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Optimized perturbation method for the propagation in the anharmonic oscillator potential

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Abstract

The optimized expansion is applied to quantum-mechanical propagation in the anharmonic potential λx^4. First-order results in the imaginary time formalism provide approximations to the free energy and particle density which agree well with the exact results in a whole range of temperatures. © 1998 Published by Elsevier Science B.V.

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The quantum mechanical anharmonic oscillator (AO) with a Hamiltonian

$$H = \frac{p^2}{2} + \frac{m^2 x^2}{2} + \lambda x^4 \tag{1}$$

is widely used as a model of interactions in solid state physics and quantum chemistry. The system cannot be solved exactly but the energy spectrum, as well as the time-evolution amplitude, can be calculated numerically to an arbitrary accuracy. For realistic systems with many degrees of freedom, however, calculation becomes impractically time-consuming and approximation methods are desirable.

A very promising and simple approximation method is generated by the optimized expansion (OE). OE has been formulated in the quantum theory of scalar field with quartic interaction in the space-time of arbitrary dimension to calculate the effective potential [1] and the free-energy density [2]. In the space-time of one-dimension (time) the field theory is equivalent to the AO with the Euclidean action given by

$$A[x] = \int_0^\beta \{\tfrac{1}{2}[\dot{x}^2(\tau) + m^2 x^2(\tau)] + \lambda x^4(\tau)\}\, d\tau, \tag{2}$$

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and the method can be used to generate a systematic approximation scheme called the optimized expansion for the free energy (OEF). It has been shown that the lowest orders of the OEF provide good approximations to the free energy [2] and the series converges to the exact result [3].

Here we generalize the method to describe local properties of the system by the application of the OE to the evolution amplitude. In the imaginary time formalism the propagator from $\tau = 0$ to $\tau = \beta$ can be expressed by the integral

$$(x_b, \beta | x_a, 0) = \mathrm{e}^{W(x_b, x_a, \beta)} = \int_{(x_a,0)}^{(x_b,\beta)} \mathrm{D}x\, \mathrm{e}^{-A[x]}, \tag{3}$$

taken over the functions which begin at $x(0) = x_a$ and end at $x(\beta) = x_b$. The most popular perturbation method gives asymptotic series for the AO energies [4], keeping thus a few lowest terms in the expansion of the propagator (3) in powers of λ provides reasonable approximations only for very small anharmonicities and short propagation times. We shall show that the OE for the propagator has a much broader region of applicability.

The OE consists of modifying the classical action to the form

$$A^{\mathrm{mod}}[x] = \int_0^\beta \{\tfrac{1}{2}[\dot{x}^2(\tau) + \omega^2 x^2(\tau)] + \epsilon[\tfrac{1}{2}(m^2 - \omega^2)x^2(\tau) + \lambda x^4(\tau)]\}\, \mathrm{d}\tau, \tag{4}$$

where the unperturbed part corresponds to the harmonic oscillator with an arbitrary frequency, ω. To obtain the evolution amplitude (3) we calculate $W(x_b, x_a, \beta)$ to the nth order in the formal expansion parameter ϵ. The given order approximation, $W^{(n)}(x_a, x_b, \beta)$ is obtained after setting $\epsilon = 1$, since only in this case does the modified action (4) become equal to the classical one (2). The exact result, obtained as a sum of an infinite approximation series cannot depend on ω, but a finite-order truncation does. The freedom of the choice of ω can be turned to advantage. We make the nth-order approximant as insensitive as possible to a small variation of the arbitrary frequency by choosing the value of ω to render the approximant stationary,

$$\frac{\partial W^{(n)}(x_a, x_b, \beta)}{\partial \omega^2} = 0. \tag{5}$$

The optimal frequency changes from order to order, which ensures that the propagator about which we expand captures the essential features of the system. One has to note that the real time-evolution amplitude can be calculated in a similar way, the results of the OE can be simply obtained by an analytic continuation of our results.

Expanding the time-evolution amplitude (3) into a series in ϵ, we have

$$\begin{aligned}(x_b, \beta | x_a, 0) &= \int_{(x_a,0)}^{(x_b,\beta)} \mathrm{D}x \exp\left(- \int_0^\beta \{\tfrac{1}{2}[\dot{x}^2(t) - \omega^2 x^2(t)] + \epsilon[\tfrac{1}{2}(\omega^2 - m^2)x^2(t) - \lambda x^4(t)]\}\, \mathrm{d}t \right) \\ &= \int_{(x_a,0)}^{(x_b,\beta)} \mathrm{D}x \exp\left(\int_0^\beta \tfrac{1}{2}[\dot{x}^2(t) - \omega^2 x^2(t)] \right) \left[1 - \epsilon \int_0^\beta \left((\omega^2 - m^2)\frac{x^2(t)}{2} - \lambda x^4(t) \right) \mathrm{d}t + \mathrm{O}(\epsilon^2) \right]\end{aligned}$$

$$= \frac{\sqrt{\omega}}{\sqrt{(2\pi \sinh \omega\beta)}} \exp\left(\frac{-\omega[(x_a^2 + x_b^2)\cosh \omega\beta - 2x_a x_b]}{2 \sin \omega\beta} \right)$$

$$\times \left(1 - \epsilon \frac{\omega^2 - m^2}{2} \int_0^\beta [L^2(t) + K(t)]\, dt - \epsilon\lambda \int_0^\beta [L^4(t) + 6L^2(t)K(t) - 3K^2(t)]\, dt + O(\epsilon^2) \right), \quad (6)$$

where

$$L(t) = \frac{x_a \sinh \omega t + x_b \sinh \omega(\beta - t)}{\sinh \omega\beta}, \qquad K(t) = \frac{\sinh \omega t \sinh \omega(\beta - t)}{\omega \sinh \omega\beta}. \quad (7)$$

The first-order approximation is given by

$$W^{(1)}(x_a, x_b, \beta) = W^{(0)}(x_a, x_b, \beta)$$

$$- \frac{m^2 - \omega^2}{2} \int_0^\beta [L^2(t) + K(t)]\, dt - \lambda \int_0^\beta [L^4(t) + 6L^2(t)K(t) + 3K^2(t)]\, dt, \quad (8)$$

where

$$W^{(0)}(x_a, x_b, \beta) = \tfrac{1}{2} \ln \left(\frac{\omega}{2\pi \sinh \omega\beta} \right) - \frac{\omega[(x_a^2 + x_b^2)\cosh \omega\beta - 2x_a x_b]}{2 \sinh \omega\beta} \quad (9)$$

corresponds to a harmonic oscillator with a frequency ω. The optimization condition (5) reduces to

$$\frac{(m^2 - \omega^2)}{2} \frac{\partial}{\partial \omega^2} \int_0^T [L^2(t) + K(t)]\, dt + \lambda \frac{\partial}{\partial \omega^2} \int_0^T [L^4(t) + 6L^2(t)K(t) - 3K^2(t)]\, dt = 0 \quad (10)$$

because of

$$\frac{\partial W^{(0)}}{\partial \omega^2} = -\tfrac{1}{2} \int_0^T [L^2(t) + K(t)]\, dt. \quad (11)$$

For the harmonic oscillator with a frequency m ($\lambda = 0$) the optimization condition (10) is solved by $\omega = m$, so that the exact propagator is recovered in the discussed approximation.

The imaginary time propagator can be used to describe equilibrium properties of the system at temperature β^{-1}. The trace of the imaginary time propagator defines the partition function

$$Z_\beta = \int dx_a (x_a, \beta | x_a, 0) = \int dx_a \int_{(x_a,0)}^{(x_a,\beta)} Dx\, e^{-A[x]} = \int dx_a\, e^{W(x_a,\beta)}, \quad (12)$$

where $W(x_a, \beta) = W(x_a, x_a, \beta)$. The free energy can be obtained as $F_\beta = -\ln Z_\beta/\beta$. The density matrix can be expressed as

$$\rho(x_a, x_b) = Z_\beta^{-1} \int_{(x_b,0)}^{(x_a,\beta)} Dx\, e^{-A[x]} \quad (13)$$

and the particle density is given by its diagonal element, $\rho(x_a) = \rho(x_a, x_a)$.

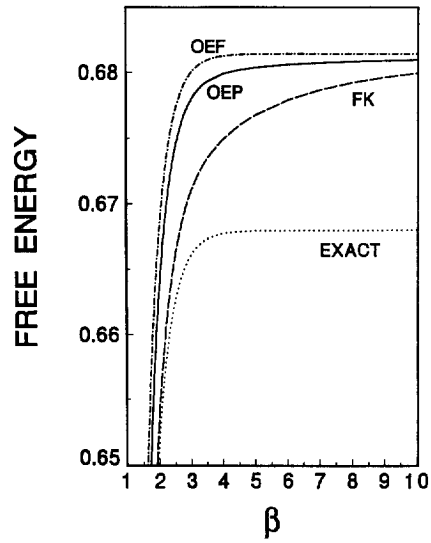

Fig. 1. The free energy F of the quartic oscillator ($m^2 = 0, \lambda = 1$), in the first order of the OE, obtained by optimization of the imaginary time propagator (OEP, solid line), and of the free energy (OEF, dashed-dotted line) compared with the FK approximation (dashed line) and the EXACT result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

If we calculate the free energy expanding the subintegral expression in Eq. (12) in powers of ϵ and performing Gaussian integrals over x_a, we would obtain the series for the free energy

$$F_\beta = \frac{\omega}{2} + \frac{1}{\beta}\ln(1 - e^{-\beta\omega}) + \epsilon\left[\frac{m^2 - \omega^2}{2\omega}\left(\frac{1}{2} + \frac{1}{e^{\beta\omega} - 1}\right) + \frac{3\lambda}{\omega^2}\left(\frac{1}{2} + \frac{1}{e^{\beta\omega} - 1}\right)^2\right] + O(\epsilon^2), \tag{14}$$

which coincides with OEF [2] when ω is determined as a stationary point of the nth-order approximation for the free energy $F_\beta^{(n)}$. The OEF provides information on global properties of the system only.

To discuss local properties we perform here the optimized expansion for the propagator (OEP), imposing a local optimization condition (5) which determines ω as a function of β, x_a and x_b. This approach directly yields approximations to the density matrix and to the particle density in a natural way. The given order approximation to the partition function (12) is obtained by performing integration over x_a numerically and the free energy is derived afterwards. Care should be taken, however, of the non-uniqueness of the solution of the local optimization condition. In the first-order calculation for the one-dimensional AO we have chosen solutions with the largest positive real part. These can be taken as starting points for solving the optimization conditions in higher orders of the OE, since the values of ω cannot differ much between orders for the expansion to converge.

In Fig. 1 we show the first-order results for the quartic oscillator ($m = 0, \lambda = 1$): the free energy OEP (obtained by optimization of the imaginary time propagator) is compared with OEF (obtained by optimization of the free energy) and with 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 a boundary between the single well ($m^2 > 0$) and double well ($m^2 < 0$) AO. The approximations to the free energy for the single-well oscillator are better than that for the quartic oscillator, the accuracy improves for increasing $m^2/\lambda^{2/3}$. 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 too deep. The particle densities, calculated in the first order

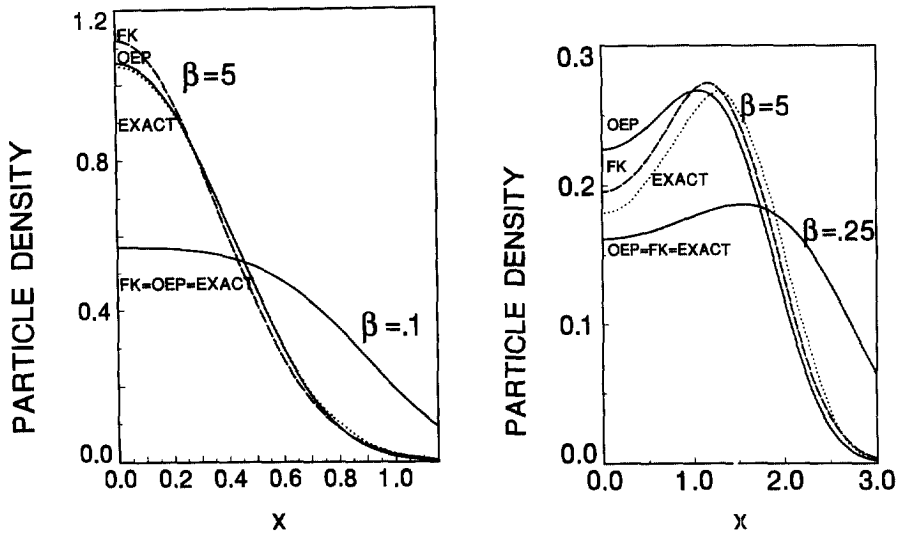

Fig. 2. The particle distribution of the single-well oscillator ($m^2 = 1$, $\lambda = 10$), obtained in the OE for the imaginary time propagator (OEP, solid line), compared with the FK approximation (dashed line) and the EXACT result (dotted line) at $\beta = 0.1$ and $\beta = 5$.

Fig. 3. Same as in Fig. 2, but for the double-well oscillator ($m^2 = -1$, $\lambda = 0.1$) at $\beta = 0.25$ and $\beta = 5$.

of the OE for the single-well ($m^2 = 1$ and $\lambda = 10$) and double-well potential ($m^2 = -1$ and $\lambda = 0.1$) are shown in Figs. 2 and 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

$$Z_\beta = \int \frac{dx_0}{\sqrt{2\pi\beta}} e^{-\beta V_{cl}(x_0,\beta)}, \tag{15}$$

with the classical effective potential, $V_{cl}(x_0, \beta)$, defined by

$$e^{-\beta V_{cl}(x_0,\beta)} = \int Dx \sqrt{2\pi\beta}\delta(x_0 - \overline{x})\, e^{-A[x]}, \tag{16}$$

where $x_0 = \overline{x} = \int d\tau\, x(\tau)/\beta$. In the variational perturbation theory the same modified action (4) is used, but the partition function is obtained by performing numerical integration over x_0 in (15) with $V_{cl}(x_0, \beta)$ calculated to the given order in ϵ, 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 (12) 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. Higher orders of both approximation schemes differ also, 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 additional numerical integration. The results of the FK method for particle densities, which are shown in Figs. 2 and 3, are of similar accuracy to 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 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 which is necessary 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 in a systematic way. In this way the convergence properties of the approximation scheme can be estimated, which is of great importance for systems where the exact result is difficult to obtain.

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References

[1] A. Okopińska, Phys. Rev. D 35 (1987) 1835.
[2] A. Okopińska, Phys. Rev. D 36 (1987) 2415.
[3] A. Duncan, H.F. Jones, Phys. Rev. D 47 (1993) 2560, R.Guida, K. Konishi, M. Suzuki, Ann. Phys. (N.Y.) 249 (1995) 106.
[4] C.M. Bender, T.T. Wu, Phys. Rev. 184 (1969) 1231.
[5] R. Giachetti, V. Tognetti, Phys. Rev. Lett. 55 (1985) 912, Int. J. Magn. Mater. 54–57 (1986) 861; Phys. Rev. B 33 (1986) 7647.
[6] R. P. Feynman, H. Kleinert, Phys. Rev. A 34 (1986) 5080.
[7] H. Kleinert, Path Integrals in Quantum Mechanics, Statistical and Polymer Physics, 2nd Ed. (World Scientific, Singapore, 1995).
[8] H. Kleinert, Phys. Lett. A 118 (1986) 267.