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# Improving the Variational Approach to Path Integrals*

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**Abstract**

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 $V(x) = m^2x^2/2 + gx^4/4$ where it yields not only a better approximation to the low-temperature part of the partition function but delivers, in addition, all bound-state energies uniformly well for any principal quantum number $n$ and coupling constant $g$.

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1) Some time ago, Feynman and Kleinert [1, 2] have considerably improved a crude variational approach to euclidean path integrals developed earlier by Feynman in his textbook on statistical mechanics [3]. (A similar improvement was given by Giacetti and Tognetti [4]). This made it possible to calculate quite accurately the *effective classical potential* [5] 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 [2, 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

$$Z = \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{-\beta[p^2/2M + V_{eff,cl}(x_0)]} = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\hbar^2\beta/M}} e^{-\beta V_{eff,cl}(x_0)} \tag{1}$$

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

$$e^{-\beta V_{eff,cl}(x_0)} \equiv \int \mathcal{D}x\, \delta(\bar{x} - x_0) e^{-\mathcal{A}/\hbar} \tag{2}$$

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

$$\mathcal{A} = \int_0^{\hbar\beta} d\tau \left[ M\frac{\dot{x}^2}{2} + V(x(\tau)) \right] \tag{3}$$

and $\bar{\delta}$ the modified $\delta$-function

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

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 $\hbar/2\sqrt{MV''(x_{\min})}$ (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). 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

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

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

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

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

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

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.,

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

Using (5) and (7) one can write

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

and apply the Jensen-Peierls inequality

$$\langle e^{-\mathcal{A}/\hbar - \mathcal{A}_\Omega^{x_0}/\hbar} \rangle_\Omega^{x_0} \geq e^{-\langle \mathcal{A}/\hbar - \mathcal{A}_\Omega^{x_0}/\hbar \rangle_\Omega^{x_0}} \tag{9}$$

to derive the Feynman-Kleinert approximation $W_1(x_0)$ to the effective classical potential [1, 2, 4]

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

The last two terms are the expectations

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

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

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

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 $a^2(x_0)$:

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

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 $V_{eff,cl}(x_0)$.

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

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

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, 2]). 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

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

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

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

Since the exponent in (16) is the average of $V(x) - M\Omega^2(x-x_0)^2/2$ 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

$$\int \mathcal{D}x\,\delta(\bar{x}-x_0)e^{-\mathcal{A}/\hbar} \geq Z_\Omega^{x_0} e^{-\beta\langle V(x) - \frac{\Omega^2(x_0)}{2}(x-x_0)^2\rangle_\Omega^{x_0}}, \tag{18}$$

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

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

where the averages $\langle\langle n|\ldots|n\rangle\rangle_\Omega^{x_0}$ are to be defined precisely below in Sec. 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

$$\begin{aligned}\int \mathcal{D}x\,\delta(\bar{x}-x_0)e^{-\mathcal{A}/\hbar} \;\geq\; & \sum_{n=0}^{\infty} \hbar\beta\Omega(x_0)e^{-\hbar\beta\Omega(x_0)(n+1/2)} \\ & \times e^{-\beta\langle\langle n|V(x) - \frac{\Omega^2(x_0)}{2}(x-x_0)^2|n\rangle\rangle_\Omega^{x_0}}.\end{aligned} \tag{20}$$

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

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

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

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

with

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

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

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

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 $(a^\dagger)^n|0\rangle/\sqrt{n!}$):

$$n_2 = (n+1/2),$$

$$
\begin{aligned}
n_4 &= \frac{3}{2}(n^2+n+1/2), \\
n_6 &= \frac{5}{4}(2n^3+3n^2+4n+3/2), \\
n_8 &= \frac{1}{16}(70n^4+140n^3+344n^2+280n+105), \\
&\vdots
\end{aligned}
\tag{26}
$$

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 $V_{eff,cl}(x_0)$ as follows:

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

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

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

This approximation is presently of a heuristic nature and justified only by its success to be exhibites 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 $V(x) = m^2x^2/2 + gx^4/4$ and $m^2 > 0$ which becomes after smearing

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

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

$$Z_2 = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\hbar^2\beta/M}} e^{-\beta W_2(x_0)} \equiv \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi\hbar^2\beta/M}} \sum_{n=0}^{\infty} e^{-\beta W_{2,n}(x_0)} \tag{31}$$

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 [12]

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

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

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

contains all $\beta$-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 $e^{-\beta W_2(x_0)}$ reduces to $[\beta m/2\sinh(\beta m/2)]e^{-\beta V(x_0)}$ with the partition function $Z_2$ given by the classical integral

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

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 [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

$$\Omega_n(x_0) = \begin{cases} s(x_0)\cosh\left\{\frac{1}{3}\mathrm{acosh}[c(x_0)]\right\} & \text{for} \quad c(x_0) > 1 \\ -s(x_0)\sin\left\{\frac{1}{3}\arcsin[c(x_0)]\right\} & \phantom{\text{for}} \quad c(x_0) < 1 \end{cases} \tag{36}$$

with

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

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

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

In the saddle point approximation, the partition function is

$$Z \approx \sum_{n=0}^{\infty} e^{-\beta E_n^{\mathrm{app}}}. \tag{39}$$

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

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

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

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

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

A comparison of our energies with the precise numerical solutions [13] 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

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

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

$$c \to c\,(1 - \frac{n_2}{gn_4} \times \text{r.h.s.}). \tag{43}$$

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. A further improvement will be necessary to correct for this.

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

First we rewrite (7) as

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

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

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

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 $\lambda$-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

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

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 $\lambda$-integral. With the wave functions havin disappeared there is no more $\lambda$-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

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

as stated above. The higher powers are treated likewise.

In the final approximation leading to $W_2(x_0)$ the expectation (46) 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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[5] 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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[11] 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 $\Omega^2(x_0)$.

[12] 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.

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The top entries of our table are from Table 4 of the first of these papers.

Table 1: Energies of the $n$th excited states of the anharmonic oscillator with potential $V(x) = x^2/2 + gx^4/4$ 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.

| $g/4$ | $E_0$ | $E_1$ | $E_2$ | $E_3$ | $E_4$ | $E_5$ | $E_6$ | $E_7$ | $E_8$ |
|---|---|---|---|---|---|---|---|---|---|
| 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 | 11.313 2 | 13.5249 | 15.8222 |
| | 0.604 901 | 1.958 04 | 3.534 89 | 5.278 55 | 7.158 70 | 9.156 13 | 11.257 3 | 13.4522 | 15.7328 |
| 0.3 | 0.637 992 | 2.094 64 | 3.844 78 | 5.796 57 | 7.911 75 | 10.1665 | 12.544 3 | 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 | 13.552 0 | 16.2642 | 19.0889 |
| | 0.673 394 | 2.229 62 | 4.099 59 | 6.194 95 | 8.471 69 | 10.9028 | 13.469 8 | 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 | 17.32204 | 20.3452 |
| | 0.701 667 | 2.339 19 | 4.323 52 | 6.554 75 | 8.983 83 | 11.5809 | 14.3257 | 17.20293 | 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 81 | 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 |

Table 1: Energies of the $n$th excited states of the anharmonic oscillator with potential $V(x) = x^2/2 + gx^4/4$ 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.

| $g/4$ | $E_0$ | $E_1$ | $E_2$ | $E_3$ | $E_4$ | $E_5$ | $E_6$ | $E_7$ | $E_8$ |
|---|---|---|---|---|---|---|---|---|---|
| 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 |
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| | 0.604 901 | 1.958 04 | 3.534 89 | 5.278 55 | 7.158 70 | 9.156 13 | 11.257 3 | 13.4522 | 15.7328 |
| 0.3 | 0.637 992 | 2.094 64 | 3.844 78 | 5.796 57 | 7.911 75 | 10.1665 | 12.544 3 | 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 | 13.552 0 | 16.2642 | 19.0889 |
| | 0.673 394 | 2.229 62 | 4.099 59 | 6.194 95 | 8.471 69 | 10.9028 | 13.469 8 | 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 | 17.32204 | 20.3452 |
| | 0.701 667 | 2.339 19 | 4.323 52 | 6.554 75 | 8.983 83 | 11.5809 | 14.3257 | 17.20293 | 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 |