Optimized Expansion for Density Matrix

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Abstract. The optimized expansion is applied to the quantum mechanical evolution amplitude, providing approximations to the density matrix and to the particle density. For the anharmonic oscillator and for the electron in the hydrogen atom the first order approximations to particle density agree well with the exact results.

The optimized expansion (OE) has been formulated as a method to generate non-perturbative approximations for the effective action in quantum field theory [1]. The method is equivalent to a systematic resummation of the perturbative series and gives the Hartree-Fock-Bogolubov approximation in the leading order. Local properties of a quantum mechanical system will be studied applying the OE to the evolution amplitude [2]. The imaginary time formalism is used in order to discuss quantum statistical applications. Given the Euclidean Lagrangian of a particle

$$L[x] = \frac{\dot{x}^2}{2} + V(x), \tag{1}$$

the imaginary time evolution amplitude can be represented as a path integral

$$(x_b, \beta | x_a, 0) = e^{W(x_b, x_a, \beta)} = \int_{x(0)=x_a}^{x(\beta)=x_b} Dx\, e^{-\int_0^\beta L[x]dt} \tag{2}$$

over all functions which begin at $x(0) = x_a$ and end at $x(\beta) = x_b$. The evolution amplitude enables one to obtain the canonical ensemble partition function

$$Z_\beta = \int dx_a (x_a, \beta | x_a, 0), \tag{3}$$

the normalized density matrix

$$\rho(x_b, x_a, \beta) = Z_\beta^{-1}(x_b, 0 | (x_a, \beta). \tag{4}$$

and the particle density $\rho(x_a, \beta) = \rho(x_a, x_a, \beta)$.

The OE is generated by modifying the classical Lagrangian to the form

$$L[x] = L_\omega + \epsilon V_{int} = \frac{\dot{x}^2}{2} + \frac{\omega x^2}{2} + \epsilon \left(V(x) - \frac{\omega x^2}{2} \right), \tag{5}$$

where the harmonic oscillator with an arbitrary frequency is chosen as the unperturbed system, and calculating the quantities of interest in powers of ϵ. The series for $W(x_b, x_a, \beta)$ is given by the cumulant expansion

$$W(x_b, x_a, \beta) = W_0(x_b, x_a, \beta, \omega) - \epsilon < V_{int}(x) >_\omega$$
$$+ \frac{\epsilon}{2}(< V_{int}^2(x) >_\omega - < V_{int}(x) >_\omega < V_{int}(x) >_\omega) - ... \tag{6}$$

where

$$W_0(x_b, x_a, \beta, \omega) = \frac{1}{2} \ln \left(\frac{\omega}{2\pi \sinh \omega\beta} \right) - \frac{\omega \left[(x_a^2 + x_b^2) \cosh \omega\beta - 2x_a x_b \right]}{2 \sinh \omega\beta} \tag{7}$$

and the expectation values are calculated for the unperturbed Lagrangian

$$< ... >_\omega = \int_{x(0)=x_a}^{x(\beta)=x_b} Dx ... e^{-\int_0^\beta L_\omega[x]dt}. \tag{8}$$

The N-th order approximant, $W^{(N)}(x_b, x_a, \beta, \omega)$, is obtained by truncating the series (6) after the N-th term and setting $\epsilon = 1$, since only in this case does the modified action agree with the classical one. The exact result does not depend on arbitrary frequency, hence in each order calculation ω is chosen to make the approximant as insensitive as possible to small variation of ω, by requiring

$$\frac{\delta W^{(N)}}{\delta \omega} = 0. \tag{9}$$

This determines the optimal value of ω as a function of β, x_a and x_b, which changes from order to order, improving the convergence of the approximation scheme.

The path integrals for the expectation values in $W^{(N)}$ (6) can be represented in terms of ordinary Gaussian integrals which can be calculated numerically [3]. In the case of a particle moving in an anharmonic potential, $V(x) = \lambda x^n$, the Gaussian integrals can be easily performed, resulting in an analytic expression for $W^{(N)}$. For the Duffing's oscillator ($n = 4$) the first order approximant is given by

$$W^{(1)}(x_a, x_b, \beta) = W_0(x_a, x_b, \beta, \omega) - \frac{m^2 - \omega^2}{2} \int_0^\beta [L^2(\tau) + K(\tau)]d\tau$$
$$- \lambda \int_0^\beta [L^4(\tau) + 6L^2(\tau)K(\tau) - 3K^2(\tau)]d\tau \tag{10}$$

where

$$L(\tau) = \frac{x_a \sinh \omega\tau + x_b \sinh \omega(\beta - \tau)}{\sinh \omega\beta} \quad \text{and} \quad K(\tau) = \frac{\sinh \omega\tau \sinh \omega(\beta - \tau)}{\omega \sinh \omega\beta} \quad (11)$$

and the optimization condition (9) reduces to

$$\frac{(m^2 - \omega^2)}{2} \frac{\partial}{\partial \omega^2} \int_0^T [L^2(\tau) + K(\tau)]d\tau$$
$$+ \lambda \frac{\partial}{\partial \omega^2} \int_0^T [L^4(\tau) + 6L^2(\tau)K(\tau) - 3K^2(\tau)]d\tau = 0. \quad (12)$$

The results for particle density, calculated in the first order of the OE for the anharmonic oscillator [2] show a good agreement with the exact ones obtained by numerical integration of Schrödinger equation and approach the exact results in the limit of high temperature. The approximation to the free energy, $F_\beta = lnZ_\beta$, is also in agreement with the numerical result in the whole range of temperatures. The agreement worsens with increasing anharmonicity of the oscillator, but even in the double well case the approximation is satisfactory provided the wells are not too deep. Higher order calculation in the OE improve the approximation in a systematic way. Moreover the accuracy of the approximation in the double well case can be significantly improved by introducing an additional parameter ξ which describes the shift from the origin of the harmonic potential $\frac{\omega(x-\xi)^2}{2}$ in the unperturbed system [3].

The systems with more than one degree of freedom can be handled by a similar approach using an anisotropic harmonic oscillator with the potential $\frac{1}{2}\sum_{i,j=1}^{\infty} x_i\omega_{ij}x_j$ as the unperturbed system in the OE. In the simplest case of a particle in a radially-symmetric potential the formulas for expectation values have been obtained [3]. The first order approximation to the electron density in a Coulomb potential has been shown to agree with the exact results [3]. The application of the OE for calculating the density matrix of realistic systems will be interesting to study.

One has to note that the real time evolution amplitude can be calculated in a similar way in the OE, and the method can be used for approximate description of wave packet dynamics.

REFERENCES

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