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Improving the variational approach to path integrals [★]

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We improve the Feynman–Kleinert variational approach to euclidean path integrals rendering it much more powerful in the low-temperature regime. The new power is illustrated by an application to the anharmonic oscillator with a potential $V(x) = \frac{1}{2}m^2x^2 + \frac{1}{4}gx^4$, where it yields not only a better approximation to the low-temperature part of the partition function but delivers, in addititition, all bound-state energies uniformly well for any principal quantum number n and coupling constant g.

1. Some time ago, Feynman and Kleinert [1] [#1] [3] have considerably improved a crude variational approach to euclidean path integrals developed earlier by Feynman in his textbook on statistical mechanics [4]. (A similar improvement was given by Giacetti and Tognetti [5].) This made it possible to calculate quite accurately the *effective classical potential* [#2] of a quantum mechanical system at all temperatures by means of a single numerical integration. This quantity contains information on particle distributions [6] and correlation functions [3,7]. The method has been applied to a variety of more complicated physical systems, most recently with success to anharmonic quantum chains [8] and quantum crystals [9]. It also has important applications to tunneling processes [10].

The purpose of this note is to present an essential improvement to this approach in the low temperature regime. As an illustration of the new power we calculate with great accuracy the energies of all excited states of the anharmonic oscillator for small and large couplings and any principal quantum number.

2. The Feynman–Kleinert approach is based on the following observation: 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,

$$Z = \int_{-\infty}^{\infty} \mathrm{d}x_0 \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar} \exp\left[-\beta\left(\frac{p^2}{2M} + V_{\mathrm{eff,cl}}(x_0)\right)\right] = \int_{-\infty}^{\infty} \frac{\mathrm{d}x_0}{\sqrt{2\pi\hbar^2\beta/M}} \exp[-\beta V_{\mathrm{eff,cl}}(x_0)] \tag{1}$$

with $\beta \equiv 1/k_B T$. The variable of integration x_0 coincides with the time-averaged position $\bar{x} \equiv (1/\hbar\beta)\int_0^{\hbar\beta}\mathrm{d}\tau\, x(\tau)$

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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 ref. [2].

[#2] This is not to be confused with the standard *effective potential* of quantum field theory whose extremum represents the fully fluctuating theory and whose functional derivatives are the complete vertex functions. The effective classical potential, on the other hand, does not yet contain the purely thermal fluctuation which are taken care of by the integral (1).

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of the fluctuating path. The function $V_{\mathrm{eff,cl}}(x_0)$ appearing in the Boltzmann factor is called the *effective classical potential.* It has the obvious path integral representation

$$\exp[-\beta V_{\mathrm{eff,cl}}(x_0)] \equiv \int \mathcal{D}x\, \tilde{\delta}(\bar{x}-x_0)\exp(-\mathcal{A}/\hbar)\,, \tag{2}$$

where $\mathcal{A}$ is the euclidean action

$$\mathcal{A} = \int_0^{\hbar\beta} \mathrm{d}\tau\,[\tfrac{1}{2}M\dot{x}^2 + V(x(\tau))] \tag{3}$$

and $\tilde{\delta}$ the modified δ-function

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

which restricts $\bar{x}$ to the value x_0. The paths have the same values at initial and final imaginary times $\tau = 0$ and $\tau = \hbar\beta$, so that the path integral yields the quantum mechanical trace.

The usefulness of this decomposition 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 $\hbar/2\sqrt{MV''(x_{\mathrm{min}})}$ (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 $1/\beta V''(x_{\mathrm{min}})$. Thus, at larger temperatures these must be integrated out, exactly which is done in (1). At low temperatures the $\bar{x} = x_0$ integral can be evaluated in a saddle point expansion. The fluctuations $x(\tau)-\bar{x}$, on the other hand, can be treated 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 action

$$\mathcal{A}_\Omega^{x_0} = \int_0^{\hbar\beta} \mathrm{d}\tau\, M[\tfrac{1}{2}\dot{x}^2 + \tfrac{1}{2}\Omega^2(x_0)(x-x_0)^2] \tag{4}$$

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

$$Z_\Omega^{x_0} = \exp[-\beta V_\Omega^{x_0}(x_0)] \equiv \int \mathcal{D}x\,\tilde{\delta}(\bar{x}-x_0)\exp(-\mathcal{A}_\Omega^{x_0}/\hbar) = \frac{\frac{1}{2}\hbar\beta\Omega(x_0)}{\sinh[\frac{1}{2}\hbar\beta\Omega(x_0)]}\,. \tag{5}$$

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

$$Z_{\Omega(x_0)} = \frac{1}{2\sinh[\frac{1}{2}\hbar\beta\Omega(x_0)]} \tag{6}$$

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

$$\langle\ldots\rangle_\Omega^{x_0} \equiv [Z_\Omega^{x_0}]^{-1}\int \mathcal{D}x\,\tilde{\delta}(\bar{x}-x_0)\exp(-\mathcal{A}_\Omega^{x_0}/\hbar)\ldots\,. \tag{7}$$

Using (5) and (7) one can write

$$\begin{aligned}\int \mathcal{D}x\,\tilde{\delta}(\bar{x}-x_0)\exp(-\mathcal{A}/\hbar) &\equiv \int \mathcal{D}x\,\tilde{\delta}(\bar{x}-x_0)\exp(-\mathcal{A}_\Omega^{x_0}/\hbar)\exp[-(\mathcal{A}-\mathcal{A}_\Omega^{x_0})/\hbar]\\ &= \langle\exp(-\mathcal{A}/\hbar - \mathcal{A}_\Omega^{x_0}/\hbar)\rangle_\Omega^{x_0}\end{aligned} \tag{8}$$

and apply the Jensen–Peierls inequality

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

to derive the Feynman–Kleinert approximation $W_1(x_0)$ to the effective classical potential [1,3,5]

$$V_{\text{eff,cl}}(x_0) \approx W_1(x_0) \equiv V_\Omega^{x_0}(x_0) + V_{a^2}(x_0) - \tfrac{1}{2}\Omega^2(x_0) a^2(x_0) . \tag{10}$$

The last two terms are the expectations

$$\frac{1}{\beta}\langle \mathcal{A}/\hbar \rangle_\Omega^{x_0} = \langle V(x) \rangle_\Omega^{x_0} = V_{a^2}(x_0) , \quad \frac{1}{\beta}\langle \mathcal{A}_\Omega^{x_0}/\hbar \rangle_\Omega^{x_0} = \tfrac{1}{2}M\Omega^2(x_0)\langle (x-x_0)^2 \rangle_\Omega^{x_0} \equiv \tfrac{1}{2}M\Omega^2(x_0) a^2(x_0) . \tag{11}$$

It is easy to see that the restricted square deviation $\langle (x-x_0)^2 \rangle_\Omega^{x_0}$ is given by

$$a^2(x_0) = \frac{\hbar}{2M\Omega(x_0)} \coth \tfrac{1}{2}\hbar\beta\Omega(x_0) - \frac{1}{M\beta\Omega^2(x_0)} . \tag{12}$$

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 is $V_{a^2}(x_0)$ obtained by a simple gaussian smearing process of width $a^2(x_0)$:

$$V_{a^2}(x_0) \equiv \int_{-\infty}^{\infty} \frac{dx_0'}{\sqrt{2\pi a^2(x_0)}} \exp[-(x_0' - x_0)^2/2a^2(x_0)]\, V(x_0') . \tag{13}$$

The best approximation is reached by minimizing the function $W_1(x_0)$ of eq. (10) with respect to $\Omega(x_0)$ which gives

$$\Omega^2(x_0) = \frac{2}{M}\frac{\partial V_{a^2}(x_0)}{\partial a^2} . \tag{14}$$

The approximate effective classical potential $W_1(x_0)$ is always slightly larger than the exact $V_{\text{eff,cl}}(x_0)$.

Eqs. (12) and (14) are solved numerically, most comfortably by iteration. The resulting approximation to the partition function

$$Z_1 = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\hbar^2\beta/M}} \exp[-\beta W_1(x_0)] \tag{15}$$

leads to a free energy $F_1 \equiv k_B T \log Z_1$ which describes the true free energy $F \equiv k_B T \log Z$ 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% [1,3]). 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, response functions to an external source, and, thus, to correlation functions.

3. The improvement to be proposed in this note comes about in the following way: First we write the integrand of the approximate partition function (15) with (10) explicitly as

$$\exp[-\beta W_1(x_0)] = Z_\Omega^{x_0} \exp\{-\beta[V_{a^2}(x_0) - \tfrac{1}{2}M\Omega^2(x_0)a^2(x_0)]\}. \tag{16}$$

Then we expand the local partition function $Z_\Omega^{x_0}$ given by (5) into its spectral content

$$Z_\Omega^{x_0} = \hbar\beta\Omega(x_0)\sum_{n=0}^{\infty}\exp[-\hbar\beta\Omega(x_0)(n+\tfrac{1}{2})]. \tag{17}$$

Since the exponent in (16) is the average of $V(x) - \frac{1}{2}M\Omega^2(x-x_0)^2$ with respect to this partition function it is suggestive to try and apply the Jensen–Peierls inequality (9) *separately* at each level n. Thus, instead of

$$\int \mathcal{D}x\,\bar{\delta}(\bar{x}-x_0)\exp(-\mathcal{A}/\hbar) \geqslant Z_\Omega^{x_0}\exp[-\beta\langle V(x) - \tfrac{1}{2}\Omega^2(x_0)(x-x_0)^2\rangle_\Omega^{x_0}], \tag{18}$$

we resolve the expectation on the left-hand side into the contributions of eigenstates of the harmonic oscillator with quantum number n and write

$$\int \mathcal{D}x\,\bar{\delta}(\bar{x}-x_0)\exp(-\mathcal{A}/\hbar) = \sum_{n=0}^{\infty}\hbar\beta\Omega(x_0)\exp[-\hbar\beta\Omega(x_0)(n+\tfrac{1}{2})]\langle\langle n|\exp[-(\mathcal{A}/\hbar - \mathcal{A}_\Omega^{x_0}/\hbar)]|n\rangle\rangle_\Omega^{x_0}, \tag{19}$$

where the averages $\langle\langle n|\dots|n\rangle\rangle_\Omega^{x_0}$ are to be defined precisely below in section 5. At this point we appeal to their intuitive meaning and present what we expect to happen, postponing its verification. Applying the Jensen–Peierls inequality to each term in the sum gives

$$\int \mathcal{D}x\,\bar{\delta}(\bar{x}-x_0)\exp(-\mathcal{A}/\hbar)$$
$$\geqslant \sum_{n=0}^{\infty}\hbar\beta\Omega(x_0)\exp[-\hbar\beta\Omega(x_0)(n+\tfrac{1}{2})]\exp[-\beta\langle\langle n|V(x) - \tfrac{1}{2}\Omega^2(x_0)(x-x_0)^2|n\rangle\rangle_\Omega^{x_0}]. \tag{20}$$

The exponent contains now the contribution to the expectation (11) of the state of principal quantum number n. We now separate, as in (12), all restricted expectations into a contribution from the ordinary unrestricted quantum mechanical fluctuations and the fluctuations of $\bar{x}$. All unrestricted expectations are then resolved into their spectral content. For $a^2(x_0)$ the separation is by (12)

$$a^2(x_0) \equiv x_2(x_0) - \frac{1}{M\hbar\beta\Omega^2(x_0)} \tag{21}$$

and the spectral decomposition of the first term is

$$x_2 = (Z_{\Omega(x_0)})^{-1}\sum_{n=0}^{\infty}\exp[-\hbar\beta\Omega(x_0)(n+\tfrac{1}{2})]\frac{\hbar}{M\Omega(x_0)}(n+\tfrac{1}{2}). \tag{22}$$

Thus, for any given value of n, we replace $a^2(x_0)$ is by its spectral content:

$$a^2(x_0) \to a_n^2(x_0) \equiv x_{2,n} - \frac{1}{M\beta\Omega^2(x_0)} \tag{23}$$

with

$$x_{2,n} \equiv \frac{\hbar}{M\Omega(x_0)}(n + \tfrac{1}{2}) . \tag{24}$$

For polynomial interactions, the smeared potential will contain increasing powers of $a^2(x_0)$ [each term x^{2n} in $V(x)$ is being smeared out to a sum $\sum_{l=0}^{n}\binom{2n}{2l}x_0^{2(n-l)}(2l-1)!!a^{2l}(x_0)$]. We express the $a^{2l}(x_0)$'s via (21) in terms of powers $x_2^k(x_0)$ and observe that these have the spectral decompositions

$$(2k-1)!!x_2^k(x_0) = (Z_{\Omega(x_0)})^{-1}\sum_{n=0}^{\infty}\exp[-\hbar\beta\Omega(n+\tfrac{1}{2})]\frac{\hbar^k}{[M\Omega(x_0)]^k}n_{2k} , \tag{25}$$

where n_{2k} are the expectations of $[M\beta\Omega^2(x_0)(x-x_0)^2]^k$ in the states $|n\rangle$ (i.e., the diagonal matrix elements of the creation and annihilation operators $[(a^\dagger + a)/\sqrt{2}]^{2k}$ between states $(a^\dagger)^n|0\rangle/\sqrt{n!}$):

$$n_2 = (n+\tfrac{1}{2}) , \quad n_4 = \tfrac{3}{2}(n^2+n+\tfrac{1}{2}) , \quad n_6 = \tfrac{5}{4}(2n^3+3n^2+4n+\tfrac{3}{2}) ,$$
$$n_8 = \tfrac{1}{16}(70n^4+140n^3+344n^2+280n+105) , \quad \ldots . \tag{26}$$

With these rules, $3a^4(x_0)$ is to be replaced by

$$3a^4(x_0) \to \frac{n_4\hbar^2}{[M\Omega(x_0)]^2} - \frac{n_2\hbar}{M\Omega(x_0)}\frac{6}{M\beta\Omega^2(x_0)} + \frac{3}{[M\beta\Omega^2(x_0)]^3} . \tag{27}$$

Expanding $V_{a^2}(x_0)$ in powers of $a^2(x_0)$ and treating each expansion term in this way yields the spectral content $V_{a^2,n}(x_0)$. Thus, we obtain an approximation $\tilde{W}_2(x_0)$ to the effective classical potential $V_{\text{eff,cl}}(x_0)$ as follows:

$$\exp[-\beta\tilde{W}_2(x_0)] \equiv \max_{\Omega(x_0)}\sum_{n=0}^{\infty}\hbar\beta\Omega(x_0)\exp(-\beta\{\hbar\Omega(x_0)(n+\tfrac{1}{2}) + [V_{a^2,n}(x_0) - \tfrac{1}{2}M\Omega^2(x_0)a_n^2(x_0)]\}) . \tag{28}$$

This expression suggests now a further improvement which leads to a more powerful low-temperature approximation to be proposed in this note: Instead of finding a *single* optimal $\Omega(x_0)$ we may try and minimize *each term* in the spectral decomposition with an own $\Omega_n(x_0)$. Then we arrive at the approximation $W_2(x_0)$ defined by

$$\exp[-\beta W_2(x_0)] \equiv \sum_{n=0}^{\infty}\max_{\Omega_n(x_0)}\hbar\beta\Omega_n(x_0)\exp(-\beta\{\hbar\Omega_n(x_0)(n+\tfrac{1}{2}) + [V_{a^2,n}(x_0) - \tfrac{1}{2}M\Omega_n^2(x_0)a_n^2(x_0)]\}) . \tag{29}$$

This approximation is presently of a heuristic nature and justified only by its success to be exhibited in the next section. Hopefully, some modification of it may eventually be derived by proper analysis.

4. As a first application take an anharmonic oscillator with the potential $V(x) = \frac{1}{2}m^2x^2 + \frac{1}{4}gx^4$ and $m^2 > 0$ which becomes after smearing

$$V_{a^2}(x_0) = \tfrac{1}{2}m^2x_0^2 + \tfrac{1}{4}gx_0^4 + \tfrac{1}{2}m^2a^2 + \tfrac{3}{2}gx_0^2a^2 + \tfrac{3}{4}ga^4 . \tag{30}$$

With (23), (27) we obtain the new approximate effective classical partition function

$$Z_2 = \int_{-\infty}^{\infty}\frac{\mathrm{d}x_0}{\sqrt{2\pi\hbar^2\beta/M}}\exp[-\beta W_2(x_0)] \equiv \int_{-\infty}^{\infty}\frac{\mathrm{d}x_0}{\sqrt{2\pi\hbar^2\beta/M}}\sum_{n=0}^{\infty}\exp[-\beta W_{2,n}(x_0)] , \tag{31}$$

where $W_{2,n}(x_0)$ is the sum of three terms:

$$W_{2,n}(x_0) = W^0_{2,n}(x_0) + W^\beta_{2,n}(x_0) + V(x_0) . \tag{32}$$

In natural units with $\hbar = 1$, $k_B = 1, M = 1$, the first term reads [#3] [#4]

$$W^0_{2,n}(x_0) = \frac{1}{2}\left(\Omega_n(x_0) + \frac{m^2 + 3gx_0^2}{\Omega_n(x_0)}\right)n_2 + \frac{g}{4}\frac{n_4}{\Omega_n^2(x_0)} \tag{33}$$

and collects all parts of $W_{2,n}(x_0)$ with no explicit dependence on β, while the second term

$$W^\beta_{2,n}(x_0) = -\frac{1}{\beta}\log[\beta\Omega_n(x_0)] + \frac{1}{2\beta} - \frac{m^2 + 3gx_0^2}{2\beta\Omega_n^2(x_0)} + \frac{g}{4}\left(-\frac{6}{\beta\Omega_n^3(x_0)}n_2 + \frac{3}{\beta^2\Omega_n^4(x_0)}\right) \tag{34}$$

contains all β-dependent parts.

In the limit $g \to 0$ where the system becomes harmonic, the minima lie all at $\Omega_n(x_0) \equiv 1$ and $\exp[-\beta W_2(x_0)]$ reduces to $[\beta m/2\sinh(\frac{1}{2}\beta m)]\exp[-\beta V(x_0)]$ with the partition function Z_2 given by the classical integral

$$Z_2 = \frac{\frac{1}{2}\beta m}{\sinh(\frac{1}{2}\beta m)}\int_{-\infty}^{\infty}\frac{dx_0}{\sqrt{2\pi\beta/M}}\exp(-\tfrac{1}{2}\beta m^2 x_0^2) = \frac{1}{2\sinh(\frac{1}{2}\beta m)} ,$$

as expected. Both $W_2(x_0)$ and Z_2 are exact in this limit and coincide, of course, with the former approximations $W_1(x_0), Z_1$ of refs. [1,2].

To judge the quality of the new effective classical potential we observe that it contains precise information on the energies of all the excited states of the anharmonic oscillator. At low temperatures, we can ignore $W^\beta_{2,n}(x_0)$ and all $\Omega_n(x_0)$-dependence rests in $W^0_{2,n}(x_0)$. Its minimization gives the cubic equation

$$\Omega_n^3(x_0) - (m^2 + 3gx_0^2)\Omega_n(x_0) - g\frac{n_4}{n_2} = 0 \tag{35}$$

solved by

$$\begin{aligned}\Omega_n(x_0) &= s(x_0)\cosh\{\tfrac{1}{3}\mathrm{acosh}[c(x_0)]\} \quad \text{for}\, c(x_0) > 1 ,\\ &= -s(x_0)\sin\{\tfrac{1}{3}\arcsin[c(x_0)]\} \quad \text{for}\, c(x_0) < 1\end{aligned} \tag{36}$$

with

$$s(x_0) \equiv \frac{2}{\sqrt{3}}\sqrt{m^2 + 3gx_0^2} , \quad c \equiv \frac{4gn_4}{s^3(x_0)n_2} . \tag{37}$$

At small temperatures, the integrals over x_0 in (31) will be dominated by the minima of $W^0_{2,n}(x_0)$ which lie at $x_0 = 0$ and have the values

$$E_n^{\mathrm{app}} \equiv W^0_{2,n}(0) = \frac{1}{2}\left(\Omega_n(0) + \frac{m^2}{\Omega_n(0)}\right)n_2 + \frac{g}{4}\frac{n_4}{\Omega_n^2(0)} . \tag{38}$$

[#3] This is most easily seen by noting that $a^2(x_0)$ of (12) and $\Omega^2(x_0)$ of (14) extremize $W_1(x_0)$ *independently* in $a^2(x_0)$ and $\Omega^2(x_0)$.

[#4] Note that at $x_0 = 0$ this is the expectation of the difference of the potential and the trial potential in the states $|n\rangle$ of the harmonic oscillator.

In the saddle point approximation, the partition function is

$$Z \approx \sum_{n=0}^{\infty} \exp(-\beta E_n^{\text{app}}) . \tag{39}$$

Hence E_n^{app} are approximations to the bound-state energies E_n of the anharmonic oscillator.

For large g or large n (or both) we find $\Omega_n(0) \to (\frac{3}{2})^{1/3} g^{1/3} n^{1/3}$ and the energies E_n^{app} grow like

$$E_n^{\text{app}} \to \kappa g^{1/3} n^{4/3} , \quad \kappa = \tfrac{1}{2}(\tfrac{3}{2})^{1/3} + \tfrac{3}{8}(\tfrac{2}{3})^{2/3} \approx 0.858\,536 . \tag{40}$$

This agrees extremely well with the exact growth behaviour which can be obtained from the semiclassical expansion and has the same power law as (40) but with the slightly ($\approx$ 1%) larger proportionality factor

$$\kappa_{\text{exact}} = \left(\frac{2}{\pi}\right)^{2/3} (\tfrac{3}{4})^{4/3} \Gamma^{8/3}(\tfrac{3}{4}) \approx 0.867\,145 . \tag{41}$$

A comparison of our energies with the precise numerical solutions [11,12] of the Schrödinger equation is shown in table 1. The agreement is seen to be quite good.

For larger temperatures, the optimal values of $\Omega_n(x_0)$ obey eq. (35) with a non-vanishing right-hand side:

$$\text{RHS} = -\frac{2\Omega_n^3(x_0)}{n_2} \frac{\partial W_{2,n}^{\beta}(x_0)}{\partial \Omega_n(x_0)} \tag{42}$$

and can no longer be found analytically. For not too large temperatures (those are relatively uninteresting in this context being described by the classical limit), however, we make use of the smallness of (42) (being of the order of T) and iterate the equation, by inserting the $T \neq 0$ value of $\Omega_n(x_0)$ into (42) and solving once more the cubic equation at the non-zero value of the right-hand side. The solution is given by (36) with c in (37) replaced by

$$c \to c\left(1 - \frac{n_2}{g n_4} \times \text{RHS}\right) . \tag{43}$$

The new value is again inserted into (42), etc. The numerical values of $W_2(x_0)$ are a better approximation to the true effective classical potential than $W_1(x_0)$. As an example take $g = 40$ and $x_0 = 0$ (the worst possible place). There $(W_1(0), W_2(0))$ have for $\beta = 2, 3, 4, 5$ the values (0.514 599 465, 0.514 534 682), (0.712 742 725, 0.712 741 086) (0.843 466 072, 0.843 466 038), (0.935 482 984, 0.935 482 983), respectively. There is no improvement at $\beta = \infty$ ($T = 0$) since there $W_2(x_0) \equiv W_1(x_0)$.

The new approximation still has the defect that at high temperatures it does not properly reduce to the classical limit. The heuristic minimization in $\Omega(x_0)$ at each n has obviously destroyed this property.

5. Let us end this note by giving a simple explicit procedure for calculating the total restricted averages $\langle \dots \rangle_{\Omega}^{x_0}$ of (7) used above, as well as a precise definition and evaluation procedure of the projected restricted expectations $\langle\langle n| \dots |n\rangle\rangle_{\Omega}^{x_0}$.

First we rewrite (7) as

$$\langle \dots \rangle_{\Omega}^{x_0} \equiv (Z_{\Omega}^{x_0})^{-1} \sqrt{\frac{2\pi\hbar^2\beta}{M}} \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \frac{\mathrm{d}\lambda}{2\pi\mathrm{i}} \int \mathcal{D}x \exp[-\mathcal{A}_{\Omega}^{x_0}/\hbar + \lambda(\bar{x} - x_0)] \dots \tag{44}$$

and complete the potential part of $\mathcal{A}_{\Omega}^{x_0}$ quadratically to

Table 1

Energies of the nth excited states of the anharmonic oscillator with potential $V(x) = \frac{1}{2}x^2 + \frac{1}{4}gx^4$ for various g and n. In each entry, the top number is the precise numerical value obtained by solving the Schrödinger equation, the second is our variational result. The top entries of this table are from table 4 of ref. [11].

$\frac{1}{4}g$	E_0	E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8
0.1	0.559 146	1.769 50	3.138 62	4.628 88	6.220 30	7.899 77	9.657 84	11.4873	13.3790
	0.560 307	1.773 39	3.138 24	4.621 93	6.205 19	7.875 22	9.622 76	11.4407	13.3235
0.2	0.602 405	1.950 54	3.536 30	5.291 27	7.184 46	9.196 34	11.3132	13.5249	15.8222
	0.604 901	1.958 04	3.534 89	5.278 55	7.158 70	9.156 13	11.2573	13.4522	15.7328
0.3	0.637 992	2.094 64	3.844 78	5.796 57	7.911 75	10.1665	12.5443	15.0328	17.6224
	0.641 630	2.104 98	3.842 40	5.779 48	7.878 23	10.1151	12.473 63	14.9417	17.5099
0.4	0.668 773	2.216 93	4.102 84	6.215 59	8.511 41	10.9631	13.5520	16.2642	19.0889
	0.673 394	2.229 62	4.099 59	6.194 95	8.471 69	10.9028	13.4698	16.1588	18.9591
0.5	0.696 176	2.324 41	4.327 52	6.578 40	9.028 78	11.6487	14.4177	17.322 04	20.3452
	0.701 667	2.339 19	4.323 52	6.554 75	8.983 83	11.5809	14.3257	17.202 93	20.2009
0.6	0.721 039	2.421 02	4.528 12	6.901 05	9.487 73	12.2557	15.1832	18.2535	21.4542
	0.727 296	2.437 50	4.523 43	6.874 77	9.438 25	12.1816	15.0828	18.1256	21.2974
0.7	0.743 904	2.509 23	4.710 33	7.193 27	9.902 61	12.8039	15.8737	19.0945	22.4530
	0.750 859	2.527 29	4.705 01	7.164 64	9.849 11	12.7240	15.7658	18.9573	22.2852
0.8	0.765 144	2.590 70	4.877 93	7.461 45	10.2828	13.3057	16.5053	19.8634	23.3658
	0.772 736	2.610 21	4.872 04	7.430 71	10.2257	13.2206	16.3907	19.7179	23.1880
0.9	0.785 032	2.666 63	5.033 60	7.710 07	10.6349	13.7700	17.0894	20.5740	24.2091
	0.793 213	2.687 45	5.027 18	7.677 39	10.5744	13.6801	16.9687	20.4209	24.0221
1	0.803 771	2.737 89	5.179 29	7.942 40	10.9636	14.2031	17.6340	21.2364	24.9950
	0.812 500	2.759 94	5.172 37	7.907 93	10.9000	14.1090	17.5076	21.0763	24.7996
10	1.504 97	5.321 61	10.3471	16.0901	22.4088	29.2115	36.4369	44.0401	51.9865
	1.531 25	5.382 13	10.3244	15.9993	22.2484	28.9793	36.1301	43.6559	51.5221
50	2.499 71	8.915 10	17.4370	27.1926	37.9385	49.5164	61.8203	74.7728	88.3143
	2.547 58	9.023 38	17.3952	27.0314	37.6562	49.1094	61.2842	74.1029	87.5059
100	3.131 38	11.1873	21.9069	34.1825	47.7072	62.2812	77.7708	94.0780	111.128
	3.192 44	11.3249	21.8535	33.9779	47.3495	61.7660	77.0924	93.2307	110.106
500	5.319 89	19.0434	37.3407	58.3016	81.4012	106.297	132.760	160.622	189.756
	5.425 76	19.2811	37.2477	57.9489	80.7856	105.411	131.595	159.167	188.001
1000	6.694 22	23.9722	47.0173	73.4191	102.516	133.877	167.212	202.311	239.012
	6.827 95	24.2721	46.9000	72.9741	101.740	132.760	165.743	200.476	236.799

$$\tfrac{1}{2}M\Omega^2(x_0)\int_0^{\hbar\beta} \mathrm{d}\tau\,[x(\tau) - x_0 - x_\lambda]^2 - \hbar\frac{\lambda^2}{2M\beta\Omega^2(x_0)}$$

with $x_\lambda \equiv \lambda/M\beta\Omega^2(x_0)$. Now the path integral over $x(\tau)$ can be done *without* the restriction of $\bar{x}$ to x_0, the trial oscillator being recentered at $x_0 + x_\lambda$. Within this path integral, the expectation of $x^2(\tau)$ is calculated as follows: First we replace $x^2(\tau)$ by $[x(\tau)-x_0-x_\lambda]^2+(x_0+x_\lambda)^2$ since the odd powers in $[x(\tau)-x_0-x_\lambda]$ do not contribute. Now $[x(\tau)-x_0-x_\lambda]^2$ has the expectation x_2. Then we do the gaussian λ-integral which replaces $(x_0+x_\lambda)^2$ by $x_0^2-1/M\beta\Omega^2(x_0)$. Thus, x^2 has the expectation $x_0^2+x_2-1/M\beta\Omega^2(x_0)=x_0^2+a^2(x_0)$ which coincides with x^2 when smeared via (13). The higher powers are treated likewise with the result given after eq. (25).

We are finally ready to define and calculate the projected expectations $\langle\langle n|\dots|n\rangle\rangle_\Omega^{x_0}$ which play the principal role in the present work. We decompose the path integral over the shifted trial harmonic oscillators in (44) into its spectral content and write

$$\begin{aligned}&\langle\langle n|f(x(\tau))|n\rangle\rangle_\Omega^{x_0}\\ &\equiv (Z_\Omega^{x_0})^{-1}\sqrt{\frac{2\pi\hbar^2\beta}{M}}M\beta\Omega^2(x_0)\int_{-i\infty}^{i\infty}\frac{dx_\lambda}{2\pi i}\int_{-\infty}^{\infty}dx_a\,\psi_n(x_a-x_0-x_\lambda)f(x_a)\psi_n(x_a-x_0-x_\lambda)\\ &\quad\times\exp[-\hbar\beta\Omega(x_0)(n+\tfrac{1}{2})]\exp[\tfrac{1}{2}M\beta\Omega^2(x_0)x_\lambda^2]\end{aligned}\tag{45}$$

with the standard *real* oscillator wave functions. As an example, the expectation of $x^2(\tau)$ is found by replacing x_a^2 by $(x_a-x_0-x_\lambda)^2+(x_0+x_\lambda)^2$, since odd powers in $(x_a-x_0-x_\lambda)$ change n of one wave function by one unit and, thus, cannot contribute between states of equal n. After this we substitute $(x_a-x_0-x_\lambda)^2$ in front of $\psi_n(x_a-x_0-x_\lambda)$ by its diagonal matrix elements $x_{2,n}$. Now we integrate over dx_a and the wave functions disappear. Finally we perform the λ-integral. With the wave functions having disappeared there is no more λ-dependence except in the gaussian exponential. Hence $(x_0+x_\lambda)^2$ may be replaced by $x_0^2+x_\lambda^2$ which becomes $x_0^2-1/M\beta\Omega^2(x_0)$. Thus, we find for $x^2(\tau)$ the spectral content of the restricted expectation value

$$\langle\langle n|x^2(\tau)|n\rangle\rangle_\Omega^{x_0}=x_0^2+x_{2,n}-\frac{1}{M\beta\Omega^2(x_0)}=x_0^2+a_n^2(x_0)\,,$$

as stated above. The higher powers are treated likewise.

In the final approximation leading to $W_2(x_0)$ the expectation (45) is replaced by the same expression with $\Omega(x_0)$ replaced by $\Omega_n(x_0)$, also in each term of the sum in $Z_\Omega^{x_0}$.

6. Just as in the case of the earlier approximation $W_1(x_0)$ it is possible to apply the present scheme to systems with several minima, such as the double-well potential. Also evaluations of particle distributions and response functions to external sources present no problem. Such applications and further developments would carry us beyond the size limitations of a letter and will be discussed elsewhere.

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