Optimized perturbation method
for the propagation in the anharmonic
oscillator potential

Anna Okopińska
Institute of Physics, Bialystok University,
Lipowa 41, 15-424 Bialystok, Poland
e-mail: okopin@fuw.edu.pl

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Abstract

The application of the optimized expansion for the quantum-mechanical
propagation in the anharmonic potential $\lambda x^4$ is discussed for real and
imaginary time. The first order results in the imaginary time formal-
ism provide approximations to the free energy and particle density
which agree well with the exact results in the whole range of temper-
atures.

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variational perturbation method, time evolution amplitude, particle density
1. The quantum mechanical Hamiltonian

$$H = \frac{p^2}{2} + \frac{m^2 x^2}{2} + \lambda x^4$$

(1)

provides the simplest representation of anharmonic effects and is widely used in solid state physics, quantum chemistry and even in paraxial optics (where the Helmholtz equation reduces to the Schrödinger equation). Although the anharmonic oscillator (AO) cannot be solved exactly, the energy spectrum, as well as the time evolution amplitude can be calculated numerically to an arbitrary accuracy. For systems with many degrees of freedom such calculation become impractically time-consuming, especially in the case of the time evolution, so that approximation methods are desirable.

A very promising and simple approximation method is generated by the optimized expansion (OE). The method has been formulated for the effective potential in quantum field theory in the space-time of arbitrary dimension \[1\]. Since the AO is equivalent to the theory of a scalar field in the space-time of one-dimension (time) with a classical action given by

$$A[x] = \int_0^T \left[ \frac{1}{2} (\dot{x}^2(t) - m^2 x^2(t)) - \lambda x^4(t) \right] dt,$$

(2)

the OE for the effective potential can be used to generate a systematic approximation scheme for the free energy of the system \[2\], in the following called the optimized expansion for the free energy (OEF). It has been shown that the lowest orders of the OEF provide good approximations \[2\] and the series converges to the exact free energy \[3\].

2. Here we generalize the method to describe local properties of the system, applying the OE to the evolution amplitude. The real time propagator can be represented by

$$\langle x_b, T | x_a, 0 \rangle = \int_{x(0) = x_a}^{x(T) = x_b} Dx e^{iA[x]},$$

(3)

where the integral is taken over the functions which begin at \(x(0) = x_a\) and end at \(x(T) = x_b\).

The most popular perturbation method is generated by expanding the propagator \(\langle x_b, T | x_a, 0 \rangle\) into a series in the coupling constant \(\lambda\) and performing the
path integrals analytically, order by order. Unfortunately the perturbation series for energy eigenvalues of the AO is asymptotic [4], keeping thus a few lowest terms in the expansion provides reasonable approximation for very small values of $\lambda$ and short propagation times $T$ only. Since the OE for the free energy shows much better convergence properties than the perturbation method, we expect also the approximations to the propagator generated in the OE to have much broader region of applicability.

The OE consists in modifying the classical action to the form

$$A^{\text{mod}}[x] = \int_0^T \left[ \frac{1}{2} \left( \dot{x}^2(t) - \omega^2 x^2(t) \right) + \epsilon \left( \frac{1}{2} (\omega^2 - m^2) x^2(t) - \lambda x^4(t) \right) \right] dt, \quad (4)$$

where the unperturbed part corresponds to the harmonic oscillator with an arbitrary frequency, $\omega$. The formal expansion parameter, $\epsilon$, has been introduced in such a way that for $\epsilon = 1$ the dependence on $\omega$ cancels and the modified action becomes equal to the classical one (2); therefore, after calculating the quantity of interest to the given order in $\epsilon$ we set $\epsilon = 1$. The exact result, obtained as a sum of an infinite series, does not depend on an arbitrary frequency, but a finite order truncation does. The advantage of the freedom can be taken to optimize the expansion: we make the $n$th-order approximant as insensitive as possible to small variation of $\omega$, choosing the value of $\omega$ which renders the approximant stationary. The optimal frequency changes from order to order, which improves convergence properties of the expansion scheme.

The OE for the time evolution can be generated by expanding the amplitude (3) into a series

$$\langle x_b, T | x_a, 0 \rangle = \int_{(x_a, 0)}^{(x_b, T)} Dx e^{i \int_0^T \frac{1}{2} \left( \dot{x}^2(t) - \omega^2 x^2(t) \right) + \epsilon \left( \frac{1}{2} (\omega^2 - m^2) x^2(t) - \lambda x^4(t) \right) dt}$$

$$= \int_{(x_a, 0)}^{(x_b, T)} Dx e^{i \int_0^T \frac{\dot{x}^2(t) - \omega^2 x^2(t)}{2} dt} \left[ 1 + i \epsilon \int_0^T \left( \omega^2 - m^2 \right) \frac{x^2(t)}{2} - \lambda x^4(t) \right] dt + O(\epsilon^2)$$

$$= \frac{\sqrt{\omega}}{\sqrt{(2 \pi) \sin \omega T}} e^{i \omega \frac{(x_b^2 + x_a^2) \cos \omega T - 2x_a x_b}{2 \sin \omega T}} \left[ 1 + i \epsilon \frac{\omega^2 - m^2}{2} \int_0^T [L^2(t) + i \mathcal{K}(t)] dt \right.$$

$$- i \epsilon \lambda \int_0^T [L^4(t) + 6i L^2(t) \mathcal{K}(t) - 3 \mathcal{K}^2(t)] dt + O(\epsilon^2) \right] \quad (5)$$
where
\[
\mathcal{L}(t) = \frac{x_a \sin \omega t + x_b \sin \omega (T - t)}{\sin \omega T} \quad \text{and} \quad \mathcal{K}(t) = \frac{\sin \omega t \sin \omega (T - t)}{\omega \sin \omega T}.
\] (6)

Representing the evolution amplitude by
\[
(x_b, T|x_a, 0) = e^{i\mathcal{W}(x_b, x_a, T)},
\] (7)
we calculate \( W \) to \( n \)-th order in \( \epsilon \) and upon setting \( \epsilon = 1 \) we optimize the approximant, \( \mathcal{W}^n(x_b, x_a, T) \), choosing \( \omega \) to fulfill
\[
\frac{\delta \mathcal{W}^n(x_a, x_b, T)}{\delta \omega} = 0.
\] (8)

The optimal choice of \( \omega \) in each order calculation, ensures that the propagator about which we expand captures essential features of the system under investigation.

The first order approximation is calculated to be given by
\[
\mathcal{W}^{(1)}(x_a, x_b, T) = \mathcal{W}^0(x_a, x_b, T) - m^2 - \frac{\omega^2}{2} \int_0^T \mathcal{L}^2(t) + i\mathcal{K}(t) dt
\]
\[
- i\omega \int_0^T \mathcal{L}^4(t) + 6i\mathcal{L}^2(t)\mathcal{K}(t) - 3\mathcal{K}^2(t) \] dt,
\] (9)
where
\[
\mathcal{W}^0(x_a, x_b, T) = \frac{1}{2} \ln \left( \frac{\omega}{2\pi i \sin \omega T} \right) + \frac{i\omega}{2} \left[ (x_a^2 + x_b^2) \cos \omega T - 2x_a x_b \right] \] \] \sin \omega T \]
\] (10)
corresponds to a harmonic oscillator with a frequency \( \omega \). The optimization condition (8) reduces to
\[
\frac{m^2 - \omega^2}{2} \int_0^T [\mathcal{L}^2(t) + i\mathcal{K}(t)] dt + \frac{1}{2} \int_0^T [\mathcal{L}^4(t) + 6i\mathcal{L}^2(t)\mathcal{K}(t) - 3\mathcal{K}^2(t)] dt = 0
\] (11)
because of
\[
\frac{\delta \mathcal{W}^0}{\delta \omega^2} = \frac{1}{2} \int_0^T [\mathcal{L}^2(t) + i\mathcal{K}(t)] dt.
\] (12)

For the harmonic oscillator with a frequency \( m \) (\( \lambda = 0 \)) the optimization condition (11) is solved by \( \omega = m \), so that the exact propagator is recovered.
in the discussed approximation. Numerical results for the AO propagator
\((\lambda \neq 0)\) can be easily obtained, calculating however the integral for wave
function evolution
\[
\psi(x_b,T) = \int (x_b,T|x_a,0)\psi(x_a,0)dx_a
\]  
(13)
the problem of highly oscillatory behavior is encountered. We decided there-
fore to discuss first the quality of the approximation for the imaginary time
propagator.

3. The imaginary time evolution amplitude
\[
(x_b,\beta|x_a,0) = e^{W(x_b,x_a,\beta)} = \int_{(x_a,0)}^{(x_b,\beta)} Dxe^{-A[x]},
\]
(14)
where \(\tau = it\) and the Euclidean action is given by
\[
A[x] = \int_0^\beta \left[ \frac{1}{2}(\dot{x}^2(\tau) + m^2x^2(\tau)) + \lambda x^4(\tau) \right] d\tau,
\]
(15)
describes equilibrium properties of the system at temperature \(\beta^{-1}\). The trace
of the imaginary time propagator defines the partition function
\[
Z_\beta = \int dx_a(x_a,\beta|x_a,0) = \int dx_a \int_{(x_a,0)}^{(x_a,\beta)} Dxe^{-A[x]} = \int dx_a e^{W(x_a,\beta)}.
\]
(16)
where \(W(x_a,\beta) = W(x_a,x_a,\beta)\) and the free energy can be obtained as
\(F_\beta = -\ln Z_\beta/\beta\). The density matrix can be expressed as
\[
\rho(x_a,x_b) = Z_\beta^{-1} \int_{(x_b,0)}^{(x_a,\beta)} Dxe^{-A[x]},
\]
(17)
and the average particle density is given by its diagonal element, \(\rho(x_a) =
\rho(x_a,x_a)\).

The OE is generated by modifying the Euclidean action to the form
\[
A^{mod}[x] = \int_0^\beta \left[ \frac{1}{2}(\dot{x}^2(\tau) + \omega^2x^2(\tau)) + \epsilon \left[(m^2 - \omega^2)x^2(\tau) + \lambda x^4(\tau)\right] \right] d\tau.
\]
(18)
The first order approximation for the imaginary time amplitude (14), obtained by an analytic continuation of the real time result (9), reads

$$W^{(1)}(x_a, x_b, \beta) = \frac{1}{2} \ln \left( \frac{\omega}{2\pi \sinh \omega \beta} \right) + \frac{\omega (x_a^2 + x_b^2) \cosh \omega \beta - 2x_a x_b}{2 \sinh \omega \beta}$$

$$- \frac{m^2 - \omega^2}{2} \int_0^\beta [L^2(t) + K(t)] dt - \lambda \int_0^\beta [L^4(t) + 6L^2(t)K(t) + 3K(t)^2] dt$$

(19)

where

$$L(t) = \frac{x_a \sinh \omega t + x_b \sinh \omega (\beta - t)}{\sinh \omega \beta}$$

and

$$K(t) = \frac{\sinh \omega t \sinh \omega (\beta - t)}{\omega \sinh \omega \beta}$$

(20)

If we calculate the free energy by expanding the subintegral expression in Eq. 16 to the given order in $\epsilon$ and performing the Gaussian integrals over $x_a$ we would obtain the series for the free energy

$$F_\beta = \frac{\omega}{2} + \frac{1}{\beta} \ln(1-e^{-\beta \omega}) + \epsilon \left[ \frac{m^2 - \omega^2}{2\omega} \left[ \frac{1}{2} + \frac{1}{e^{\beta \omega} - 1} \right] + \frac{3\lambda}{\omega^2} \left[ \frac{1}{2} + \frac{1}{e^{\beta \omega} - 1} \right]^2 \right] + O(\epsilon^2)$$

(21)

which coincides with OEF [2]. The $n$-th order approximation is obtained by requiring

$$\frac{\delta F_\beta}{\delta \omega} = 0$$

(22)

which determines $\omega$ as a function of $\beta$. The OEF provides information on global properties of the system only. To discuss local properties we proceed differently in this paper: we perform the optimized expansion for the propagator (OEP), imposing a local optimization condition

$$\frac{\delta W^{(n)}(x_a, x_b, \beta)}{\delta \omega} = 0$$

(23)

which determines $\omega$ as a function of $\beta, x_a$ and $x_b$. This approach yields approximations to the density matrix (17) in a natural way. The given order approximation to the partition function is obtained by performing integration over $x_a$ in Eq. 16 numerically and the free energy is derived afterwards.

Here we discuss approximations to the free energy and to the particle density for the one-dimensional AO, generated in the first order of the OE.
In Fig. 1 we show the results for the quartic oscillator \((m = 0, \lambda = 1)\): the free energy OEP (obtained by optimization of the imaginary time amplitude) is compared with OEF (obtained by optimization of the free energy) and the exact result calculated numerically. In the limit of high temperature both OEP and OEF approach the exact result, at zero temperature the approximations coincide also, but the accuracy is the worst. At finite temperature OEP appears slightly better than OEF, differences between approximations are not large owing to the fact that only a small region of \(x_a\) contributes to the partition function and it does not make a big difference whether the integration over \(x_a\) is performed before or after optimization. The quartic oscillator is on the border between the single well \((m^2 > 0)\) and double well \((m^2 < 0)\) AO. Since the accuracy improves for increasing \(m^2 \lambda^2 / 3\), the approximations to the free energy for \(m^2 > 0\) are better than in the case of quartic oscillator. For the double well oscillator the accuracy is worse, but even in this case both OEF and OEP are satisfactory provided the wells are not very deep. The OEP has a great advantage of yielding directly the approximations to the density matrix (17) and the particle density. The particle densities, calculated in the first order of the OE for the single well \((m^2 = 1\) and \(\lambda = 10)\) and double well potential \((m^2 = -1\) and \(\lambda = .1)\) are shown in Fig.2 and Fig.3, respectively. They are in good agreement with the exact densities calculated from the Schrödinger wave functions.

The OE for the imaginary time propagation amplitude bears some similarities with the Feynman-Kleinert (FK) variational method [5, 6], extended to a systematic variational perturbation theory for the free energy [7]. In the FK approach the exact partition function is expressed as

\[
Z_\beta = \int \frac{dx_0}{\sqrt{(2\pi \beta)}} e^{-\beta V_d(x_0, \beta)}, \tag{24}
\]

with the classical effective potential, \(V_d(x_0, \beta)\), defined by

\[
e^{-\beta V_d(x_0, \beta)} = \int Dx \sqrt{(2\pi \beta)} \delta(x_0 - \bar{x}) e^{-\mathcal{A}[x]}, \tag{25}
\]

where \(x_0 = \bar{x} = \frac{\int dx x(\tau)}{\beta}\). In the variational perturbation theory the same modified action [18] is used, but the partition function is obtained by performing numerical integration over \(x_0\) in (24) with \(V_d(x_0, \beta)\) calculated to
the given order in $\epsilon$, i.e., the OE is applied to the classical effective potential, while in our approach the partition function is expressed by $W(x_a, \beta)$ and integration over $x_a$ in (14) is performed. The free energy for the quartic oscillator obtained in the first order of the FK approach is compared in Fig.1 with our results. In the limits of high and low temperature the FK results coincide with OEP, for intermediate temperatures the former agree better with the exact free energy than the later. To any finite order in $\epsilon$ the results of the methods are different, the difference comes from the fact that $V_{cl}(x_0, \beta)$ is a function of the mean value of the coordinate, $x_0$, and $W(x_a, \beta)$ is a function of a starting point on periodic trajectory, $x_a = x_b = x(t = 0)$.

The OEP can be thus directly applied to calculate the particle density which is a function of $x_a$. In the FK approach the relation between $x_0$ and $x_a$ can be taken into account to calculate the particle density [8], but this requires an additionary numerical integration. The results of the FK method for particle densities which are shown in Fig.2 and 3 are of similar accuracy as that obtained in the OEP, the later are even better for the single well oscillator. This is remarkable since the FK approach requires two numerical integrations, while in the OEP only the integral for the partition function has to be performed numerically, which is an important advantage of our method in view of further applications to the systems with many degrees of freedom.

It is worthwhile to note that the FK method cannot be extended to the case of non-periodic trajectories in order to obtain non-diagonal terms of the density matrix and the propagation amplitude in the real time formalism. The OEP offers such a possibility in a natural way, we shall present a detailed discussion of the real time propagation in a separate paper. Both in the imaginary and in the real time formalism, the OEP gives a possibility to calculate corrections to the propagation amplitude, improving generated approximations in a systematic way. In this way the convergence properties of the approximation scheme can be estimated which is of great importance for the systems where the exact result is difficult to obtain.

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References

[1] A. Okopińska, Phys. Rev. D35 (1987) 1835.
[2] A. Okopińska, Phys. Rev. D36 (1987) 2415.
[3] A. Duncan and H. F. Jones, Phys. Rev. D47 (1993) 2560, R. Guida, K. Konishi and M. Suzuki, Ann. Phys. (N.Y.) 249 (1995) 106.
[4] C. M. Bender and T. T. Wu, Phys. Rev. 184 (1969) 1231.
[5] R. Giachetti and V. Tognetti, Phys. Rev. Lett. 55 (1985) 912, Int. Jour. Magn. Mater. 54-57 (1986) 861, Phys. Rev. B 33 (1986) 7647.
[6] R. P. Feynman and H. Kleinert, Phys. Rev. A 34 (1986) 5080.
[7] H. Kleinert, Path Integrals in Quantum Mechanics, Statistical and Polymer Physics, 2nd edition (World Scientific, Singapore, 1995);
[8] H. Kleinert, Phys. Lett. A 118 (1986) 267.
Figure captions

Figure 1. The free energy $F$ of the quartic oscillator, $(m^2 = 0, \lambda = 1)$ in the first order of the OE, obtained by optimization of the imaginary time propagator (OEP, *solid line*), and of the free energy (OEF, *dashed-dotted line*) compared with the FK approximation (*dashed line*) and the EXACT result (*dotted line*), plotted vs. the inverse temperature $\beta$.

Figure 2. The particle distribution of the single well oscillator $(m^2 = 1, \lambda = 10)$, obtained in the OE for the imaginary time propagator (OEP, *solid line*), compared with the FK approximation (*dashed line*) and the EXACT result (*dotted line*) at $\beta = .1$ and $\beta = 5$.

Figure 3. Same as in Fig.2, but for the double-well oscillator $(m^2 = -1, \lambda = .1)$ at $\beta = .25$ and $\beta = 5$. 
Figure 1

FREE ENERGY

\[ \beta \]

OEF
OEP
FK
EXACT
Figure 2

Particle Density

\( \beta = 5 \)

\( \beta = .1 \)
