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Variational interpolation algorithm between weak- and strong-coupling expansions – application to the polaron

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Abstract

For many physical quantities, theory supplies weak- and strong-coupling expansions of the types $\sum a_n \alpha^n$ and $\alpha^p \sum b_n (\alpha^{-2/4})^n$, respectively. Either or both of these may have a zero radius of convergence. We present a simple interpolation algorithm which rapidly converges for an increasing number of known expansion coefficients. The accuracy is illustrated by calculating the ground state energies of the anharmonic oscillator using only the leading large-order coefficient b_0 (apart from the trivial zeroth-order expansion coefficient $a_0 = 1/2$). The errors are less than 0.5% for all g . The algorithm is then applied to find energies and masses of the Fröhlich–Feynman polaron. While our energies are very close to Feynman’s variational results (although more accurate), our masses are quite different from his, calling for a calculation of at least one more weak- or strong-coupling expansion coefficient to decide which are correct.

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1. Recently, the Feynman–Kleinert variational approximation to path integrals [1] has been extended to a systematic variational perturbation expansion [2]. This expansion converges uniformly and rapidly (for the anharmonic oscillator exponentially fast like $\exp(-\text{const} \times N^{1/3})$, where N is the order of the approximation [3]². Due to the uniformity of the

convergence, it has given rise to an efficient method for extracting strong-coupling expansions from a weak-coupling expansions [10,6,8].

For many physical systems, there exists an independent knowledge of expansion coefficients for weak and strong couplings. Important examples are most lattice models of statistical mechanics (see for example Refs. [11]). The purpose of this note is to propose a simple algorithm by which the variational perturbation expansion can be used to find a systematic convergent interpolation between the weak- and the strong-coupling expansions.

The algorithm is completely general and holds for any physical system whose quantities possess expan-

stood understood only recently in Ref. [8] and proved rigorously in Ref. [9].

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² As far as energy values and not entire path integrals are concerned, similar expansions have been proposed and investigated in Ref. [4]. Rigorous proofs of convergence were first given in Ref. [5], which did not, however, explain the exponentially fast convergence at strong couplings discovered in Ref. [6]. (Ref. [6] contains references to earlier less accurate calculations of strong-coupling expansion coefficients from weak-coupling perturbation theory, in particular Refs. [7]. Those works did not extract the exponential law of convergence from their data.) This was under-

sions in some coupling constant α of the type $\sum a_n \alpha^n$ for weak, and of the type $\alpha^p \sum b_n (\alpha^{-2/q})^n$ for strong couplings, where either or both of these expansions may have a zero radius of convergence.

A typical example is the ground state energy of the anharmonic oscillator with $p = 1/3, q = 3$. It illustrates the power of the algorithm. We calculate the energy for all coupling strengths using only the leading large-order coefficient b_0 , apart from the trivial coefficient $a_0 = 1/2$. The errors are everywhere less than 0.5% (see Fig. 1).

To make a prediction, we apply the algorithm to the Fröhlich–Feynman polaron [12,13]. Its ground state energy is known with three terms in the weak-coupling expansion, and two terms in the strong-coupling expansion; for the polaron mass, the corresponding numbers are 2 and 1. Apart from these exactly known expansion terms, there exists Feynman’s famous variational solution whose leading expansion coefficients are exact, and which interpolates energy and mass for all coupling constants. The Feynman energy is an upper bound to the correct one. Numerically, it is known to be quite accurate. For the mass, the knowledge is more scarce. It will turn out that our interpolation for the mass displays an interesting drastic shape discrepancy with Feynman’s (see Figs. 2 and 3), calling for a calculation of at least one more weak- or strong-coupling coefficients to decide which shape is correct.

2. Following the method explained in Ref. [3], we rewrite the weak-coupling expansion of order N

$$E_N = \sum_{n=0}^N a_n \alpha^n \tag{1}$$

as

$$E_N^\omega = \omega^p \sum_{n=0}^N a_n \left(\frac{\alpha}{\omega^q} \right)^n. \tag{2}$$

where ω is an auxiliary parameter whose value is eventually set equal to 1, whereas p, q are two parameters determined by general properties of the strong-coupling expansion to be specified below. Then we replace ω by the identical expression

$$\omega \rightarrow \sqrt{\Omega^2 + \omega^2 - \Omega^2}. \tag{3}$$

and reexpand E_N^ω in powers of λ , treating $\omega^2 - \Omega^2$ as a quantity of order α . The reexpanded series is truncating after the order $n > N$.

The resulting expansion has the form

$$W_N(\alpha, \Omega) = \Omega^p \sum_{n=1}^N a_n f_n(\Omega) \left(\frac{\alpha}{\Omega^q} \right)^n, \tag{4}$$

where

$$f_n(\Omega) = \sum_{j=0}^{N-n} \binom{\frac{1}{2}(p - qn)}{j} (-1)^j \left(1 - \frac{\omega^2}{\Omega^2} \right)^j. \tag{5}$$

Forming the first and second derivatives of $W_N(\alpha, \Omega)$ with respect to Ω , we calculate the positions of the extrema and the turning points. The smallest among these is denoted by Ω_N . The resulting $W_N(\alpha) \equiv W_N(\alpha, \Omega_N)$ constitutes the desired approximation to the energy.

It is easy to take this approximation to the strong-coupling limit $\alpha \rightarrow \infty$. For dimensional reasons, Ω_N increases with α like $\Omega_N \approx \alpha^{1/q} c_N$, so that

$$W_N(\alpha, \Omega_N) \approx \alpha^{p/q} c_N^p w_N^{(0)}, \tag{6}$$

where

$$w_N^{(0)} = \sum_{n=0}^N a_n f_n(\infty) \left(\frac{1}{c_N^q} \right)^n. \tag{7}$$

The full strong-coupling expression is obtained by writing $W_N(\alpha, \Omega) = \Omega^p w_N(\hat{\alpha}, \omega^2/\Omega^2)$, with $\hat{\alpha} \equiv \alpha/\Omega^q$, and expanding w_N in powers of ω^2/Ω^2 , which behaves for $\alpha \rightarrow \infty$ like $(1/c^2)(\alpha/\omega^q)^{-2/q}$. The result is

$$W_N(\alpha) = \alpha^{p/q} \left[b_0(c) + b_1(c) \left(\frac{\alpha}{\omega^q} \right)^{-2/q} + b_2(c) \left(\frac{\alpha}{\omega^q} \right)^{-4/q} + \dots \right], \tag{8}$$

with

$$b_n(c) = \frac{1}{n!} w_N^{(n)}(\hat{\alpha}, 0) \hat{\alpha}^{(2n-p)/q} |_{\hat{\alpha}=1/c^q}, \tag{9}$$

and the superscript (n) denotes the n th derivative with respect to $\hat{\omega}^2$.

The parameters p and q in expansion (2) are now determined to render the correct leading and the successive powers of α in the strong-coupling expansion (8).

The leading coefficient c_N in the optimal frequency Ω_n is found by searching for the extrema of the leading coefficient $b_0(c)$ as a function of c and choosing the smallest of them.

Explicitly

$$b_n(c) = \sum_{l=0}^N a_l \sum_{j=0}^{N-n} \binom{\frac{1}{2}(p-lq)}{j} \binom{j}{n} \times (-1)^{j-n} c^{p-lq-2n}. \tag{10}$$

Next we have to correct for the fact that for large but finite α , the trial frequency Ω has corrections to the behavior $\alpha^{1/q}c$. The coefficient c will depend on α like

$$c(\alpha) = c + c_1 \left(\frac{\alpha}{\omega^q}\right)^{-2/q} + c_2 \left(\frac{\alpha}{\omega^q}\right)^{-4/q} + \dots \tag{11}$$

requiring a reexpansion of c -dependent coefficients b_n^c in (8). The expansion coefficients γ_n are determined by extremizing $b_{2n}(c)$. The final result can again be written in the form (8) with b_n^c replaced by b_n , which are determined by the equations shown in Table 1. The two leading coefficients receive no correction and are omitted.

It is now obvious that the knowledge of any strong-coupling coefficients b_0, b_1 can be exploited to determine approximately further coefficients a_{N+1}, a_{N+2}, \dots and thus carry $W_N(\alpha)$ to higher orders. We merely have to solve Eq. (10) for as many b_n as are available.

3. The weak-coupling expansion of the anharmonic oscillator looks like (1) with $\alpha = g/4$ (for a potential is $gx^4/4$). The lowest coefficient a_0 is trivially determined by the ground state energy of the harmonic oscillator, being equal to $1/2$.

The strong-coupling behavior is known from general scaling arguments to start out like $g^{1/3}$ followed by powers of $g^{-1/3}, g^{-1}, g^{-5/3}$. Inspection of (8) shows that this corresponds to $p = 1$ and $q = 3$. The leading coefficient is known extremely accurately [6,14], $b_0 = 0.667\,986\,259\,155\,777\,108\,270\,962\,016\,919\,860 \dots$. This is now used to determine an approximate a_1

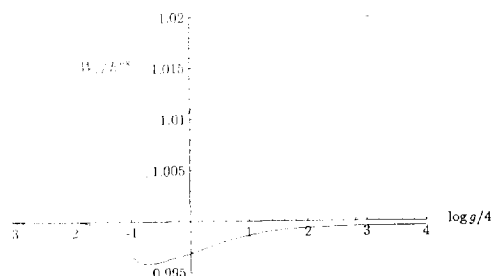


Fig. 1. Plot of the ratio of the interpolation energy with respect to the exact energy as a function of the coupling constant. The accuracy is everywhere better than 99.5%. For comparison, we also plot the variational perturbation result using the exact $a_1 = 3/4$.

(forgetting that we know the exact value $a_1^{ex} = 3/4$). The energy (4) reads for $N = 1$

$$W_1(\alpha, \Omega) = \left(\frac{1}{2}\Omega + \frac{1}{2\Omega}\right)a_0 + \frac{a_1}{\Omega^2}\alpha. \tag{12}$$

Eq. (10) yields, for $n = 0$,

$$b_0 = \frac{1}{2}ca_0 + \frac{a_1}{c^2}. \tag{13}$$

Minimizing b_0 with respect to c we find $c = c_1 \equiv 2(a_1/2a_0)^{1/3}$ with $b_0 = 3a_0c_1/4 = 3(a_0^2a_1/2)^{1/3}/2$. Inserting this into (13) fixes $a_1 = 2(2/3b_0)^3/a_0^2 = 0.773\,970 \dots$, quite close to the exact value. With our approximate a_1 we calculate $W_1(\alpha, \Omega)$ at its minimum, where

$$\begin{aligned} \Omega_1 &= \frac{2}{\sqrt{3}}\omega \cosh\left[\frac{1}{3}\operatorname{acosh}(g/g^{(0)})\right] & \text{for } g > g^{(0)}, \\ &= \frac{2}{\sqrt{3}}\omega \cos\left[\frac{1}{3}\arccos(g/g^{(0)})\right] & \text{for } g < g^{(0)}, \end{aligned} \tag{14}$$

with $g^{(0)} \equiv 2\omega^3a_0/3\sqrt{3}a_1$. The result is shown in Fig. 1. Since the difference with respect to the exact solution would be too small to be visible on a direct plot of the energy, we display the ratio with respect to the exact energy $W_1(\alpha)/E^{ex}$. The accuracy is everywhere better than 99.5%. For comparison, we also display the much worse (although also quite good) variational perturbation result using the exact $a_1^{ex} = 3/4$.

4. Let us now turn to the polaron model. The Hamiltonian operator reads

Table 1

Equations determining the coefficients b_n in the strong-coupling expansion from the functions $b_n(c)$ and their derivatives. For brevity, we have suppressed the argument c in the entries

n	b_n	$-c_{n-1}$
2	$b_2 - c_1 b_1' + \frac{1}{2} c_1^2 b_0''$	b_1'/b_0''
3	$b_3 - c_2 b_1' + c_1 b_2' + c_1 c_2 b_0'' + \frac{1}{2} c_1^2 b_1'' + \frac{1}{6} c_1^3 b_0^{(3)}$	$b_2' + c_1 b_1'' + \frac{1}{2} c_1^2 b_0^{(3)}/b_0''$
4	$b_4 - c_3 b_1' + c_2 b_2' + c_1 b_3' + (\frac{1}{2} c_2^2 + c_1 c_3) b_0'' - c_1 c_2 b_1'' + \frac{1}{2} c_1^2 b_2'' + \frac{1}{2} c_1^3 c_2 b_0^{(3)} + \frac{1}{6} c_1^3 b_1^{(3)} + \frac{1}{24} c_1^4 b_0^{(4)}$	$(b_3' + c_2 b_1'' + c_1 b_2'' + c_1 c_2 b_0^{(3)} + \frac{1}{2} c_1^2 b_1^{(3)} + \frac{1}{6} c_1^3 b_0^{(4)})/b_0''$

$$H = \frac{\mathbf{p}^2}{2m_b} + \sum_{\mathbf{k}} \hbar \omega_0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}} (V_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} + \text{h.c.}) \quad (15)$$

where m_b is the effective mass of the electron in the conduction band, \mathbf{p} is the electron momentum, ω_0 is the frequency of optical phonons which are created and annihilated by $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$, and

$$V_{\mathbf{k}} = -i \frac{\hbar \omega}{|\mathbf{k}|} \left(\frac{4\pi\alpha}{V} \right)^{1/2} \left(\frac{\hbar}{2m_b \omega_0} \right)^{1/4} \quad (16)$$

specifies the electron–phonon interaction in the volume V . The Fröhlich coupling constant

$$\alpha = \frac{e^2}{\hbar c} \sqrt{\frac{m_b c^2}{2\hbar \omega_0}} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) \quad (17)$$

involves the fundamental constants e , c , \hbar and the electronic and static dielectric constants ϵ_∞ and ϵ_0 , respectively. This form of $V_{\mathbf{k}}$ assumes the size of the polaron to be large with respect to the lattice spacing. It further ignores spin and relativistic effects and the dispersion of the electron band.

In natural units with $\hbar = c = m_b = \omega_0 = 1$, the partition function of the polaron in thermal equilibrium at a fixed temperature T is described by the path integral

$$Z(\beta) = \int \mathcal{D}\mathbf{x}(\tau) \exp \left(- \frac{1}{2} \int_0^\beta d\tau \dot{\mathbf{x}}^2 + \frac{\alpha}{2^{3/2}} \int_0^\beta \int_0^\beta d\tau d\tau' \frac{e^{-|\tau-\tau'|}}{\mathbf{x}(\tau) - \mathbf{x}(\tau')} \right), \quad (18)$$

where $\beta = 1/T$ is the inverse temperature (at Boltzmann constant $k_B = 1$). The weak-coupling expansion

of the energy of the polaron is known up to the order α^3 [15],

$$E^w = -\alpha - 0.0159196220\alpha^2 - 0.000806070048\alpha^3 - O(\alpha^4). \quad (19)$$

For strong couplings the energy is [17]

$$E^s = -0.108513\alpha^2 - 2.836 - O(\alpha^{-2}). \quad (20)$$

The polaron mass has the corresponding expansions [18,17]

$$m^w = 1 + \frac{1}{6}\alpha + 0.02362763\alpha^2 + O(\alpha^4), \quad (21)$$

$$m^s = 0.0227019\alpha^4 + O(\alpha^2). \quad (22)$$

Feynman was the first to find a uniform all-coupling constant expressions from a variational approximation to the path integral (18),

$$E^F = \text{Min}_{v,w} \frac{3}{4v} (v-w)^2 - \frac{\alpha}{\sqrt{\pi}} \int_0^\infty \frac{d\tau e^{-\tau}}{[\omega^2 \tau + (v^2 - w^2)(1 - e^{-v\tau})/v]^{1/2}} \quad (23)$$

and

$$m^F = 1 + \frac{1}{3\sqrt{\pi}} \alpha v^3 \times \int_0^\infty \frac{d\tau \tau^2 e^{-\tau}}{[\omega^2 \tau + (v^2 - \omega^2)(1 - e^{-\tau})/v]^{1/2}}, \quad (24)$$

the latter being evaluated at the parameters $v(\alpha)$, $w(\alpha)$ obtained in minimizing E^F . For weak coupling,

Feynman's expressions are exact only to the order α . They have the expansions [15]

$$E^{F,w} = -\alpha - 0.012345\alpha^2 - 6.34366 \times 10^{-4}\alpha^3 - 4.64315 \times 10^{-5}\alpha^4 - 3.957 \times 10^{-6}\alpha^5 - \dots, \quad (25)$$

$$m^{F,w} = 1 + \frac{1}{6}\alpha + 2.469136 \times 10^{-2}\alpha^2 + 3.566719 \times 10^{-3}\alpha^3 + 5.073952 \times 10^{-4}\alpha^4 + \dots \quad (26)$$

For strong couplings, the expansions are

$$E^{F,s} \approx -0.106103\alpha^2 - 2.829422 - 4.863866/\alpha^2 - 34.195252/\alpha^4 + \dots, \quad (27)$$

$$m^{F,s} \approx 0.020141\alpha^4 - 1.012775\alpha^2 + 11.85579 + \dots \quad (28)$$

With the help of the interpolation algorithm based on the variational perturbation expansion we shall find new expressions for E and m which share with Feynman's the validity for all α , but are more reliable at small and large α by possessing the presently most precise weak- and strong-coupling expansions (19), (20) and (21), (22).

5. We now apply our interpolation algorithm the expansions (19) and (20) for the energy. To make the series start out with α^0 as required by the general ansatz (2), we remove an overall factor $-\alpha$ from E and deal with $-E/\alpha$.

Then we see from (20) that the correct leading power in the strong-coupling expansion requires taking $p = 1, q = 1$. The knowledge of b_0 and b_1 allows us to extend the known weak coupling expansion (19) by two further expansion terms. Their coefficients a_3, a_4 are solutions of the equations

$$b_0 = \frac{35}{128}a_0c + a_1 + \frac{15}{8}\frac{a_2}{c} + \frac{2a_3}{c^2} + \frac{a_4}{c^3}, \quad (29)$$

$$b_1 = \frac{35}{32}\frac{a_0}{c} - \frac{5}{4}\frac{a_2}{c^3} + \frac{a_3}{c^3}. \quad (30)$$

The constant c governing the growth of Ω_N for $\alpha \rightarrow \infty$ is obtained by extremizing b_0 in c , which yields the equation

$$\frac{35}{128}a_0 - \frac{15}{8}\frac{a_2}{c^2} - \frac{4a_3}{c^3} - \frac{4a_4}{c^5} = 0. \quad (31)$$

The simultaneous solution of (29)–(31) renders

$$c_4 = 0.09819868, \quad a_3 = 6.43047343 \times 10^{-4}, \\ a_4 = -8.4505836 \times 10^{-5}. \quad (32)$$

The reexpanded energy (4) reads explicitly (for E including the earlier removed factor $-\alpha$)

$$W_4(\alpha, \Omega) = a_0\alpha \left(-\frac{35}{128}\Omega - \frac{35}{32\Omega} + \frac{35}{64\Omega^3} - \frac{7}{32\Omega^5} + \frac{5}{128\Omega^7} \right) - a_1\alpha^2 + a_2\alpha^3 \left(-\frac{15}{8\Omega} + \frac{5}{4\Omega^3} - \frac{3}{8\Omega^5} \right) + a_3\alpha^4 \left(-\frac{2}{\Omega^2} + \frac{1}{\Omega^4} \right) - a_4\alpha^5 \frac{1}{\Omega^3}. \quad (33)$$

Extremizing this we find Ω_4 as a function of α (it turns out to be quite well approximated by the simple function $\Omega_4 \approx c_4\alpha + 1/(1 + 0.07\alpha)$). This is to be compared with the optimal frequency obtained from minimizing the lower approximation $W_2(\alpha, \Omega)$,

$$\Omega_2^2 = 1 + \frac{4a_2}{3a_0}x^2 + \sqrt{\left(1 + \frac{4a_2}{3a_0}x^2\right)^2 - 1}, \quad (34)$$

which behaves likes $c_2\alpha + 1 + \dots$ with $c_2 = \sqrt{8a_2/3a_0} \approx 0.120154$. The resulting energy is shown in Fig. 2, where it is compared with the Feynman variational energy. For completeness, we have also plotted the weak-coupling expansion, the strong-coupling expansion, the lower approximation $W_2(\alpha)$, and two Padé approximants which were given in Ref. [16] as upper and lower bounds to the energy.

6. Consider now the polaron mass, where the strong-coupling behavior (22) fixes $p = 4, q = 1$. The coefficient b_0 allows us to determine an approximate coefficient a_3 and to calculate the variational perturbation expansion $W_3(\alpha)$. From (10) we find the equation

$$b_0 = -a_1c^3/8 + a_3c, \quad (35)$$

whose minimum lies at $c_3 = \sqrt{8a_2/3a_0}$ (this value follows, of course, also directly from (37)), where $b_0 = \sqrt{32a_3^3/27a_1}$. Using b_0 from (22), we obtain $a_3 = (27a_1b_0^2/32)^{1/3} \approx 0.0416929$.

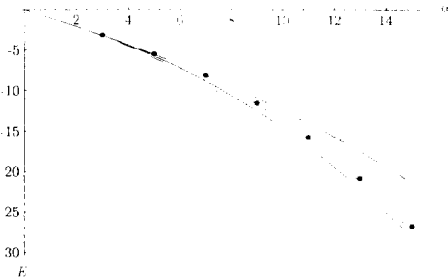


Fig. 2. The polaron energy obtained from our variational interpolation (solid line) between the weak-coupling expansion (dashed) and the strong-coupling expansion (short-dashed) to be compared with Feynman's variational approximation (fat dots), which is known to be an upper bound to the energy. The dotted curves are Padé approximants which were given in Ref. [16] as upper and lower bounds. The dot-dashed curve shows the variational perturbation theory $W_2(\alpha)$, which does not make use of the strong-coupling information.

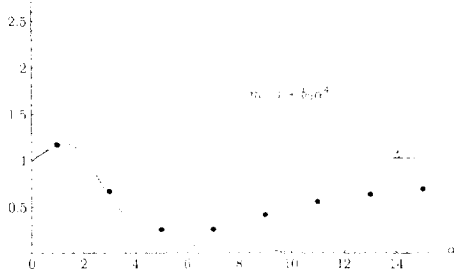


Fig. 3. The polaron mass curve interpolating optimally between the weak- (dashed) and strong-coupling expansions (short-dashed). To see better the differences between the strongly rising functions, we have divided out the asymptotic behavior $m_{as} = 1 + b_0\alpha^4$ before plotting the curves. The fat dots show Feynman's variational approximation. The dotted curves are Padé approximants which were given in Ref. [16] as upper and lower bounds to the mass.

From (4) we have

$$W_3(\alpha, \omega) = a_0 + a_1\alpha \left(-\frac{\Omega^3}{8} - \frac{3\Omega}{4} + \frac{3}{8\Omega} \right) + a_2\alpha^2 + a_3\alpha^3\Omega. \tag{36}$$

This is extremal at

$$\Omega_3^2 = 1 + \frac{4a_3}{3a_1}x^2 + \sqrt{\left(1 + \frac{4a_3}{3a_1}x^2 \right)^2 - 1}. \tag{37}$$

The approximation $W_3(\alpha) = W_3(\alpha, \Omega_3)$ for the polaron mass is shown in Fig. 3, where it is compared

with the weak and strong-coupling expansions and with Feynman's variational result. To see better the differences between the curves which all grow fast with α , we have divided out the asymptotic behavior $m_{as} = 1 + b_0\alpha^4$ before plotting the data. As for the energy, we have again displayed two Padé approximants given by Ref. [16] as upper and lower bounds to the energy. Note that our interpolation differs considerably from Feynman's and higher order expansion coefficients in the weak or the strong coupling expansions will be necessary to find out which is the true behavior of the model.

Our curve has, incidentally, the strong-coupling expansion

$$m^s = 0.0227019\alpha^4 + 0.125722\alpha^2 + 1.15304 + O(\alpha^{-2}), \tag{38}$$

the α^2 -term being in sharp contrast with Feynman's expression (28). On the weak-coupling side, a comparison of our expansion with Feynman's in Eq. (26) shows that our coefficient $a_3 \approx 0.0416929$ is about ten times larger than his.

Both differences are the reason for our curve forming a pronounced peak in Fig. 3, whereas Feynman's has a valley. It will be interesting to find out how the polaron mass really behaves. This would be possible by calculating one or more terms of either the weak- or the strong-coupling expansion.

Our interpolation algorithm is more flexible and accurate than Padé's. First, we can account for an arbitrary fractional leading power behavior α^p as $\alpha \rightarrow \infty$. Second, the successive lower powers in the strong-coupling expansion can be spaced by an arbitrary amount $2/q$. Third, our functions have in general a cut in the complex α -plane approximating the cuts in the function to be interpolated [19]. Padé approximants, in contrast, have always an integer power behavior in the strong-coupling limit, a unit spacing in the strong-coupling expansion, and poles to approximate cuts.

Note added. While this paper was being prepared, we found a method of incorporating the exact large-order behavior into the present expansion scheme [20].

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