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 \( V(x) = \frac{1}{2} m^2 x^2 + \frac{1}{4} g x^4 \), 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 \( g \).

1. Some time ago, Feynman and Kleinert [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 \(^*\) 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,

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

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

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\(^*\) For a detailed appreciation of the accuracy of the Feynman–Kleinert approach in comparison with several other approximation schemes, see ref. [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).
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

$$\exp[-\beta V_{\text{eff, cl}}(x_0)] = \int D\chi \delta(\tilde{x} - x_0) \exp(-A/h),$$

(2)

where $A$ is the euclidean action

$$A = \int_0^{\hbar/\beta} d\tau \left[ \frac{1}{2} M \dot{\chi}^2 + V(x(\tau)) \right]$$

(3)

and $\delta$ the modified $\delta$-function

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

which restricts $\tilde{x}$ to the value $x_0$. The paths have the same values at initial and final imaginary times $\tau = 0$ and $\tau = \beta$, 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 $\tilde{x}$: the square deviations $[x(\tau) - \tilde{x}]^2$ 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 $\hbar^2 \sqrt{MV''}(x_{\text{min}})$ (with $x_{\text{min}}$ being the position of the potential minimum). The main thermal fluctuations take place in $\tilde{x}$ with the average square deviation of $\tilde{x}$ from the potential minimum being of the order of $1/\beta V''(x_{\text{min}})$. Thus, at larger temperatures these must be integrated out, exactly which is done in (1). At low temperatures the $\tilde{x} = x_0$ integral can be evaluated in a saddle point expansion. The fluctuations $x(\tau) - \tilde{x}$, 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

$$A_{\Omega}^{x_0} = \int_0^{\hbar/\beta} d\tau \left[ \frac{1}{2} \dot{\chi}^2 + \frac{1}{2} \Omega^2(x_0)(x - x_0)^2 \right]$$

(4)

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

$$Z_{\Omega}^{x_0} = \exp[-\beta V_{\Omega}^{x_0}(x_0)] = \int D\chi \delta(\tilde{x} - x_0) \exp(-A_{\Omega}^{x_0}/h) = \frac{1}{2} \frac{\hbar \beta \Omega(x_0)}{\sinh[1/2 \hbar \beta \Omega(x_0)]}.$$  

(5)

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

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

(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.,

$$\langle \ldots \rangle_{\Omega}^{x_0} \equiv \left[ Z_{\Omega}^{x_0} \right]^{-1} \int D\chi \delta(\tilde{x} - x_0) \exp(-A_{\Omega}^{x_0}/h) \ldots.$$  

(7)

Using (5) and (7) one can write

$$\int D\chi \delta(\tilde{x} - x_0) \exp(-A/h) \equiv \int D\chi \delta(\tilde{x} - x_0) \exp(-A_{\Omega}^{x_0}/h) \exp[-(A - A_{\Omega}^{x_0})/h]$$

$$\quad = \langle \exp(-A/h - A_{\Omega}^{x_0}/h) \rangle_{\Omega}^{x_0}$$

(8)
and apply the Jensen–Peierls inequality

$$\langle \exp(-A/\hbar - A_0/\hbar) \rangle_{\hat{A}} \geq \exp(-\langle A/\hbar - A_0/\hbar \rangle_{\hat{A}})$$

(9)

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

$$V_{\text{eff,cl}}(x_0) \approx W_1(x_0) \equiv V_{\hat{A}}(x_0) = V_{a_0}^2(x_0) + V_{a_2}(x_0) - \frac{1}{2} \Omega^2(x_0) a^2(x_0).$$

(10)

The last two terms are the expectations

$$\frac{1}{\beta} \langle A_0/\hbar \rangle_{\hat{A}} = \langle V(x) \rangle_{\hat{A}} = V_{a_0}^2(x_0), \quad \frac{1}{\beta} \langle A_0/\hbar \rangle_{\hat{A}} = \frac{1}{2} M \Omega^2(x_0) \langle (x - x_0)^2 \rangle_{\hat{A}} \equiv \frac{1}{2} M \Omega^2(x_0) a^2(x_0).$$

(11)

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

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

(12)

The first term is the well-known unrestricted average while the second term subtracts from this the square deviations of $\hat{x}$ from $x_0$. The restricted expectation of the potential is $V_{a_2}(x_0)$ obtained by a simple gaussian smearing process of width $a^2(x_0)$:

$$V_{a_2}(x_0) \equiv \int_{-\infty}^{\infty} \frac{dx_0'}{\sqrt{2\pi a^2(x_0)}} \exp(-\frac{(x_0' - x_0)^2}{2a^2(x_0)}) V(x_0').$$

(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

$$\Omega^2(x_0) = \frac{2}{M} \frac{\partial V_{a_2}(x_0)}{\partial a^2}.$$  

(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

$$Z_1 = \int_{-\infty}^{\infty} dx_0 \exp(-\beta W_1(x_0))$$

(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

\[ \exp[-\beta W(x)] = Z_{\Omega}^{(0)} \exp\{-\beta[V_{\text{a}}(x_0) - \frac{1}{2} M \Omega^2(x_0) a^2(x_0)]\}. \]  

Then we expand the local partition function \( Z_{\Omega}^{(0)} \) given by (5) into its spectral content

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

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

\[ \int \mathcal{D}x \delta(\tilde{x} - x_0) \exp(-\mathcal{A}/\hbar) \geq Z_{\Omega}^{(0)} \exp\{-\beta(V(x) - \frac{1}{2} \Omega^2(x_0)(x - x_0)^2)^{\mathcal{A}]_{\Omega}}^{(0)}\}, \]

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

\[ \int \mathcal{D}x \delta(\tilde{x} - x_0) \exp(-\mathcal{A}/\hbar) = \sum_{n=0}^{\infty} \hbar \beta \Omega (x_0) \exp\{-\hbar \beta \Omega (x_0) (n + \frac{1}{2})\} \langle \langle n \rangle \exp\{-\mathcal{A}/\hbar - \mathcal{A}^{(0)}_{\Omega}/\hbar \}\rangle^{\mathcal{A}]_{\Omega}}^{(0)}, \]

where the averages \( \langle \langle n \rangle \rangle^{\mathcal{A}]_{\Omega}} \) 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

\[ \int \mathcal{D}x \delta(\tilde{x} - x_0) \exp(-\mathcal{A}/\hbar) \]

\[ \geq \sum_{n=0}^{\infty} \hbar \beta \Omega (x_0) \exp\{-\hbar \beta \Omega (x_0) (n + \frac{1}{2})\} \exp\{-\beta(V(x) - \frac{1}{2} \Omega^2(x_0)(x - x_0)^2|n\rangle)^{\mathcal{A}]_{\Omega}}^{(0)}\}. \]

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 \( x \). All unrestricted expectations are then resolved into their spectral content. For \( a^2(x_0) \) the separation is by (12)

\[ a^2(x_0) \equiv x^2_2(x_0) - \frac{1}{M \hbar \beta \Omega^2(x_0)} \]  

and the spectral decomposition of the first term is

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

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

\[ a^2(x_0) \rightarrow a^2_n(x_0) \equiv x_{2n} - \frac{1}{M \hbar \beta \Omega^2(x_0)} \]

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with
\[ x_{2n} = \frac{\hbar}{M \Omega(x_0)} (n + \frac{1}{2}). \quad (24) \]

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 to a sum \( \sum_{n=0}^{\infty} \frac{2^n a_{2n}^{(n)}}!(2l-1)!(l-1)!a^{2l}(x_0) \)]. We express the \( a^{2l}(x_0) \)'s via (21) in terms of powers \( x^k(x_0) \) and observe that these have the spectral decompositions
\[
(2k - 1)! x^k(x_0) = (Z_{\Omega(x_0)})^{-1} \sum_{n=0}^{\infty} \exp[-\hbar \beta \Omega(n + \frac{1}{2})] \frac{\hbar^k}{[M \Omega(x_0)]^k} n_{2k},
\]
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 \( \{(a^\dag + a)/\sqrt{2}\}^{2k} \) between states \( (a^\dag)^n|0\rangle/\sqrt{n!} \):
\[
\begin{align*}
 n_2 &= (n + \frac{1}{2}), \quad n_4 = \frac{3}{2}(n^2 + n + \frac{1}{2}), \quad n_6 = \frac{1}{2}(2n^3 + 3n^2 + 4n + \frac{1}{2}), \\
 n_8 &= \frac{1}{16}(70n^4 + 140n^3 + 344n^2 + 280n + 105), \quad \ldots .
\end{align*}
\]
(26)

With these rules, \( 3a^4(x_0) \) is to be replaced by
\[
3a^4(x_0) \rightarrow \frac{n_4 \hbar^2}{[M \Omega(x_0)]^2} = \frac{n_2 \hbar^2}{M \Omega(x_0) M \beta \Omega^2(x_0)} + \frac{3}{[M \beta \Omega^2(x_0)]^2}.
\]
(27)

Expanding \( V_{\alpha^2}(x_0) \) in powers of \( a^2(x_0) \) and treating each expansion term in this way yields the spectral content \( V_{\alpha^2,\alpha}(x_0) \). Thus, we obtain an approximation \( \tilde{W}_2(x_0) \) to the effective classical potential \( V_{\text{eff,cl}}(x_0) \) as follows:
\[
\exp[-\beta \tilde{W}_2(x_0)] = \max_{\Omega(x_0)} \sum_{n=0}^{\infty} \exp[-\hbar \beta \Omega(x_0)(n + \frac{1}{2}) + [V_{\alpha^2}(x_0) - \frac{1}{2} M \Omega^2(x_0) a_0^2(x_0)]]).
\]
(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
\[
\exp[-\beta W_2(x_0)] = \max_{\Omega_n(x_0)} \sum_{n=0}^{\infty} \exp[-\hbar \beta \Omega_n(x_0)(n + \frac{1}{2}) + [V_{\alpha^2}(x_0) - \frac{1}{2} M \Omega_n^2(x_0) a_0^2(x_0)]].
\]
(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 \( V(x) = \frac{1}{2} m^2 x^2 + \frac{1}{4} g x^4 \) and \( m^2 > 0 \) which becomes after smearing
\[
V_{\alpha^2}(x_0) = \frac{1}{2} m^2 x_0^2 + \frac{1}{4} g x_0^4 + \frac{1}{2} m^2 a^2 + \frac{1}{2} g x_0^2 a^2 + \frac{1}{2} g a^4.
\]
(30)

With (23), (27) we obtain the new approximate effective classical partition function
\[
Z_2 = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi \hbar^2 \beta/M}} \exp[-\beta W_2(x_0)] = \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi \hbar^2 \beta/M}} \sum_{n=0}^{\infty} \exp[-\beta W_{2,n}(x_0)].
\]
(31)
where $W_{2,n}(x_0)$ is the sum of three terms:
\[
W_{2,n}(x_0) = W_{2,n}^0(x_0) + W_{2,n}^\beta(x_0) + V(x_0) .
\] (32)

In natural units with $\hbar = 1$, $k_B = 1$, $M = 1$, the first term reads \(^3\) \(^4\)
\[
W_{2,n}^0(x_0) = \frac{1}{2} \left( \Omega_n(x_0) + \frac{m^2 + 3g x_0^2}{\Omega_n(x_0)} \right) n_2 + g \frac{n_4}{4 \Omega_n^2(x_0) }.
\] (33)

and collects all parts of $W_{2,n}(x_0)$ with no explicit dependence on $\beta$, while the second term
\[
W_{2,n}^\beta(x_0) = -\frac{1}{\beta} \log[\beta \Omega_n(x_0)] + \frac{1}{2\beta} \frac{m^2 + 3g x_0^2}{2\beta \Omega_n^2(x_0)} + g \frac{6}{\beta \Omega_n^3(x_0)} n_2 + \frac{3}{\beta^2 \Omega_n^4(x_0)}
\] (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 $\exp\{-\beta W_2(x_0)\}$ 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
\[
Z_2 = \frac{\frac{1}{2} \beta m}{\sinh(\frac{1}{2} \beta m)} \int_{-\infty}^{\infty} \frac{dx_0}{\sqrt{2\pi} / M} \exp(-\frac{1}{2} \beta m^2 x_0^2) = \frac{1}{2 \sinh(\frac{1}{2} \beta m)} ,
\]
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 $W_{2,n}^\beta(x_0)$ and all $\Omega_n(x_0)$-dependence rests in $W_{2,n}^0(x_0)$. Its minimization gives the cubic equation
\[
\Omega_n^3(x_0) - (m^2 + 3g x_0^2) \Omega_n(x_0) - g \frac{n_4}{n_2} = 0
\] (35)
solved by
\[
\Omega_n(x_0) = s(x_0) \cosh\left[\frac{1}{3} \cosh^{-1}[c(x_0)]\right] \quad \text{for } c(x_0) > 1 ,
\]
\[
= -s(x_0) \sinh\left[\frac{1}{3} \sinh^{-1}[c(x_0)]\right] \quad \text{for } c(x_0) < 1
\] (36)
with
\[
s(x_0) = \frac{2}{\sqrt{3}} \sqrt{m^2 + 3g x_0^2} , \quad c = \frac{4gn_4}{s^3(x_0)n_2} .
\] (37)

At small temperatures, the integrals over $x_0$ in (31) will be dominated by the minima of $W_{2,n}^0(x_0)$ which lie at $x_0 = 0$ and have the values
\[
E_n^{\text{pp}} = W_{2,n}^0(0) = \frac{1}{2} \left( \Omega_n(0) + \frac{m^2}{\Omega_n(0)} \right) n_2 + g \frac{n_4}{4 \Omega_n^2(0)} .
\] (38)

\(^3\) This is most easily seen by noting that $a^2(x_0)$ of (12) and $\Omega^2(x_0)$ of (14) extremize $W_1(x_0)$ \textit{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

\[ Z \approx \sum_{n=0}^{\infty} \exp(-\beta E_n^{\text{app}}). \]  \hspace{1cm} (39)

Hence \( E_n^{\text{app}} \) 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 \( E_n^{\text{app}} \) grow like

\[ E_n^{\text{app}} \to \kappa g^{1/3} n^{4/3}, \quad \kappa = \frac{1}{2} (\frac{3}{2})^{1/3} + \frac{1}{6} (\frac{3}{2})^{2/3} \approx 0.858536. \]  \hspace{1cm} (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

\[ \kappa_{\text{exact}} = \left( \frac{2}{\pi} \right)^{2/3} \left( \frac{3}{2} \right)^{2/3} r^{8/3} \left( \frac{3}{2} \right) \approx 0.867145. \]  \hspace{1cm} (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:

\[ \text{RHS} = -\frac{2\Omega^2_n(x_0)}{n_2} \frac{\partial W^\beta_{2,n}(x_0)}{\partial \Omega_n(x_0)} \]  \hspace{1cm} (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

\[ c \to c \left( 1 - \frac{n_2}{g n_4} \times \text{RHS} \right). \]  \hspace{1cm} (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 \((0.514599465, 0.514534682), (0.712742.725, 0.712741086), (0.843466072, 0.843466038), (0.935482984, 0.935482983)\), 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 \( \langle \ldots \rangle_{Q_0} \) of (7) used above, as well as a precise definition and evaluation procedure of the projected restricted expectations \( \langle \langle n \ldots | n \rangle \rangle_{Q_0} \).

First we rewrite (7) as

\[ \langle \ldots \rangle_{Q_0} = (Z_{Q_0})^{-1} \int_{-\infty}^{\infty} \frac{d^\beta}{2\pi} \int D\Omega \exp\left[ -A_{Q_0}^{Q_0} / \hbar + \lambda (\overline{x} - x_0) \right] \ldots \]  \hspace{1cm} (44)

and complete the potential part of \( A_{Q_0}^{Q_0} \) quadratically to

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Table 1
Energies of the nth excited states of the anharmonic oscillator with potential $V(x) = \frac{1}{2}x^2 + \frac{1}{4}g x^4$ 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 in this table are from table 4 of ref. [11].

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<th>$\frac{1}{4}g$</th>
<th>$E_0$</th>
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<th>$E_2$</th>
<th>$E_3$</th>
<th>$E_4$</th>
<th>$E_5$</th>
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$$\frac{1}{2}M\Omega^2(x_0) \int_{0}^{\frac{\hbar}{\beta}} d\tau [x(\tau) - x_0 - x_1]^2 - \hbar \frac{\lambda}{2M\beta\Omega^2(x_0)}$$

with $x_1 \equiv \lambda/M\beta\Omega^2(x_0)$. Now the path integral over $x(\tau)$ can be done without the restriction of $x$ to $x_0$, the trial oscillator being recentered at $x_0 + x_1$. Within this path integral, the expectation of $x^2(\tau)$ is calculated as
follows: First we replace \( x^2(\tau) \) by \([x(\tau) - x_0 - x_i]^2 + (x_0 + x_j)^2\) since the odd powers in \([x(\tau) - x_0 - x_i]\) do not contribute. Now \([x(\tau) - x_0 - x_i]^2\) has the expectation \(x_2\). Then we do the gaussian \(\lambda\)-integral which replaces \((x_0 + x_i)^2\) by \(x_0^2 - 1/M\beta\Omega^2(x_0)\). Thus, \(x_2\) has the expectation \(x_0^2 + x_2 - 1/M\beta\Omega^2(x_0) = x_0^2 + a(x_0)\) 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 \(\langle n|\ldots|n\rangle_0^0\) 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

\[
\langle n|f(x(\tau))|n\rangle_0^0 = \left(\frac{Z_0^0}{\hbar}\right)^{-1} \int \frac{dx_2}{2\pi i} \int \frac{dx_3}{2\pi i} \int dx_4 \psi_n(x_4 - x_0 - x_i) f(x_4) \psi_n(x_4 - x_0 - x_i) \times \exp[-\hbar\beta\Omega(x_0)(n + \frac{1}{2})] \exp\left[\frac{1}{2}M\beta\Omega^2(x_0)x_2^2\right]
\]

with the standard real oscillator wave functions. As an example, the expectation of \(x^2(\tau)\) is found by replacing \(x_2^2\) by \((x_4 - x_0 - x_i)^2 + (x_0 + x_i)^2\), since odd powers in \((x_4 - x_0 - x_i)^2\) change \(n\) of one wave function by one unit and, thus, cannot contribute between states of equal \(n\). After this we substitute \((x_4 - x_0 - x_i)^2\) in front of \(\psi_n(x_4 - x_0 - x_i)\) by its diagonal matrix elements \(x_{2,n}\). Now we integrate over \(dx_4\) and the wave functions disappear. Finally we perform the \(\lambda\)-integral. With the wave functions having disappeared there is no more \(\lambda\)-dependence except in the gaussian exponential. Hence \((x_0 + x_i)^2\) may be replaced by \(x_0^2 + x_i^2\) 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

\[
\langle n|x^2(\tau)|n\rangle_0^0 = x_0^2 + x_{2,n} - \frac{1}{M\beta\Omega^2(x_0)} = x_0^2 + a_n(x_0),
\]

as stated above. The higher powers are treated likewise.

In the final approximation leading to \(W_1(x_0)\) 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 \(Z_0^0\).

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.

The author thanks Dr. A. M. J. Schakel and Mr. R. Goetz for several discussions.

References

1638; 
see also the review R. Giachetti, V. Tognetti, A. Cuocoli and R. Vaia, lecture presented at XXVI Karpacz School of 
Theoretical Physics (Karpacz, Poland, 1990).


