from the standpoint of selling path integrals is that it is one of the few places where the path integral not only helps you discover an answer, but also remains the best way to calculate the answer even after you know it."

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