On the Best Quadratic Approximation in Feynman’s Path Integral Treatment of the Polaron

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Abstract

The best quadratic approximation to the retarded polaron action due to Adamowski et al. and Saitoh is investigated numerically for a wide range of coupling constants. The non-linear variational equations are solved iteratively with an efficient method in order to obtain the ground-state energy and the effective mass of the polaron. The virial theorem and expansions for small and large couplings are used to check the high accuracy of the numerical results. Only small improvements over Feynman’s (non-optimal) results are observed. For a moving polaron it is shown that the most general quadratic trial action may contain anisotropic terms which, however, do not lead to improvements for the ground-state energy and effective mass.

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1. The polaron problem is a non-relativistic field theory for an electron moving in a crystal and has received a lot of attention in the past decades (for reviews see [1], [2]). Among the many theoretical treatments Feynman’s approach [3] is still outstanding: he first integrated out the phonons to obtain an effective action for the electron which for large Euclidean times reads

\[ S_{\text{eff}} = \int_0^\beta dt \frac{1}{2} \dot{x}^2 - \frac{\alpha}{2\sqrt{2}} \int_0^\beta dt \int_0^\beta dt' \frac{e^{-(t-t')}}{|x(t) - x(t')|}. \]  

He then performed a variational approximation with a quadratic retarded trial action

\[ S_t = \frac{1}{2} \int_0^\beta dt \dot{x}^2 + \frac{1}{2} \int_0^\beta dt \int_0^\beta dt' f(t-t') \left[ x(t) - x(t') \right]^2, \]

choosing \( f_F(\sigma) = C \exp(-w\sigma) \), where \( C \) and \( w \) are two variational parameters (the strength parameter \( C \) is usually written as \( w(v^2 - w^2)/4 \)). This yields one of the best analytical approximations for the ground-state energy of the polaron for all values of the dimensionless coupling constant \( \alpha \). The best possible, rotationally invariant, quadratic trial action is obtained by replacing the exponential retardation by an arbitrary function \( f(\sigma) \) and was proposed by Adamowski et al. [4] and Saitoh [5]. Surprisingly for both small and strong coupling this best isotropic quadratic approximation only yields very small improvements for the ground-state energy \( E_0 \)

\[ E_0 \xrightarrow{\alpha \to 0} -\alpha - a \alpha^2 + O(\alpha^3) \]

\[ E_0 \xrightarrow{\alpha \to \infty} -\bar{a} \alpha^2 + O(1). \]

One finds at small coupling \( a_F = 0.0123457, a_{\text{iso}} = 0.0125978 \) whereas the exact value is \( a = 0.0159196 \) and for strong coupling \( \bar{a}_F = \bar{a}_{\text{iso}} = 0.106103 \) compared to \( \bar{a} = 0.108513 \). Probably discouraged by these analytical results the best isotropic quadratic approximation has never been investigated systematically for a whole range of couplings, in particular for intermediate coupling.

It is the purpose of the present Letter to do this for the ground-state energy and the effective mass of the polaron and to point out that an easy, efficient method exists to solve the non-linear variational equations. Although numerical results have been reported in the literature [4, 6], it will turn out that they are unreliable and considerably overestimate the improvement on Feynman’s approach. We also investigate the question whether the inclusion of anisotropic terms in the quadratic trial action leads to further improvements. This work is an outgrow of recent attempts to generalize Feynman’s polaron approach to four-dimensional field theories [7-11] in the context of the worldline formalism [12]. The nomenclature is the one used in Ref. [7].

2. We start with the expression for the ground-state energy using the quadratic trial action (2):

\[ E_0 = \frac{3}{2\pi} \int_0^\infty dE \left[ \ln A(E) + \frac{1}{A(E)} - 1 \right] - \frac{\alpha}{\sqrt{\pi}} \int_0^\infty d\sigma \frac{e^{-\sigma}}{\mu(\sigma)} \equiv \Omega + V. \]

Here

\[ \mu^2(\sigma) = \frac{4}{\pi} \int_0^\infty dE \frac{\sin^2(E\sigma/2)}{E^2} \frac{1}{A(E)} \]

(6)
is the “pseudotime” corresponding to the “profile function” $A(E)$ which is linked to the retardation function through

$$A(E) = 1 + \frac{8}{E^2} \int_0^\infty d\sigma f(\sigma) \sin^2 \left( \frac{E\sigma}{2} \right).$$

(7)

With Feynman’s choice one obtains the standard expression $A_F(E) = (v^2 + E^2)/(w^2 + E^2)$ for the profile function and the pseudotime can also be given analytically. However, one can do better by not imposing a special form for the retardation function \[4, 5\]. Indeed, by varying Eq. (5) with respect to $f(\sigma)$ or, equivalently, with respect to $A(E)$, one finds that the best variational profile function is determined by

$$A_{iso}(E) = 1 + \frac{4\alpha}{3\sqrt{\pi}} \int_0^\infty d\sigma \frac{e^{-\sigma}}{\mu_{iso}^3(\sigma)} \frac{\sin^2(E\sigma/2)}{E^2}.$$ \(8\)

By comparing with Eq. (7) one sees that the retardation function has the form \[\footnote{It should be kept in mind that for the ground-state energy we only consider the $\beta \to \infty$ limit which leads to the already simplified expression given in Eq. (1).}\]

$$f_{iso}(\sigma) = \frac{\alpha}{6\sqrt{\pi}} \frac{e^{-\sigma}}{\mu_{iso}^3(\sigma)}.$$ \(9\)

In particular, since for small $\sigma$ the pseudotime $\mu^2(\sigma)$ behaves like $\sigma$, we see that the retardation function $f_{iso}(\sigma)$ has a $\sigma^{-3/2}$-singularity at small relative times in marked contrast to Feynman’s Ansatz. Equivalently, the profile function at large $E$ does not approach unity like $1/E^2$ as Feynman’s parametrization suggests but slower, like $A_{iso}(E) \to 1 + 2\sqrt{2}\alpha/(3E^{3/2})$. The wrong small-time behaviour of Feynman’s Ansatz is responsible for the awkward behaviour of his variational parameters for $\alpha \to 0$: both $v$ and $w$ tend to 3 in this limit whereas one would have expected $w \to 1$ by comparison with the exact effective action (1).

For a quantitative description at arbitrary $\alpha$ one has to solve the coupled non-linear variational equations (8) and (6) numerically. This can be done as follows [8]: one maps the infinite intervals to finite ones by substituting $E = \tan^2 \theta$, $\sigma = \tan^2 \psi$ and solves the variational equations on a grid of Gaussian points. In this way the required integrals both in the variational equations and in the evaluation of the ground-state energy can be evaluated directly by Gauss-Legendre quadrature. The above choice of mapping is made to eliminate the integrable but numerically slowly convergent square-root behaviour near $\sigma \to 0$ in the various $\sigma$-integrals. The variational equations are then solved iteratively by starting either from the perturbative values $A(E) = 1$, $\mu^2(\sigma) = \sigma$ or from Feynman’s parametrization using the known values of the variational parameters [13]. For larger coupling the latter method gives faster initial convergence as seen in Fig. 1. The convergence rate was monitored by calculating the maximal relative deviation between two iterations, both for $A(E)$ and for $\mu^2(\sigma)$ for all Gaussian points, i.e. for all discrete values $\theta_i$ and $\psi_i$. In the numerical calculations reported in Table 1 the allowed maximal relative deviation was set to $10^{-7}$ and reached after 7 - 70 iterations, depending on the coupling constant (see Fig. 1). Furthermore, the $[0, \pi/2]$-range for the variables $\theta, \psi$ was subdivided into $n_e$ intervals and Gaussian integration with $n_g$ points was applied in the subintervals. Typically values of $(n_e, n_g) = (6, 72)$ were needed to obtain a ground-state energy accurate to six digits. It turned out that solving the non-linear variational equations by this method is numerically not more demanding than minimizing the energy functional with respect to the Feynman parameters $v$ and $w$.
Figure 1: Convergence rate for solving the variational equations (8, 6) iteratively at two different values of the coupling constant. The open symbols denote the case when the starting values are the free ones, the full symbols when Feynman’s parametrization is used for initialization.

To check the numerical stability of the method the ground-state energy was also calculated in a different way: the variational equations for \(A_{\text{iso}}(E)\) can be used to re-express the kinetic term \(\Omega\) in terms of the potential \(V\) (see the Appendix of Ref. [8] where this is detailed for the relativistic case):

\[
\Omega_{\text{iso}} = \int_0^\infty d\sigma \frac{\delta V}{\delta \mu^2(\sigma)} \mu^4(\sigma) \frac{\partial}{\partial \sigma} \left( \frac{\sigma}{\mu^2(\sigma)} \right) \bigg|_{\mu^2 = \mu^2_{\text{iso}}}.
\]

This can be combined with the potential term and after elimination of the derivative of the pseudotime one obtains the expression

\[
E_{\text{virial}} = -\frac{\alpha}{\sqrt{\pi}} \int_0^\infty d\sigma \left( \frac{3}{2} - \sigma \right) e^{-\sigma} \mu^2_{\text{iso}}(\sigma).
\]

This may be called “virial energy” since it also arises from evaluating the virial theorem for two-time actions [14]. In the numerical calculations an agreement in six digits between the two expressions for the energy was demanded and obtained.

Table 1 collects the results for coupling constants from \(\alpha = 1\) to \(\alpha = 15\). Note that convergence is obtained in all cases whereas in the relativistic case for coupling constants larger than a critical coupling the relative maximal deviations started to grow again with increasing number of iterations [8]. This was a signal for the instability of the scalar Wick-Cutkosky model whereas the polaron has a well-known strong coupling limit [15]. Also included is the effective mass of the polaron, defined by the expansion \(E(p) = E_0 + p^2/(2m^*) + \cdots\). It is given by [6]

\[
m^*_\text{iso} = 1 + \frac{\alpha}{3\sqrt{\pi}} \int_0^\infty d\sigma \frac{\sigma^2}{\mu^2_{\text{iso}}(\sigma)} e^{-\sigma}.
\]
and coincides with the value of the profile function $A_{iso}(E)$ at $E = 0$ (see Eq. (8)).

Being a variational calculation the values for the ground-state energy should lie below Feynman’s result which is non-optimal. Table 1 shows that for small coupling the relative change of the energy follows the behaviour $(a_F - a_{iso}) \alpha = -2.52 \cdot 10^{-4} \alpha$ which is expected from the small-coupling expansion (3). But also for intermediate coupling the best isotropic quadratic approximation gives only a slight improvement, maximally 0.15 %, for the ground-state energy.

| $\alpha$ | $E_0^{iso}$ | $10^3 \cdot \frac{E_0^{iso} - E_0}{E_0^{iso}}$ | $\alpha^2 \cdot (E_0^{iso} - E_0^F)$ | $m_{iso}^*$ | $10^3 \cdot \frac{m_{iso}^* - m_F^*}{m_F^*}$ | $m_{iso}^* - m_F^*$ |
|---------|-------------|---------------------------------|---------------------------------|-----------|---------------------------------|-----------------|
| 1       | -1.013296   | 0.26                            |                                 | 1.19615   | 0.53                            |                 |
| 2       | -2.056467   | 0.54                            |                                 | 1.47515   | 2.21                            |                 |
| 3       | -3.135951   | 0.84                            |                                 | 1.89862   | 5.12                            |                 |
| 4       | -4.261309   | 1.13                            |                                 | 2.60234   | 8.93                            |                 |
| 5       | -5.447781   | 1.40                            |                                 | 3.93259   | 12.1                            |                 |
| 6       | -6.72130    | 1.55                            |                                 | 6.9081    | 10.2                            |                 |
| 7       | -8.12440    | 1.44                            |                                 | 14.416    | 1.52                            |                 |
| 8       | -9.70625    | 1.12                            | -0.70                           | 31.479    | -2.86                           | -0.09           |
| 9       | -11.49505   | 0.81                            | -0.75                           | 62.597    | -2.46                           | -0.15           |
| 10      | -13.4982    | 0.58                            | -0.78                           | 111.65    | -1.48                           | -0.17           |
| 11      | -15.7163    | 0.41                            | -0.79                           | 182.96    | -0.90                           | -0.16           |
| 12      | -18.1489    | 0.30                            | -0.79                           | 281.47    | -0.54                           | -0.15           |
| 13      | -20.7954    | 0.23                            | -0.80                           | 412.65    | -0.32                           | -0.13           |
| 14      | -23.6554    | 0.17                            | -0.81                           | 582.47    | -0.20                           | -0.11           |
| 15      | -26.7285    | 0.13                            | -0.81                           | 797.4     | -0.12                           | -0.10           |

Table 1: The polaron ground state energy and effective mass in the best isotropic quadratic approximation as a function of the coupling constant $\alpha$. The third and sixth column display the relative deviation from the results using Feynman’s parametrization (see Ref. [13] and Table 2), while the entries in the fourth and last columns should approach a constant value in the large coupling limit (see text).

In contrast, the numerical values for this approximation reported by Adamowski et al. claim to be below the Feynman energy by as much as 0.75 % at $\alpha = 11$.\(^2\) That this is incorrect and probably due to insufficient convergence and/or numerical instability is shown in Fig. 2 where the present results for this specific coupling constant are plotted as function of the number of Gaussian points. It is clearly seen that with sufficient subdivisions of the intervals both expressions (5) and (11) for the ground-state energy converge to the same value which is far away from the one given in Ref. [4].

\(^2\)The difference might not seem much, however it should be remembered that Feynman’s energy is itself only a little more than 2 % above the exact energy at asymptotically large couplings; see Eq. (4).
Figure 2: Ground-state energy of the polaron for $\alpha = 11$ as a function of the number $n_e$ of subdivisions used in the 72-point Gauss-Legendre integrations. Open circles denote the energy evaluated from Eq. (5), full circles from the virial theorem (11). The inset shows the convergence of both numerical values in more detail. The value using Feynman’s parametrization and the result reported by Adamowski et al. [4] are shown by dashed lines.

An additional check on the accuracy of the numerical results is provided by the large coupling limits of $E_{\text{iso}}^0$ and $E_F^0$, which may be calculated analytically from Eq. (5). A systematic expansion around $\alpha \to \infty$ may be developed by making use of the fact that as the coupling constant increases the pseudotime remains constant over an increasing range of $\sigma$ (see Sec. 3.2 as well as the Appendix of Ref. [9]). One finds, after some effort, that not only the leading $O(\alpha^2)$ term of $E_{\text{iso}}^0$ and $E_F^0$ is identical (see Eq. (4)), but also the first subleading term:

$$E_{0,\text{iso}}^{F} = -\frac{1}{3\pi}\alpha^2 - 3\left(\frac{1}{4} + \log 2\right) + O(\alpha^{-2}).$$

(13)

The numerical values in the fourth column of Table 1 indeed show that the difference between $E_{\text{iso}}^0$ and $E_F^0$ is of order $\alpha^{-2}$.

For the effective mass the corrections to Feynman’s result are somewhat larger (for small $\alpha$ the relative change follows the perturbative result $2(a_{\text{iso}} - a_F)\alpha^2 = 5.04 \cdot 10^{-4} \alpha^2$, and they are closer to the ones given in Ref. [6]. For example, at $\alpha = 5$ (their largest value) Gerlach et al. give $m_{\text{iso}}^* = 3.940$ whereas a similar increase in Gaussian points as shown in Fig. 2 stabilizes the correct value at $m_{\text{iso}}^* = 3.93259$. At larger couplings the convergence of the present method deteriorates somewhat.
(see Fig. 1) but up to $\alpha = 15$ four to five significant figures can be given also for the effective mass of Eq. (12). Surprisingly, the large coupling limits of both $m_{\text{iso}}^*$ and $m_F^*$ again coincide to the first subleading term, i.e.,

$$m_{F,\text{iso}}^* = \frac{16}{81\pi^2} \alpha^4 - \frac{4}{3\pi} (1 + \log 4) \alpha^2 + \mathcal{O}(\alpha^0),$$ (14)

the numerical values quoted in the last column of Table 1 being consistent with this. In the course of these calculations it turned out that the values of the effective mass in Feynman’s parametrization are very sensitive to the precise numbers for the parameters $v, w$ and deviate somewhat from the ones given in Table II of Ref. [13]. We have re-calculated them by solving the variational equations for $v, w$ (instead of minimizing the energy functional which is sufficient for the energy but not for the effective mass) and checked that they agree to a very high precision with the large-coupling expansion. For convenience and further reference the new values are given in Table 2.

| $\alpha$ | $v$   | $w$   | $E_F$ | $E_F$ (SC) | $m_F^*$ | $m_F^*$ (SC) |
|---------|-------|-------|-------|-----------|---------|--------------|
| 1       | 3.10850 | 2.86958 | -1.0130308 | 1.19552 |
| 2       | 3.24535 | 2.72564 | -2.0553560 | 1.47189 |
| 3       | 3.42130 | 2.56031 | -3.1333335 | 1.88895 |
| 4       | 3.66464 | 2.36792 | -4.2564809 | 2.57931 |
| 5       | 4.03434 | 2.14002 | -5.4401445 | 3.88562 |
| 6       | 4.66687 | 1.87363 | -6.710871 | 6.83836 |
| 7       | 5.80989 | 1.60365 | -8.112688 | 14.3941 |
| 8       | 7.58682 | 1.40329 | -9.695371 | 31.5693 |
| 9       | 9.85025 | 1.28230 | -11.485786 | 62.7515 |
| 10      | 12.4749 | 1.20918 | -13.490437 | 111.150 |
| 11      | 15.4132 | 1.16209 | -15.709808 | 182.692 |
| 12      | 18.6483 | 1.12988 | -18.143395 | 281.327 |
| 13      | 22.1733 | 1.10676 | -20.790681 | 412.573 |
| 14      | 25.98515| 1.08952 | -23.651278 | 582.432 |
| 15      | 30.08224| 1.076285| -26.724904 | 797.385 |

Table 2: Precise values for Feynman parameters, ground state energy and effective mass. The values in columns 5 and 7 are from the strong coupling (SC) expansions $E_F(SC) = \sum_{i=0}^\infty e_i \alpha^{2-i}$, $m_F^*(SC) = \sum_{i=0}^\infty m_i \alpha^{4-i}$ for which we have calculated the following expansion coefficients: $e_0 = -0.1061033$, $e_2 = -2.829442$, $e_4 = -4.86387$, $e_6 = -34.1953$, $e_8 = 533.141$, $e_{10} = 51525.2$, $e_{12} = 6.61224 \cdot 10^6$, $e_{14} = 9.53627 \cdot 10^8$ and $m_0 = 0.02001406$, $m_2 = -1.012775$, $m_4 = 11.8558$, $m_6 = 43.0986$. Most of these coefficients, except $e_{12}$ and $e_{14}$, have also been obtained in Ref. [16].
3. For a moving polaron Eq. (2) is not the most general quadratic trial action. Indeed, there is now a preferred direction \( \hat{p} = p/|p| \) which may be used for constructing a trial action which makes use of this directionality, i.e.,

\[
S_{\text{aniso}} = S_{\text{iso}} - i(\lambda' - 1) p \cdot \int_0^\beta dt \dot{x}(t) + \frac{1}{2} \int_0^\beta dt dt' g(t - t') \left( \hat{p} \cdot [x(t) - x(t')] \right)^2 .
\] (15)

This the most general quadratic trial action which is scalar and invariant under time and space translations as well as time-reversal. Time-translational invariance requires that the retardation functions in the quadratic terms are functions of the relative time and allows only a constant parameter (written as \( \lambda' - 1 \)) in the linear term. Space-translational invariance leads to a dependence on coordinate differences or derivatives \(^3\). Finally, time-reversal invariance requires the linear term to be purely imaginary. In Eq. (15) it has been written in such a way that it may be combined with the exponential in the Fourier transform of the partition function projected on momentum \( p \) \([14]\). For \( p \neq 0 \) we thus have a new variational parameter \( \lambda' \) and two profile functions at our disposal

\[
A(E) \rightarrow A_{ij}(E) = A_L(E) \hat{p}_i \hat{p}_j + A_T(E) (\delta_{ij} - \hat{p}_i \hat{p}_j) \quad i, j = 1, 2, 3 .
\] (16)

Here the subscripts “L” and “T” denote longitudinal and transverse components with respect to the direction of the polaron momentum. Using the methods developed in Ref. \([17]\) it is straightforward to calculate the various averages needed in the Feynman variational principle and to evaluate the limit \( \beta \rightarrow \infty \). One finds that the energy

\[
E_{\text{aniso}}^p = \frac{1}{3} \left( 2 \Omega[A_T] + \Omega[A_L] \right) + V_p[\mu_L^2, \mu_T^2] + \frac{p^2}{2} (2\lambda - \lambda^2)
\] (17)

is stationary \(^4\) under variation of the parameter \( \lambda = \lambda'/A_L(0) \) and the two profile functions \( A_{L,T}(E) \) or, equivalently, the two pseudotimes \( \mu_{L,T}^2(\sigma) \). The potential term is given by

\[
V_p = -\frac{\alpha}{\sqrt{\pi}} \int_0^\infty d\sigma e^{-\sigma} \int_0^1 dx \frac{\mu_L(\sigma)}{\mu_L^2(\sigma) + [\mu_T^2(\sigma) - \mu_L^2(\sigma)]x^2} \exp \left[ \frac{\lambda^2 \sigma^2 x^2}{2\mu_L^2(\sigma)} \right] .
\] (18)

Clearly, the symmetric solution \( A_T(E) = A_L(E) \equiv A_{\text{iso}}(E) \) and hence \( \mu_T^2(\sigma) = \mu_L^2(\sigma) \), emerges when \( p^2 = 0 \) and hence, not surprisingly, \( E_{\text{aniso}}^p = E_{\text{iso}}^p \). A little less obvious is that the effective mass will, in fact, also remain unchanged. To see this, we expand the exponential in the potential to order \( p^2 \):

\[
V_p[A_T, A_L, \lambda] \equiv V_0[A_T, A_L] + \frac{\lambda^2 \sigma^2 x^2}{2\mu_L^2(\sigma)} V_1[A_T, A_L] + O \left( p^4 \right) .
\] (19)

To leading order in the momentum

\[
V_1[A_T, A_L] = V_1[A_{\text{iso}}] + O \left( p^2 \right) = 1 - m_{\text{iso}}^* + O \left( p^2 \right)
\] (20)

where Eq. (12) has been used. On the other hand, \( V_0 \) (and \( \Omega \)) contain an additional term of order \( p^2 \) because of the implicit dependence of \( A_{T,L} \) on the momentum. By writing \( A_{T,L}(E) \equiv \)

\(^3\)Terms with derivatives may be converted into the form of Eq. (15) by suitable integrations by part.

\(^4\)This is due to the use of a complex trial function and “momentum averaging” but as in Ref. \([7]\) one can show that the energy for arbitrary momentum \( p \) is also minimal. The effective mass, however, is the derivative of the energy with respect to \( p^2 \) at \( p = 0 \) and thereby has no minimum property anymore.
\[ A_{\text{iso}}(E) + p^2 \Delta A_{T,L}(E) + \ldots \] and expanding the functionals, one can make this remaining momentum dependence explicit. Hence one obtains for the energy

\[
\begin{align*}
E_{p}^{\text{aniso}} &= \Omega[A_{\text{iso}}] + V_0[A_{\text{iso}}] + \frac{p^2}{2} \int_0^\infty dE \left\{ \frac{2}{3} \Delta A_T(E) + \frac{1}{3} \Delta A_L(E) \right\} \frac{\delta}{\delta A(E)} \Omega[A] \\
&\quad + \sum_{i=L,T} \Delta A_i(E) \frac{\delta}{\delta A_i(E)} V_0[A_T, A_L] \bigg|_{A=A_{\text{iso}}} + \frac{p^2}{2} \left( 2\lambda - \lambda^2 + \lambda^2 V_1[A_{\text{iso}}] \right) + O\left( p^4 \right) \\
&= E_0^{\text{iso}} + \frac{p^2}{2} \int_0^\infty dE \frac{2\Delta A_T(E) + \Delta A_L(E)}{3} \left[ \frac{\delta}{\delta A(E)} \left( \Omega[A] + V_0[A] \right) \right]_{A=A_{\text{iso}}} \\
&\quad + \frac{p^2}{2} \left( 2\lambda - \lambda^2 + \lambda^2 V_1[A_{\text{iso}}] \right) + O\left( p^4 \right). \quad (21)
\end{align*}
\]

Figure 3: Energy difference between the variational approximation with the most general (anisotropic) and the isotropic trial action as function of the coupling constant \( \alpha \) and the polaron momentum \( p \).

The numerical results at \( \alpha = 5 \) have been multiplied by a factor 5 to make them better visible in the graph. The curves show the analytical perturbative \( O(\alpha^2) \) result: the dashed curve includes only the leading term at small momenta (i.e. \( O(p^4) \), see Eq. (23)) while the dotted line is the full second-order result without expansion in \( p^2 \).

The integral over \( E \) vanishes for any \( \Delta A_{T,L}(E) \) because of the variational equation for \( A_{\text{iso}}(E) \). On the other hand, the variational equation for \( \lambda \) yields \( \lambda^{-1} = 1 - V_1[A_{\text{iso}}] \) so that, upon substitution of
Eq. (20), one obtains

$$E_{\text{aniso}}^p = E_{\text{iso}}^p + \frac{p^2}{2m_{\text{iso}}^2} + \mathcal{O}(p^4).$$  \hspace{1cm} (22)

It is only at higher orders in $p^2$ that a difference between $E_{\text{aniso}}^p$ and $E_{\text{iso}}^p$ can show up. In fact, by solving the variational equations perturbatively, one sees that there is a difference between these two energies at $\mathcal{O}(p^4)$:

$$E_{\text{aniso}}^p - E_{\text{iso}}^p = -\left(\frac{p^2}{2}\right)^2 \left[\left(\frac{8}{225\pi} - \frac{1}{150}\right) \alpha^2 + \mathcal{O}(\alpha^3)\right] + \mathcal{O}(p^6).$$ \hspace{1cm} (23)

The anisotropic trial action has lowered the energy, as it should, however note that numerically the improvement is very small, the dimensionless coefficient of the $\alpha^2 p^4/4$ term being only 0.004651. Fig. 3 shows that for small couplings our numerical results obtained by solving the anisotropic variational equations indeed follow the analytical prediction (23) rather well.

4. In summary, we have investigated the use of the most general quadratic trial actions, both isotropic and anisotropic, in Feynman’s variational approach to the polaron problem and found out that they only lead to small numerical improvements compared to Feynman’s original parametrization of the retardation function. This is despite the fact that the variational retardation functions have quite a different small-time behaviour compared to Feynman’s Ansatz, but is consistent with results from the large-$N$ expansion \[18\], where $N$ is the number of space dimensions (similar results have been reported in Refs. \[19\]). Anisotropic terms in the trial action only become beneficial for a finite polaron momentum but not for the ground-state energy at $p = 0$ and its derivative, the effective mass.

The small improvement over Feynman’s results, even with arbitrary retardation functions, indicates that a quadratic trial action leaves out part of the correct physics of the polaron. This is most evident when the second-order expression for the ground-state energy is compared with the exact result. However, this does not imply that the optimal quadratic trial actions, both the isotropic and the anisotropic one, are useless. First, in four-dimensional relativistic field theory the correct ultraviolet behaviour of the trial action is of much greater importance \[8\] than for the polaron. Second, as shown in Ref. \[9\], the correct analytic structure of the profile function $A(E)$ is essential for describing scattering processes, where an analytic continuation to normal time is required. For these purposes Feynman’s Ansatz is totally inadequate whereas an improved parameterization $f_I(\sigma) \propto \exp(-w'\sigma)/\sigma^{3/2}$ captures the essence of the variational retardation function (9) and allows an easy analytic continuation. Third, extensions to fermionic theories like Quantum Electrodynamics require precise but subtle relations between fermionic and bosonic retardation functions \[11\] which are only fulfilled by the variational solutions if the variational Ansatz is left sufficiently general. And, finally, for a massive relativistic particle on its gerlach-mass-shell which corresponds to a moving 4-D polaron with $p^2 = M^2$, the 4-momentum is large and therefore one may expect substantial improvements in describing the physics of the system (for example, its instability) if one uses the most general, anisotropic trial action.
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