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Systematic corrections to the variational calculation of the effective classical potential ☆

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We show how the Feynman–Kleinert approximation to path integrals (which is based on a locally harmonic variational ansatz and the Jensen–Peierls inequality) can be improved systematically towards the exact result by means of two different methods. One of them leads, even at the lowest correction level, to a great accuracy for any coupling strength including the strong-coupling limit.

1. In a recent note [1] we have increased the power of the variational approach to path integrals by introducing a separate trial frequency for each principal quantum number of a quantum system. The spectral resolution of the ansatz gave detailed information on all energy levels of an anharmonic oscillator. The ground state energy, however, did not improve with respect to the simple Feynman–Kleinert approximation [2,3] [#1] which made essential use of the Jensen–Peierls inequality

$$\langle e^{-X}\rangle \geq e^{\langle -X\rangle} . \tag{1}$$

The ground state energy coincided with the expectation value of the Hamiltonian operator in a normalized Gaussian wave packet of optimized width. For the anharmonic oscillator, the deviation from the exact energy was of the order of a few percent.

Obviously, if we want to do better than that, we have to go beyond the Jensen–Peierls inequality. This is what we want to do in this note by developing two systematic graphical schemes of different complexity and quality for improving the effective classical potential.

2. For later comparison we briefly recall the Feynmann–Kleinert approach: The partition function of a quantum mechanical particle of mass M in a one-dimensional potential $V(x)$ can always be expressed as a classical phase space integral

$$Z=\int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp\{-\beta[p^2/2M+V_{\text{eff,cl}}(x_0)]\}=\int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\hbar^2\beta/M}} \exp[-\beta V_{\text{eff,cl}}(x_0)] , \tag{2}$$

with $\beta\equiv 1/k_B T$, where the variable of integration x_0 is the time-averaged position $\bar{x}\equiv(1/\hbar\beta)\int_0^{\hbar\beta} d\tau\, x(\tau)$ of the fluctuating path. The function $V_{\text{eff,cl}}(x_0)$ appearing in the Boltzmann factor is called the *effective classical potential*. It has the obvious path integral representation

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[#1] For a detailed appreciation of the accuracy of the Feynman–Kleinert approach in comparison with several other approximation schemes see the paper by Srivastava and Vishwamittar [2].

$$\exp[-\beta V_{\mathrm{eff,cl}}(x_0)] \equiv Z^{x_0} \equiv \int \mathscr{D}x\, \delta(\bar{x}-x_0) \exp(-\mathscr{A}/\hbar)\,, \tag{3}$$

where $\mathscr{A}$ is the Euclidean action

$$\mathscr{A} = \int_0^{\hbar\beta} \mathrm{d}\tau\, [\tfrac{1}{2}M\dot{x}^2 + V(x(\tau))] \tag{4}$$

and δ the modified δ function

$$\delta(\bar{x}-x_0) \equiv \sqrt{2\pi\hbar^2\beta/M}\, \delta(\bar{x}-x_0)\,,$$

which forces $\bar{x}$ to be equal to x_0. The paths have the same values at initial and final imaginary times $\tau=0$ and $\tau=\hbar\beta$. The quantity Z^{x_0} is the *local partition function*. The effective classical potential obviously coincides with the local free energy $F^{x_0} = -\beta^{-1}\log Z^{x_0} \equiv V_{\mathrm{eff,cl}}(x_0)$.

The usefulness of a separate treatment of x_0 derives from the fact that at finite temperatures the fluctuations rarely carry $x(\tau)$ far from $\bar{x}$. The square deviations $[x(\tau)-\bar{x}]^2$ are for larger temperatures only of the order of $\hbar^2\beta/12M$ and remain finite down to zero temperature where they are of the order of $\hbar/2\sqrt{MV''(x_{\min})}$ (with $x_{\min}$ being the position of the potential minimum). The main thermal fluctuations take place in $\bar{x}$ with the average square deviation of $\bar{x}$ from the potential minimum being of the order of $1/\beta V''(x_{\min})$. Thus, at larger temperatures these must be integrated out exactly, which is done in (1). The fluctuations $x(\tau)-\bar{x}$, on the other hand, can be dealt with approximately with satisfactory accuracy on the basis of a variational approach which is excellent at high and satisfactory at low temperatures.

The variational ansatz makes use of the trial partition function of a harmonic oscillator centered at x_0 with the local action

$$\mathscr{A}_{\Omega}^{x_0} = \int_0^{\hbar\beta} \mathrm{d}\tau\, M[\tfrac{1}{2}\dot{x}^2 + \tfrac{1}{2}\Omega^2(x_0)(x-x_0)^2] \tag{5}$$

for which the path integral with restricted $\bar{x}=x_0$ can be done and gives the *local harmonic partition function*

$$Z_{\Omega}^{x_0} = \exp[-\beta V_{\Omega}^{x_0}(x_0)] \equiv \int \mathscr{D}x\, \delta(\bar{x}-x_0) \exp(-\mathscr{A}_{\Omega}^{x_0}/\hbar) = \frac{\frac{1}{2}\hbar\beta\Omega(x_0)}{\sinh[\frac{1}{2}\hbar\beta\Omega(x_0)]}\,. \tag{6}$$

The right-hand side differs from the unrestricted global partition function

$$Z_{\Omega(x_0)} = \frac{1}{2\sinh[\frac{1}{2}\hbar\beta\Omega(x_0)]} \tag{7}$$

by a factor $\hbar\beta\Omega(x_0)$. Expectations within the local trial partition function will be denoted by $\langle\ \rangle_{\Omega}^{x_0}$, i.e.

$$\langle \ldots \rangle_{\Omega}^{x_0} \equiv (Z_{\Omega}^{x_0})^{-1} \int \mathscr{D}x\, \delta(\bar{x}-x_0) \exp(-\mathscr{A}_{\Omega}^{x_0}/\hbar) \ldots\,. \tag{8}$$

Using (6) and (8) one can write

$$\int \mathscr{D}x\, \delta(\bar{x}-x_0) \exp(-\mathscr{A}/\hbar) \equiv \int \mathscr{D}x\, \delta(\bar{x}-x_0) \exp(-\mathscr{A}_{\Omega}^{x_0}/\hbar) \exp[-(\mathscr{A}-\mathscr{A}_{\Omega}^{x_0})/\hbar]$$

$$= \langle \exp(-\mathscr{A}/\hbar - \mathscr{A}_{\Omega}^{x_0}/\hbar) \rangle_{\Omega}^{x_0} \tag{9}$$

and apply the Jensen–Peierls inequality

$$\langle \exp(-\mathscr{A}/\hbar - \mathscr{A}_{\Omega}^{x_0}/\hbar) \rangle_{\Omega}^{x_0} \geqslant \exp(-\langle \mathscr{A}/\hbar - \mathscr{A}_{\Omega}^{x_0}/\hbar \rangle_{\Omega}^{x_0}) \tag{10}$$

to derive the Feynman–Kleinert approximation $W_1(x_0)$ to the effective classical potential [2,3]

$$V_{\mathrm{eff,cl}}(x_0) \approx W_1(x_0) \equiv V_{\Omega}^{x_0}(x_0) + V_{a^2}(x_0) - \tfrac{1}{2}\Omega^2(x_0)a^2(x_0) \,. \tag{11}$$

The last two terms are the expectations

$$\frac{1}{\beta}\langle \mathscr{A}/\hbar \rangle_{\Omega}^{x_0} = \langle V(x) \rangle_{\Omega}^{x_0} = V_{a^2}(x_0) \,,$$

$$\frac{1}{\beta}\langle \mathscr{A}_{\Omega}^{x_0}/\hbar \rangle_{\Omega}^{x_0} = \tfrac{1}{2}M\Omega^2(x_0)\langle (x-x_0)^2 \rangle_{\Omega}^{x_0} \equiv \tfrac{1}{2}M\Omega^2(x_0)a^2(x_0) \,. \tag{12}$$

The restricted square deviation $\langle (x-x_0)^2 \rangle_{\Omega}^{x_0}$ is given by

$$a^2(x_0) = \frac{\hbar}{2M\Omega(x_0)} \coth[\tfrac{1}{2}\hbar\beta\Omega(x_0)] - \frac{1}{M\beta\Omega^2(x_0)} \,. \tag{13}$$

The first term is the well-known unrestricted average while the second term subtracts from this the square deviations of $\bar{x}$ from x_0. The restricted expectation of the potential, $V_{a^2}(x_0)$, is obtained by a simple Gaussian smearing process of width $a^2(x_0)$,

$$V_{a^2}(x_0) \equiv \int_{-\infty}^{\infty} \frac{\mathrm{d}x_0'}{\sqrt{2\pi a^2(x_0)}} \exp[-(x_0'-x_0)^2/2a^2(x_0)]V(x_0') \,. \tag{14}$$

The best approximation is reached at

$$\Omega^2(x_0) = \frac{2}{M}\frac{\partial V_{a^2}(x_0)}{\partial a^2} \,. \tag{15}$$

Equations (13) and (15) are solved numerically, most comfortably by iteration. The approximate effective classical potential $W_1(x_0)$ is always slightly larger than the exact $V_{\mathrm{eff,cl}}(x_0)$.

The resulting approximation to the partition function

$$Z_1 = \int_{-\infty}^{\infty} \frac{\mathrm{d}x_0}{\sqrt{2\pi\hbar^2\beta/M}} \exp[-\beta W_1(x_0)] \tag{16}$$

leads to a free energy $F_1 \equiv k_{\mathrm{B}}T \log Z_1$ which describes the true free energy $F \equiv k_{\mathrm{B}}T \log Z$ of the system quite well at all temperatures. At high temperatures, this is not astonishing since F_1 has the correct classical limit. At low temperatures, the accuracy is due to the fact that F_1 tends to the lowest energy of the Hamiltonian operator in a Gaussian trial wave packet. This is known to be quite accurate for potentials with a smooth minimum (even for singular potentials such as $1/r$ the variational energy is accurate to 15% [2,3]). At arbitrary temperatures the approximation is always better than that.

A simple integral leads from the approximate effective classical potential $W_1(x_0)$ to particle distributions and response functions to an external source [3].

3. The first type of systematic improvements to be developed in this note comes about as follows. We expand the action into powers of the fluctuations $x'(\tau) \equiv x(\tau) - x_0$ around the temporal average and write

$$\mathscr{A} = \mathscr{A}_0 + \mathscr{A}^{x_0} \,, \tag{17}$$

with

$$\mathscr{A}_0 = \hbar\beta V(x_0) \,, \qquad \mathscr{A}^{x_0} = \int_0^{\hbar\beta} \mathrm{d}\tau \, [\tfrac{1}{2}M\dot{x}'^2 + V^{x_0}(x'(\tau))] \tag{18}$$

and

$$V^{x_0}(x') = \frac{1}{2!} V''(x_0)x'^2 + \frac{1}{3!} V^{(3)}(x_0)x'^3 + \frac{1}{4!} V^{(4)}(x_0)x'^4 + \dots . \tag{19}$$

The $V'(x_0)$ term is absent since $\bar{x}' \equiv \int_0^{\hbar\beta} d\tau\, x'(\tau) = 0$ by definition of x'.

The action $\mathscr{A}^{x_0}$ is now extended by a bilocal external current term

$$\mathscr{A}^{\mathrm{curr}} = -\tfrac{1}{2} \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\tau'\, x(\tau) K(\tau, \tau') x(\tau') \tag{20}$$

and the local partition function can be written as

$$Z^{x_0}[K] = \exp(-W^{x_0}[K]/\hbar) , \tag{21}$$

where $W^{x_0}[K]$ is a functional of $K(\tau, \tau')$ whose derivative $\delta/\delta K(\tau, \tau')$ gives, for each x_0, the correlation function $G^{x_0}(\tau, \tau') = \langle x'(\tau) x'(\tau') \rangle^{x_0}$ via $\delta W/\delta K = -\frac{1}{2} G^{x_0}$. The property $\bar{x}' = 0$ implies also that $\langle x'(\tau) \rangle^{x_0} \equiv 0$ so that $G^{x_0}(\tau, \tau')$ is a connected correlation function. We now form the double Legendre transform

$$\Gamma^{x_0}[G^{x_0}] \equiv W^{x_0}[K] - W^{x_0}_K K \equiv W^{x_0}[K] + \tfrac{1}{2} G^{x_0} K , \tag{22}$$

where the subscript K indicates the associated functional derivative and multiplication is functional. The functional derivative of $\Gamma^{x_0}[G^{x_0}]$ with respect to G^{x_0} satisfies $\Gamma^{x_0}_{G^{x_0}}[G^{x_0}] = \frac{1}{2} K$. This shows that for the physical situation with no external current K, the functional $\Gamma^{x_0}[G^{x_0}]$ is extremal in G^{x_0}. It may be called the *local effective action of the second type* associated with the action $\mathscr{A}$. There are simple graphical rules for calculating $\Gamma^{x_0}[G^{x_0}]$ organized by powers of the coupling strength in $V(x_0)$ [4,5] [#2]. The result is

$$\Gamma^{x_0}[G^{x_0}] = \hbar\beta V(x_0) + \hbar \operatorname{Tr} \log[(G^{x_0})^{-1}\hbar/(-M\partial_\tau^2)] + \tfrac{1}{2}\hbar \operatorname{Tr}\{[-M\partial_\tau^2 + V''(x_0)] G^{x_0}(\tau, \tau') - \hbar\}$$
$$+ \tfrac{1}{8}\hbar^2 \int_0^{\hbar\beta} d\tau\, G^{x_0 2}(\tau, \tau) + \Gamma^{x_0}_{\mathrm{int}}[G^{x_0}] , \tag{23}$$

with $\Gamma^{x_0}_{\mathrm{int}}[G^{x_0}] = \Gamma^{x_0}_2[G^{x_0}] + \Gamma^{x_0}_3[G^{x_0}] + \dots$ collecting the interactions (involving 2, 3, ... powers of the coupling strength). They are given by the two-particle irreducible graphs

$$\Gamma^{x_0}_2 = -\frac{1}{12\hbar} V^{(3)}(x_0)^2 \iint G^{x_0 3}(\tau, \tau') - \frac{1}{48\hbar} V^{(4)}(x_0)^2 \iint G^{x_0 4}(\tau, \tau')$$

$$= -\frac{1}{12\hbar}$$  $$- \frac{1}{48\hbar}$$  . $$\tag{24}$$

$$\Gamma^{x_0}_3 = \frac{1}{8\hbar^2} V^{(3)}(x_0)^2 V^{(4)}(x_0) \iiint G^{x_0 5} + \frac{1}{48\hbar^2} V^{(4)}(x_0)^3 \iiint G^{x_0 6}$$

$$= \frac{1}{8\hbar}$$ $$+ \frac{1}{48\hbar^2}$$, $$\tag{25}$$

with the diagrams indicating the contractions to be performed. Each line corresponds to a Green function $G^{x_0}(\tau, \tau')$ containing the τ variables of the vertices and the integral symbols imply the integrals $\int_0^{\hbar\beta} d\tau$ over the τ variables. We now write down a general spectral decomposition for $G^{x_0}(\tau, \tau')$ respecting the $\bar{x}' = 0$:

[#2] The diagrams with the correct multiplicity are given in fig. 4 of ref. [5].

$$G^{x_0}(\tau,\tau')=\frac{2}{M\beta}\sum_{m=1}^{\infty}\exp[-i\omega_m(\tau-\tau')]\,\frac{1}{\omega_n^2+\Omega^2(x_0)}\,, \tag{26}$$

with the Matsubara frequencies $\omega_m=2\pi m k_B T/\hbar$. For $|\tau-\tau'|\leqslant\beta$ the sum is

$$G^{x_0}(\tau,\tau')=\frac{1}{M\beta\Omega^2(x_0)}\left(\tfrac{1}{2}\hbar\beta\Omega\,\frac{\cosh[\frac{1}{2}(|\tau-\tau'|-\hbar\beta)\Omega]}{\sinh(\frac{1}{2}\hbar\beta\Omega)}-1\right), \tag{27}$$

a function $G^{x_0}(\tau-\tau')$ of the time difference only. With it, (24) can be rewritten as

$$\frac{1}{\hbar}\Gamma^{x_0}[G^{x_0}]=\beta W_2(x_0)=\beta[W_1(x_0)+W_1^{\rm corr}(x_0)]\,, \tag{28}$$

where

$$W_1(x_0)=\beta^{-1}\log\left(\frac{\sinh[\frac{1}{2}\hbar\beta\Omega(x_0)]}{\frac{1}{2}\hbar\beta\Omega(x_0)}\right)+V(x_0)+\tfrac{1}{2}[V''(x_0)-M\Omega^2(x_0)]a^2+\tfrac{1}{8}V^{(4)}(x_0)a^4 \tag{29}$$

and

$$W_1^{\rm corr}(x_0)=\frac{1}{\beta\hbar}\Gamma_{\rm int}^{x_0}[G^{x_0}]=-\tfrac{1}{12}\beta V^{(3)}(x_0)^2a_3^6-\tfrac{1}{48}\beta V^{(4)}(x_0)^2a_4^8$$
$$+\tfrac{1}{8}\beta V^{(3)}(x_0)^2\beta V^{(4)}(x_0)^2a_5^{10}+\tfrac{1}{48}\beta V^{(4)}(x_0)^3a_6^{12}\,, \tag{30}$$

having defined

$$a^2(x_0)\equiv G^{x_0}(\tau,\tau)=\frac{1}{M\beta\Omega^2(x_0)}\{\tfrac{1}{2}\hbar\beta\Omega(x_0)\coth[\tfrac{1}{2}\hbar\beta\Omega(x_0)]-1\}\,, \tag{31}$$

and

$$a_3^6(x_0)\equiv\frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau\,G^{x_0\,3}(\tau)\,,\qquad a_4^8(x_0)\equiv\frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau\,G^{x_0\,4}(\tau)\,,$$
$$a_5^{10}(x_0)\equiv\frac{1}{(\hbar\beta)^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,G^{x_0}(\tau-\tau')G^{x_0\,2}(\tau')G^{x_0\,2}(\tau)\,,$$
$$a_6^{12}(x_0)\equiv\frac{1}{(\hbar\beta)^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,G^{x_0\,2}(\tau-\tau')G^{x_0\,2}(\tau')G^{x_0\,2}(\tau)\,. \tag{32}$$

Higher graphs can easily be written down using the results of ref. [5], p. 366. Note that $W_1(x_0)$ coincides with the Feynman–Kleinert approximation (11) which happens to be extremal with respect to independent variations in $\Omega^2(x_0)$ and a^2.

4. To see the improvement brought about by the corrections we shall apply this and the method to be presented in section 6 to the classical partition function of the anharmonic oscillator consisting of the integral

$$Z=\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi/\beta\omega^2}}\exp[-\beta(\tfrac{1}{2}\omega^2x^2+\tfrac{1}{4}gx^4)]\,. \tag{33}$$

It is easy to expand this in powers of g as $Z=\sum_{k=0}^{\infty}z^{(k)}g'^k$ where $g'=g/\beta\omega^4$. The coefficients are

$$z^{(k)} = \frac{(-1)^k}{k!}\frac{\Gamma(2k+\frac{1}{2})}{\Gamma(\frac{1}{2})} \tag{34}$$

starting out like $1, -\frac{3}{4}, \frac{105}{32}, -\frac{3465}{128}, \frac{675675}{2048}, \ldots$. For large k they grow like $(-1)^k 4^k k!/k\pi\sqrt{2}$. The series is divergent but Borel-summable. It can be expanded in a convergent power series in $1/\sqrt{g'}$ by rewriting it as

$$Z = g'^{-1/4}\frac{1}{\sqrt{\pi}}\int_0^\infty \frac{dy}{\sqrt{y}}\exp(-y/\sqrt{g'})\exp(-y^2) \tag{35}$$

and expanding the first exponential. The result is the absolutely convergent strong-coupling series

$$Z = g'^{-1/4}\sum_{k=0}^{\infty}\xi_k(1/\sqrt{g'})^k, \tag{36}$$

with the coefficients

$$\xi_k = \frac{1}{2\sqrt{\pi}}(-1)^k\frac{\Gamma(\frac{1}{2}k+\frac{1}{4})}{k!}. \tag{37}$$

This is the same as

$$Z = \exp(1/8g')W_{0,-1/4}(1/4g') = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{2g'}\right)^{1/2}\exp(1/8g')K_{1/4}(1/8g'), \tag{38}$$

where $W_{0,-1/4}(z)$ is Whittaker's function and $K_{1/4}(z)$ the modified Bessel function. For $g\to\infty$ the function approaches the limit

$$Z \underset{g\to\infty}{\longrightarrow} \kappa_0 g'^{-1/4}, \tag{39}$$

with

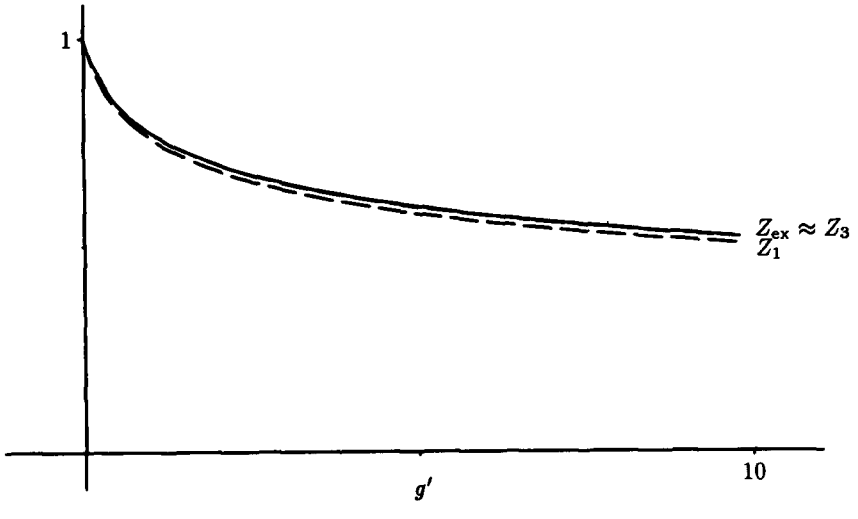

Fig. 1. The anharmonic model integral as a function of g' in comparison with the three variational approximations, Z_1 (dashed) based on the Jensen–Peierls inequality, the Padé approximation $Z_2^{\text{Padé}}$, the new variational approximation Z_3, and the exact Z_{ex}. The latter two are indistinguishable on this plot, Z_3 lying less than 0.1% below Z_{ex} at $g' = 10$.

$$\kappa_0 = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{dy}{\sqrt{y}} \exp(-y^2) = \frac{\Gamma(\frac{1}{4})}{2\sqrt{\pi}} \approx 1.0228 . \tag{40}$$

The curve is plotted in fig. 1.

5. How well is this classical partition function reproduced by the successive improvements? The correlation functions of the trial oscillator are $a^2 = \langle x^2 \rangle_\Omega = 1/\beta\Omega^2$ and the function W_2 of (28) reduces for $\beta = 1$ to

$$W_2 = W_1 + W_1^{\text{corr}} = \tfrac{1}{2} \log(\Omega^2/\omega^2) + \tfrac{1}{2}(\omega^2 - \Omega^2)a^2 + \tfrac{3}{4}ga^4 - \frac{6^2}{48} g^2 a^8 + \frac{6^3}{48} g^3 a^{12} - \frac{5 \times 6^4}{128} g^4 a^{16} + \dots . \tag{41}$$

In this simple case the different contractions in the diagrams are all the same and the coefficients of W_2 can be calculated to all orders as $6^n c_n g^n a^{4n}$ with c_n satisfying the recursion relation (see eq. (101) of ref. [5])

$$c_n = \frac{1}{2} \left(-\tfrac{1}{6} c_{n-1} (2n-2)(2n-3) + 8 \sum_{m+m'=n} m m' (2m'-1) c_{m'} \right), \tag{42}$$

so that c_5, c_6, ... are $\frac{35}{144}$, $-\frac{175}{96}$, $\frac{1925}{96}$, $-\frac{175175}{576}$, $\frac{875875}{144}$, $-\frac{14889875}{96}$, ... The value of Ω^2 where W_2 is minimal can be expanded in a power series, reinserted into $Z_2 \equiv \exp(-W_2)$, and the result is the power series $Z_2 \equiv \sum_{k=0}^\infty z_2^{(k)} g^{\prime k}$ whose coefficients agree with the exact ones to the order to which the correction terms have been included. The higher coefficients grow rapidly and have a very small radius of convergence, although they cannot quite match the factorial growth with zero radius of (34). At the Feynman–Kleinert level, $z_1^{(k)}$ start out like

$$1, \ -\tfrac{3}{4}, \ \tfrac{81}{32}, \ -\tfrac{1665}{128}, \ \tfrac{168939}{2048}, \ -\tfrac{24329889}{40960}, \ \tfrac{1526112009}{327680}, \ -\tfrac{356115654603}{9175040}, \ \tfrac{19884581106597}{58720256},$$
$$-\tfrac{3595662040811859}{1174405120}, \ \tfrac{1338018356629685889}{46976204800},$$

with the successive ratios growing like -0.75, -3.38, -5.14, -6.34, -7.20, -7.84, -8.33, -8.73, -9.04, -9.30, showing the small radius of convergence. This is to be compared with the exact ratios -0.75, -4.38, -8.25, -12.1875, -16.15, -20.13, -24.11, -28.09, -32.08, -36.08.

An important feature of the Feynman–Kleinert approximation is that it explains quite well the strong-coupling behaviour $g \to \infty$ of the system. In this limit, Ω^2 diverges like $dg^{1/2}$ and $Z_1 \to e^{1/4}/\sqrt{d} g^{1/4}$ with $d = \sqrt{3}$. The value $e^{1/4}/\sqrt{d} \approx 0.9756$ compares reasonably with the correct value κ_0 in (40). However, when trying to calculate this behaviour in the presence of the correction terms, we find a severe weakness of the present improvement scheme: The equation to be solved for d reads (correction terms in parentheses)

$$-d + \frac{3}{d} - \left(\frac{6}{d^3} - \frac{54}{d^5} + \frac{810}{d^7} + \dots \right) = 0 . \tag{43}$$

The factorial growth of the coefficients makes it impossible to extract a solution without resummation procedures. Without a knowledge on the large-order behaviour we cannot use the most powerful Borel techniques but may take recourse to a Padé approximation. Assuming that for a more complicated theory only the g^2 diagrams are calculated and the large-order behaviour is unknown we rewrite W_2 as

$$W_2^{\text{Padé}} \approx \tfrac{1}{2} \log(\Omega^2/\omega^2) + \tfrac{1}{2}(\omega^2 - 2\Omega^2)a^2 + \tfrac{1}{2}\Omega^2 a^2 + \tfrac{3}{4}ga^4 - \tfrac{3}{4}g^2 a^8 + \dots$$
$$\approx -\tfrac{1}{2} \log a^2 + \tfrac{1}{2}\omega^2 a^2 + \tfrac{1}{2}(c-1) - \tfrac{1}{2}c \frac{1 + (1 - 3/2c) g a^4}{1 + g a^4} , \tag{44}$$

with an arbitrary parameter c, the asymptotic extremum is determined by $-d + (3/d)(1 + 1/d^2)^{-2} = 0$, the corresponding Padé approximation to (43), and this has still no solution. We may, however, approximate (43)

with the different Padé approximation $-d(1-1/d^2)/(1+2/d^2)=0$ which is solved by $d=1$ and corresponds to the energy

$$\bar{W}_2^{\text{Padé}} = -\tfrac{1}{2}\log a^2 + \tfrac{1}{2}(a^2-1) - \frac{3}{4}\int_0^{ga^4} \frac{\mathrm{d}t}{t}\,\frac{1-t}{1+2t}, \tag{45}$$

The asymptotic behavior of $\bar{Z}_2^{\text{Padé}}$ is $d^{-1/2}\exp[\tfrac{1}{2}-\tfrac{3}{4}\int_0^{1/d^2}\mathrm{d}t/(1+2t)]g^{-1/4}\approx 1.0920g^{-1/4}$, which is too large by $\sim 7\%$. Also a Borel–Padé approximation

$$\bar{W}_2^{\text{Padé}} = -\tfrac{1}{2}\log a^2 + \tfrac{1}{2}(a^2-1) - \tfrac{1}{2}\int_0^{\infty} \mathrm{d}t\,\mathrm{e}^{-t}\,\frac{1-tga^4}{1+2tga^4} \tag{46}$$

is not much better, giving an equation $d=3\int_0^{\infty}\mathrm{d}t\,\mathrm{e}^{-t}t(1+t/2d^2)^{-2}$ solved by $d\approx 1.015$ and an asymptotic limit $\bar{Z}_2^{\text{Padé}}\to d^{-1/2}\exp[\tfrac{1}{2}-\tfrac{3}{4}\int_0^{\infty}\mathrm{d}t\,td^{-2}(1+t/2d^2)^{-1}]g^{-1/4}\approx 1.087g^{-1/4}$, still too large by $\sim 6\%$.

When calculating Z_2, the strong-coupling problem implies that the extremality condition has a solution only for small $g\ll 1$. For the two Padé approximations, however, the extremum exists for all g and the resulting partition functions $Z_2^{\text{Padé}}$ approach the exact ones in a similar way as Z_1 (see fig. 1), except that they do so from above with an error which slowly increases to the asymptotic values 8% and 6%, respectively. Since they do not improve Z_1, we do not plot them.

Obviously, as long as only the g^2 correction is known, the situation is quite unsatisfactory. This leads us to searching for a better improvement scheme which contains reliable information on the strong-coupling limit from the beginning.

6. The following improvement scheme is greatly superior to the previous one. It requires the evaluation of only a few correlation functions and yields, for the anharmonic oscillator, extremely good approximations to all excitation energies for all g including the strong-coupling limit. We split the action $\mathscr{A}^{x_0}$ in (17)–(19) into the local trial action $\mathscr{A}_{\Omega}^{x_0}$ of (5) plus an interaction $\mathscr{A}_{\text{int}}^{x_0}=\mathscr{A}^{x_0}-\mathscr{A}_{\Omega}^{x_0}$ and expand the exponential $\exp(-\mathscr{A}_{\text{int}}^{x_0}/\hbar)$ into a power series. Calculating the expectations within the trial partition function $Z_{\Omega}^{x_0}$ yields an expansion

$$\exp(-\mathscr{A}_0/\hbar)Z_{\Omega}^{x_0}\left(1-\frac{1}{\hbar}\langle\mathscr{A}_{\text{int}}^{x_0}\rangle_{\Omega}^{x_0}+\frac{1}{2\hbar^2}\langle\mathscr{A}_{\text{int}}^{x_0\,2}\rangle_{\Omega}^{x_0}-\frac{1}{6\hbar^3}\langle\mathscr{A}_{\text{int}}^{x_0\,3}\rangle_{\Omega}^{x_0}+\ldots\right). \tag{47}$$

This can be rewritten as an exponential function of a rearranged series which, when truncated after the cubic terms in $\mathscr{A}_{\text{int}}^{x_0}$, reads

$$\exp(-\beta W_3^{x_0}) \equiv \exp\left(-\beta V(x_0)-\beta V_{\Omega}^{x_0}-\frac{1}{\hbar}\langle\mathscr{A}_{\text{int}}^{x_0}\rangle_{\Omega}^{x_0}+\frac{1}{2\hbar^2}\langle\mathscr{A}_{\text{int}}^{x_0\,2}\rangle_{\Omega,\text{c}}^{x_0}-\frac{1}{6\hbar^3}\langle\mathscr{A}_{\text{int}}^{x_0\,3}\rangle_{\Omega,\text{c}}^{x_0}\right), \tag{48}$$

where the subscript c defines the connected correlation functions via the cumulant expansion

$$\begin{aligned}
&\langle\mathscr{A}_{\text{int}}^{x_0\,2}\rangle_{\Omega,\text{c}}^{x_0} \equiv \langle\mathscr{A}_{\text{int}}^{x_0\,2}\rangle_{\Omega}^{x_0} - \langle\mathscr{A}_{\text{int}}^{x_0}\rangle_{\Omega}^{x_0\,2},\\
&\langle\mathscr{A}_{\text{int}}^{x_0\,3}\rangle_{\Omega,\text{c}}^{x_0} \equiv \langle\mathscr{A}_{\text{int}}^{x_0 3}\rangle_{\Omega}^{x_0} - 3\langle\mathscr{A}_{\text{int}}^{x_0\,2}\rangle_{\Omega}^{x_0}\langle\mathscr{A}_{\text{int}}^{x_0}\rangle_{\Omega}^{x_0} + 2\langle\mathscr{A}_{\text{int}}^{x_0}\rangle_{\Omega}^{x_0\,3},
\end{aligned} \tag{49}$$

etc. We may carry the expansion further, but for many purposes and in this note we shall go only this far. The approximate local free energy of the system is obtained by extremizing $W_3^{x_0}$ defined by (49) with respect to the trial frequency Ω. The original Feynman–Kleinert approximation corresponds, of course, to stopping after the first expectation of $\mathscr{A}_{\text{int}}^{x_0}$.

7. To see the greatly improved accuracy brought about by the new terms consider first the partition function

Table 1
The new approximation Z_3 for the model partition function (33) as compared with the exact one Z_{ex}, the Feynman–Kleinert approximation Z_1, and the lower-order approximation Z_2.

g'	Z_{ex}	Z_1	Z_3	Z_2
1	0.772052178	0.759099639	0.771784848	0.779618732
2	0.697727989	0.682058752	0.697379209	0.707793821
3	0.652511915	0.635812008	0.652129205	0.663692090
4	0.620282560	0.603115125	0.619882812	0.632059224
5	0.595411433	0.578026028	0.595002455	0.607536290
6	0.575265822	0.557790484	0.574851763	0.587602248
7	0.558403061	0.540909512	0.557986336	0.570868994
8	0.543948145	0.526478854	0.543530246	0.556491231
9	0.531331175	0.513912161	0.530913086	0.543916527
10	0.520160764	0.502808246	0.519743112	0.532764372

Table 2
The new approximation E_3^0 for the ground state energy of the anharmonic oscillator (in units $\hbar\omega$) for various couplings g as compared with the exact one E_{ex}^0, the Feynman–Kleinert approximation E_1^0, and the lower order approximation E_2^0.

$\frac{1}{4}g'$	E_{ex}^0	E_1^0	E_3^0	E_2^0
0.1	0.559146	0.560307371	0.559154219	0.558926659
0.2	0.602405	0.604900748	0.602430628	0.601789378
0.3	0.637992	0.641629862	0.638035761	0.636984919
0.4	0.668773	0.673394715	0.668834137	0.667405766
0.5	0.696176	0.701661643	0.696253638	0.694480729
0.6	0.721039	0.727295668	0.721131779	0.719043542
0.7	0.743904	0.750857818	0.744010403	0.741631780
0.8	0.765144	0.772736359	0.765263715	0.762616228
0.9	0.785032	0.793213066	0.785163496	0.782265430
1	0.803771	0.812500000	0.803914055	0.800781250
10	1.50497	1.53125000	1.50549935	1.49462891
50	2.49971	2.54758040	2.50070646	2.48038428
100	3.13138	3.19244404	3.13265657	3.10661623
500	5.31989	5.42575605	5.32225950	5.27671970
1000	6.69422	6.82795331	6.69722906	6.63962245

of the simple integral (33). Then we can drop the locality label x_0 and the "interaction" is $\mathscr{A}_{int}=\frac{1}{4}\beta g(rx^2+x^4)$ with $r=2(\omega^2-\Omega^2)/g$. The correlation functions are simply

$$\langle \mathscr{A}_{int}\rangle_\Omega=\tfrac{1}{4}g(3a^4+ra^2)\,,\qquad \langle \mathscr{A}_{int}^2\rangle_{\Omega,c}=g^2(6a^8+\tfrac{3}{2}a^6r+\tfrac{1}{8}a^4r^2)\,,$$
$$\langle \mathscr{A}_{int}^3\rangle_{\Omega,c}=\tfrac{1}{8}g^3(1188a^{12}+288a^{10}r+27a^8r^2+a^6r^3)\,, \tag{50}$$

with $a^2=1/\beta\Omega^2$. The resulting approximation $Z_3=\exp(-\beta W_3)$ is shown in fig. 1. The curve lies so closely underneath the exact curve that it is impossible to distinguish the two without magnification. We therefore state the values in table 1. The error is everywhere less than 0.1% amounting to an improvement in accuracy of about a factor 40 with respect to the Feynman–Kleinert approximation.

Note that it is necessary to go to Z_3 to get a substantial improvement over the Feynman–Kleinert approximation Z_1. If we were to stop the expansion in (49) after the quadratic terms there would be no extremum in Ω. The reason is the alternating sign of any additional expectations in (49) which causes the trial energy of order n to diverge to $(-1)^{n-1}\times\infty$ for $\Omega\to 0$. Since it goes to positive infinity for large Ω, only the odd orders

Table 3
The new approximation E_3^g for the excited energy of the anharmonic oscillator (in units $\hbar\omega$) at various couplings g in comparison with the exact one E_{ex}^g, the Feynman–Kleinert approximation E_1^g, and the lower order approximation E_2^g.

$\frac{1}{4}g'$	E_{ex}^g	E_1^g	E_3^g	E_2^g
0.1	13.3790	13.3235257	13.3847643	13.3766211
0.2	15.8222	15.7327929	15.8275802	15.8135994
0.3	17.6224	17.5099190	17.6281810	17.6099785
0.4	19.0889	18.9591071	19.0958388	19.0742800
0.5	20.3452	20.2009502	20.3531080	20.3287326
0.6	21.4542	21.2974258	21.4629384	21.4361207
0.7	22.4530	22.2851972	22.4625543	22.4335694
0.8	23.3658	23.1879959	23.3760415	23.3451009
0.9	24.2091	24.0221820	24.2199988	24.1872711
1	24.9950	24.7995745	25.0064145	24.9720376
10	51.9865	51.5221384	51.9986710	51.9301030
50	88.3143	87.5058600	88.3500454	88.2154879
100	111.128	110.105819	111.173183	111.002842
500	189.756	188.001018	189.833415	189.540577
1000	239.012	236.799221	239.109584	238.740320

have minima. The even approximations can, however, serve to slightly improve the Feynman–Kleinert by evaluating then at the extremal Ω of the lower odd approximation, as illustrated in the last column of table 1.

8. Let us finally illustrate the quality of the new approximation for the path integral of the anharmonic oscillator. For simplicity we consider only the worst possible case of a vanishing temperature. Then x_0 is equal to zero and can be dropped in all equations, the value of W_3 at x_0 giving an approximation E_3^0 for the ground state energy. The correlation functions (50) of the interaction entering into $W_3^{x_0}$ of (49) become [#3]

$$\langle \mathscr{A}_{\rm int} \rangle_\Omega = \tfrac{1}{4}\hbar\beta g(3a^4+ra^2)\,, \qquad \langle \mathscr{A}_{\rm int}^2 \rangle_{\Omega,c} = \hbar\beta\times 2g^2(\tfrac{21}{8}a^8+\tfrac{3}{4}a^6r+\tfrac{1}{16}a^4r^2)/\hbar\Omega\,,$$
$$\langle \mathscr{A}_{\rm int}^2 \rangle_{\Omega,c} = \hbar\beta\times 6g^3(\tfrac{333}{16}a^{12}+\tfrac{105}{16}a^{10}r+\tfrac{3}{4}a^8r^2+\tfrac{1}{32}a^6r^3)/\hbar^2\Omega^2\,. \qquad (51)$$

Minimization of W_3 with respect to Ω gives the results shown in table 2. The gain in accuracy over the Feynman–Kleinert approximation is also here considerable (about a factor 40). The error is now less than 0.1%. Also shown are the numbers for the even approximation W_2 evaluated at the extremal Ω values of W_1. A full discussion of W_3 for all temperatures will be given elsewhere.

In the two examples the new approximate energies always lie above the true ones (a fact which is not true for the even approximations such as W_2). We therefore conjecture that it may be possible to prove an inequality for all odd approximations W_3, W_5, ... generalizing and sharpening the Jensen–Peierls inequality.

With the approximation being so successful we may apply it to the path integral projected into a fixed excited state of the trial oscillator. The excited energies are given by the projections of the expectations contained in W_3 to a given n. The energy shifts with respect to $E_0^n=\hbar\Omega(n+\frac{1}{2})$ are then given by the well-known Rayleigh–Schrödinger formula associated with the perturbation potential $\Delta V=\frac{1}{2}(\omega^2-\Omega^2)x^2+\frac{1}{4}gx^4$. Up to this order it reads

$$\Delta E^n=\Delta E_1^n+\Delta E_2^n+\Delta E_3^n=\Delta V_{nn}-\sum_{m\neq n}\frac{\Delta V_{nm}\Delta V_{mn}}{E_m-E_n}+\sum_{m\neq n}\sum_{k\neq n}\frac{\Delta V_{nm}\Delta V_{mk}\Delta V_{kn}}{(E_m-E_n)(E_k-E_n)}-\Delta V_{nn}\sum_{m\neq n}\frac{\Delta V_{nm}\Delta V_{mn}}{(E_m-E_n)^2}\,. \qquad (52)$$

[#3] The r^n terms are found from those with no r by replacing in them Ω by $\sqrt{\Omega^2+gr/2M}$ and expanding everything in powers of r up to r^3.

After some algebra we find [7]

$$\Delta E_1^n = \tfrac{1}{4}g[3(2n^2+2n+1)a^4+r(2n+1)a^2] ,$$

$$\Delta E_2^n = -\tfrac{1}{8}g^2[(34n^3+51n^2+59n+21)a^8+\tfrac{3}{4}(2n^2+2n+1)a^6r+\tfrac{1}{16}(2n+1)a^4r^2]/\hbar\Omega ,$$

$$\Delta E_3^n = g^3[\tfrac{3}{16}(125n^4+250n^3+472n^2+347n+111)a^{12}+\tfrac{5}{16}(34n^3+51n^2+59n+21)a^{10}r$$
$$+\tfrac{3}{4}(2n^2+2n+1)a^8r^2+\tfrac{1}{32}(2n+1)a^6r^3]/\hbar^2\Omega^2 , \qquad (53)$$

which for $n=0$ reduce to (53), apart from a factor $\hbar\beta$. Extremization gives for all n energies which lie only very little above the true ones. This is illustrated in table 3 for $n=8$ (compare with the energy table in ref. [1]). A sum over the Boltzmann factors associated with these energies yields, of course, an extremely good approximation to the partition function.

It will be interesting to see how well the particle distributions can be reproduced by applying the same approximation to the density matrices.

9. We have given two schemes for a systematic improvement scheme to the Feynman–Kleinert approximation to path integrals. The first is based on a local version of the well-known loop expansion of the effective action of the second type. The second uses a natural expansion of the partition function in powers of the trial interactions. The first method is beset with the typical problems of factorial growth of the loop diagrams. These can be overcome only by appropriate resummation techniques. A Borel resummation would be best, but a Padé approximation is seen to yield reasonable results.

The second method is extremely accurate and promises to be successful also in quantum field theories.

In a forthcoming paper we shall extend the variational principle to tunneling processes and obtain a greatly improved control over perturbation coefficients to all orders of the coupling constant [6].

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