ARTICLES

Path integrals for the quantum microcanonical ensemble

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Path integral representations for the quantum microcanonical ensemble are presented. In the quantum microcanonical ensemble, two operators are of primary interest. First, $\hat{\rho}=\delta(E-\hat{H})$ corresponds to the microcanonical density matrix and can be used to calculate expectation values. Second, $\hat{N}=\Theta(E-\hat{H})$ can give the number of states with energy $E_n<E$. We consider position matrix elements of both of these operators $\Omega(x,x',E)=\langle x'|\delta(E-\hat{H})|x\rangle$ and $\Theta(x,x',E)=\langle x'|\theta(E-\hat{H})|x\rangle$. A path integral formalism leads to exact integral representations for $\Omega(x,x',E)$ and $\Theta(x,x',E)$. We present both phase space and configuration space forms. For simple systems, such as the free particle and harmonic oscillator, exact solutions are possible. For more complicated systems, expansion schemes or numerical evaluations are required. A perturbative calculation and numerical integration results are presented for the quantum anharmonic oscillator.

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I. INTRODUCTION

The Feynman path integral, which was originally developed for the quantum propagator $K(x,x',T)=\langle x'|e^{-i\hat{H}T/\hbar}|x\rangle$, has found many applications in statistical mechanics [1,2]. In the quantum canonical ensemble, for example, the central quantity of interest is the thermal density matrix $\hat{\rho}_c=e^{-\beta\hat{H}}$. Since its position matrix elements $\langle x'|e^{-\beta\hat{H}}|x\rangle$ are isomorphic to the quantum propagator $K(x,x',T)$, path integral expressions could also be developed for it as well. Monte Carlo evaluation of this path integral has formed the basis of many quantum calculations, especially related to condensed matter systems at low temperatures [3].

For the quantum microcanonical ensemble, no such path integral expressions have been available. This fact, in part, has hampered application of the microcanonical ensemble to realistic systems. Such calculations could be of great interest for several reasons. First, since many systems at low temperatures are effectively isolated, a microcanonical approach may be more appropriate. Bose-Einstein condensates, for example, confined in a trap at very low temperatures may fall into this category. Secondly, even though the ensembles are equivalent in the thermodynamic limit, differences are expected for small, finite numbers of particles. These differences might be measurable experimentally, for example, in clusters. Thirdly, first order phase transitions are accompanied by a latent heat which gives a discontinuity in the energy at the transition. In this situation, it may be more useful to have the energy E as a control parameter rather than the temperature T [4].

In this paper, we develop exact path integral representations for the quantum microcanonical ensemble. We consider two operators $\hat{\rho}=\delta(E-\hat{H})$ and $\hat{N}=\theta(E-\hat{H})$ where E is a parameter with dimension of energy and $\hat{H}$ is the Hamiltonian operator of the system. The first operator $\hat{\rho}=\delta(E-\hat{H})$ corresponds to the microcanonical density matrix. In particular, we are interested in its position matrix elements

$$\Omega(x,x',E)=\langle x'|\delta(E-\hat{H})|x\rangle. \tag{1}$$

Notice that this quantity is the inverse Laplace transform of the Euclidian propagator $\langle x'|e^{-\hat{H}T}|x\rangle$. Knowledge of the density matrix allows calculation for statistical expectation values

$$\langle\hat{O}\rangle=\mathrm{Tr}\,\hat{O}\hat{\rho}/\mathrm{Tr}\,\hat{\rho}. \tag{2}$$

If the trace is taken in the position basis, then

$$\mathrm{Tr}\,\hat{O}\hat{\rho}=\int dx\,dx'\langle x|\hat{O}|x'\rangle\langle x'|\delta(E-\hat{H})|x\rangle, \tag{3}$$

where $\langle x'|\delta(E-\hat{H})|x\rangle$ is precisely $\Omega(x,x',E)$.

We can examine the structure of $\Omega(x,x',E)$ further by inserting a complete set of energy eigenstates $\hat{H}\psi_n=E_n\psi_n$. The following spectral form is obtained:

$$\Omega(x,x',E)=\sum_n \psi_n^*(x')\psi_n(x)\delta(E-E_n). \tag{4}$$

By taking the trace of $\Omega(x,x',E)$, we find

$$\omega(E)=\sum_n \delta(E-E_n) \tag{5}$$

which corresponds to the density of states.

The second operator we consider is $\hat{N}=\theta(E-\hat{H})$. Again, we are interested in position matrix elements

$$\Theta(x,x',E)=\langle x'|\theta(E-\hat{H})|x\rangle. \tag{6}$$

Notice that this quantity is simply related to $\Omega(x,x',E)$ since $d\Theta(E)/dE=\Omega(E)$. Taking the trace of $\Theta(x,x',E)$, we find

$$\Theta(E)=\sum_n \theta(E-E_n) \tag{7}$$

which gives the number of states with energy $E_n<E$.

This paper is organized as follows. As a preliminary calculation, $\Omega(x,x',E)$ is evaluated for the free particle. This can be done directly without recourse to path integrals. This will provide a first check for the later path integral expressions. Next, the path integral for $\Omega(x,x',E)$ is developed. Both phase space and configuration forms are presented. Similar expressions for $\Theta(x,x',E)$ follow immediately by doing an energy integral. For the case of the free particle and the harmonic oscillator, the path integrals for $\Omega(x,x',E)$ are evaluated exactly. As with the Feynman path integral, these are the only exact solutions possible. For more complicated potentials, the integrals must be evaluated approximately, either through an expansion or numerically. A perturbative calculation for the anharmonic oscillator is performed, recovering known results. Numerical evaluations are also presented. In this paper, only single particle quantum systems are considered, but generalization of these ideas to many-body systems and quantum fields is immediate.

II. FREE PARTICLE KERNELS

Before introducing path integrals, we consider the free particle directly. In this case,

$$\Omega(x,x',E)=\langle x'|\delta(E-\hat{p}^2/2m)|x\rangle, \tag{8}$$

where $\hat{H}=\hat{p}^2/2m$. Momentum eigenstates can be inserted

$$\Omega(x,x',E)=\int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}e^{ip/\hbar(x'-x)}\delta(E-p^2/2m) \tag{9}$$

and the integral evaluated to give

$$\Omega(x,x',E)=\sqrt{\frac{m}{2\pi^2\hbar^2E}}\cos\left[\frac{2}{\hbar}\sqrt{\frac{m}{2}(x'-x)^2E}\right]. \tag{10}$$

This is the exact result for the free particle. The free particle expression for $\Theta(x,x',E)$ can be found immediately by integrating with respect to E. The result is

$$\Theta(x,x',E)=\frac{1}{\pi(x'-x)}\sin\left[\frac{2}{\hbar}\sqrt{\frac{m}{2}(x'-x)^2E}\right]. \tag{11}$$

III. PATH INTEGRAL EXPRESSIONS

The path integral expression for $\Omega(x,x',E)$ for an arbitrary potential is now derived. We begin by using the integral representation for the delta function in Eq. (1)

$$\Omega(x,x',E)=\int_{-\infty}^{\infty}dz e^{iEz}\langle x'|e^{-iz\hat{H}}|x\rangle. \tag{12}$$

The matrix element $\langle x'|e^{-iz\hat{H}}|x\rangle$ inside the integral has the form of a propagator with $z=t/\hbar$. We can develop a path integral expression for it in the usual way [1,2]. First, we write $e^{-iz\hat{H}}=(e^{-iz\hat{H}\epsilon})^{N+1}$ where $\epsilon=1/(N+1)$ and is dimensionless. Notice in the usual derivation, $\epsilon=T/(N+1)$ where T is the time. Here, $z\hbar$ plays the role of the time interval which we divide into N segments of length $z\hbar\epsilon$. We insert N sets of complete position states between each product to give

$$\Omega(x,x',E)=\int dz e^{izE}\prod_{n=1}^{N}\int_{-\infty}^{\infty}dx_n\prod_{k=1}^{N+1}\langle x_k|e^{-iz\epsilon\hat{H}}|x_{k-1}\rangle, \tag{13}$$

where the fixed end points (x,x') are now labeled $x=x_o$ and $x'=x_{N+1}$. For a single particle, $\hat{H}=\hat{T}+\hat{V}$ where $\hat{T}$ and $\hat{V}$ are the kinetic and potential energy operators. The exponential $e^{-iz\epsilon\hat{H}}$ can be decomposed for small ϵ using the Trotter formula $e^{\hat{H}}=\lim_{N\to\infty}(e^{\hat{T}/N}e^{\hat{V}/N})^N$. If $\hat{T}=\hat{p}^2/2m$, and complete sets of momentum states are inserted, then

$$\langle x_k|e^{-iz\epsilon\hat{H}}|x_{k-1}\rangle=\int\frac{dp_k}{2\pi\hbar}e^{(i/\hbar)p_k(x_k-x_{k-1})}e^{-iz\epsilon H(x_k,p_k)}, \tag{14}$$

where $H(x_k,p_k)=p_k^2/2m+V(x_k)$ is the classical Hamiltonian. We find for N time slices

$$\Omega(x,x',E)=\int_{-\infty}^{\infty}dz e^{izE}\prod_{n=1}^{N}\int_{-\infty}^{\infty}dx_n\prod_{m=1}^{N+1}\int_{-\infty}^{\infty}\frac{dp_m}{2\pi\hbar}\times e^{i/\hbar\sum_{k=1}^{N+1}p_k(x_k-x_{k-1})}e^{-iz\epsilon\sum_{k=1}^{N+1}H(x_k,p_k)}, \tag{15}$$

where the summation evaluates the Hamiltonian $H(x_k,p_k)$ along a path with fixed end points (x,x') and period $z\hbar$. The z integration can be performed, and again yields a delta function:

$$\Omega(x,x',E)=\prod_{n=1}^{N}\int_{-\infty}^{\infty}dx_n\prod_{m=1}^{N+1}\int_{-\infty}^{\infty}\frac{dp_m}{2\pi\hbar}\times e^{i/\hbar\sum_{k=1}^{N+1}p_k(x_k-x_{k-1})}\times\delta\left(E-\epsilon\sum_{k=1}^{N+1}H(x_k,p_k)\right). \tag{16}$$

This is the phase space path integral for $\Omega(x,x',E)$. It becomes exact in the limit as $N\to\infty$. Since $\epsilon=1/(N+1)$, instead of the usual $\epsilon=T/(N+1)$, we have effectively set $T=1$. Thus, all paths have unit period. A path integral for $\omega(E)$, the density of states, is immediate by restricting to closed paths $x=x'=\bar{x}$ and integrating over $\bar{x}$. This corresponds to taking the trace of $\Omega(x,x',E)$

The momentum integrals can be performed exactly and give

$$\Omega(x,x',E) = \sqrt{\frac{m}{2\pi\hbar^2\epsilon}}\prod_{n=1}^{N} \times\int_{-\infty}^{\infty}\frac{dx_n}{\sqrt{2\pi\hbar^2\epsilon/m}}\frac{[E-V]^{\nu/2}}{[A_F/\hbar^2]^{\nu/2}} \times J_\nu\left(2\sqrt{\frac{A_F}{\hbar^2}(E-V)}\right)\theta(E-V), \quad (17)$$

where $\nu=(N-1)/2$, J_ν is a Bessel function of order ν, and $\theta(E-V)$ is a theta function.

$$A_F=\frac{m}{2}\epsilon\sum_{k=1}^{N+1}\frac{(x_k-x_{k-1})^2}{\epsilon^2}$$

is the free action and $V=\epsilon\Sigma_{k=1}^{N+1}V(x_k)$ is the classical potential evaluated along a given path for N time slices. Since ϵ is dimensionless, A_F and V do not have their customary units of action. V has units of energy and A_F has units of $[\hbar T]$.

This is the primary result of this paper. Equation (17) is the configuration space path integral for $\Omega(x,x',E)$. As with the phase space form, it becomes exact as $N\rightarrow\infty$. Notice that since $\Omega(x,x',E)=\langle x'|\delta(E-\hat{H})|x\rangle$ is the inverse Laplace transform of the Euclidian propagator, the path integral expressions above could have been obtained from an inverse Laplace transform of the Euclidian Feynman path integral.

A path integral expression for $\Theta(x,x',E)$ can be obtained immediately by integrating $\Omega(x,x',E)$ with respect to the energy parameter E. The configuration space result is

$$\Theta(x,x',E) = \sqrt{\frac{m}{2\pi\hbar^2\epsilon}}\prod_{n=1}^{N} \times\int_{-\infty}^{\infty}\frac{dx_n}{\sqrt{2\pi\hbar^2\epsilon/m}}\frac{[E-V]^{(\nu+1)/2}}{[A_F/\hbar^2]^{(\nu+1)/2}} \times J_{(\nu+1)}\left(2\sqrt{\frac{A_F}{\hbar^2}(E-V)}\right)\theta(E-V). \quad (18)$$

IV. FREE PARTICLE PATH INTEGRAL

As a first example, the path integral for $\Omega(x,x',E)$ is evaluated for the free particle. For the remainder of this paper, the following shorthand will be used for the path integration measure

$$\int [dx_n] = \sqrt{\frac{m}{2\pi\hbar^2\epsilon}}\prod_{n=1}^{N}\int_{-\infty}^{\infty}\frac{dx_n}{\sqrt{2\pi\hbar^2\epsilon/m}}. \quad (19)$$

We will also suppress factors of $\hbar$. The free particle ($V=0$) expression is

$$\Omega(x,x',E)=\int [dx_n]\frac{E^{\nu/2}}{A_F^{\nu/2}}J_\nu(2\sqrt{A_F E}), \quad (20)$$

where $A_F=(m/2\epsilon)\Sigma_1^{N+1}(x_k-x_{k-1})^2$ is the free particle action. A_F can be diagonalized using Fourier analysis. The resulting integrals can then be performed iteratively.

We follow a treatment which is standard for the Feynman path integral as outlined in Kleinert [2]. Each path is first decomposed

$$x(t)=x_c(t)+\delta x(t) \quad (21)$$

into a classical path (i.e., x_c obeys the classical equation of motion) plus a fluctuation piece $\delta x(t)$ about $x_c(t)$. The action breaks up into

$$A_F=A_{cl}+\frac{m}{2\epsilon}\sum_{k=1}^{N+1}(\delta x_k-\delta x_{k-1})^2, \quad (22)$$

where $A_{cl}=(m/2)(x'-x)^2$ is the classical action for a path of unit period. The path fluctuations can be Fourier analyzed using the series

$$\delta x_k(t_k)=\sum_{m=1}^{N}\sqrt{\frac{2}{N+1}}\sin(m\pi t_k)x_m,$$

where the x_m are the Fourier components. The result for the fluctuation action

$$A_{\mathrm{fl}}=\frac{m}{2}\epsilon\sum_{1}^{N+1}\Omega_m\bar{\Omega}_m x_m^2, \quad (23)$$

where

$$\Omega_m\bar{\Omega}_m=\frac{1}{\epsilon^2}\left[2-2\cos\left(\frac{\pi m}{N+1}\right)\right].$$

The Fourier transformed action is returned to the path integral, the x_m variables decouple, and the integrations can be done iteratively. The result

$$\Omega(x,x',E)=\sqrt{\frac{m}{2\pi^2 E}}\cos\left[\frac{2}{\hbar}\sqrt{\frac{m}{2}(x'-x)^2 E}\right] \quad (24)$$

agrees with the free particle solution obtained previously (10). Notice that the path integral was evaluated for finite N, but gave the continuum result. In fact, the $N=1$ path integral also gives the continuum $N=\infty$ result. This trivial N dependence is unique to the free particle as with the Feynman case.

V. HARMONIC OSCILLATOR

Next, the harmonic oscillator is considered. In this case, $V(x_k)=\frac{1}{2}m\omega_0^2x_k^2$ where m is the mass and ω_0 is the characteristic frequency. For simplicity, only the trace $\omega(s)$ is considered

$$\omega(E)=\int_{-\infty}^{\infty}d\bar{x}\,\Omega(x,x',E)|_{x=x'=\bar{x}}, \quad (25)$$

where the end points have been identified $x=x'=\bar{x}$, and the $\bar{x}$ integration implements the trace. To evaluate this quantity, we insert the path integral expression for $\Omega(x,x',E)$ in Eq. (13). An integral representation for the Bessel function is also used

$$\frac{J_\nu(2z)}{z^\nu}=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}dt\,t^{-\nu-1}e^{t-z^2/t}. \tag{26}$$

After rescaling and interchanging integrations in $\omega(E)$, we obtain

$$\omega(E)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}dt\,e^{Et}\int d\overline{x}\int [dx_n]e^{-[A_F+t^2V]}. \tag{27}$$

The path integration has the form of the trace of a Euclidian propagator. For the harmonic oscillator, the result is well known $Z=1/2\sinh[(\omega_0/2)t]$ [2]. The t integration is equivalent to an inverse Laplace transform. Assembling these results and doing the inversion yields

$$\omega(E)=\sum_{n=0}^{\infty}\frac{\nu}{E}J_\nu\left(\frac{2(N+1)E}{\hbar\omega_O}\right), \tag{28}$$

where $\nu=(2n+1)(N+1)$. This is the exact density of states for the harmonic oscillator for finite N. As $N\to\infty$, $\omega(E)$ goes over to the continuum form

$$\omega(E)=\sum_{n=0}^{\infty}\delta\left(E-\left(n+\frac{1}{2}\right)\omega_0\right) \tag{29}$$

with the harmonic oscillator spectrum $E_n=(n+\frac{1}{2})\omega_0$.

VI. ANHARMONIC OSCILLATOR: PERTURBATIVE SERIES

For more complicated potentials, the integrals must be evaluated either perturbatively or numerically. We generate a perturbation series for $\Omega(x,x',E)$, and apply it to the anharmonic oscillator with potential $V(x_k)=\frac{1}{2}m\omega_0^2x_k^2+g/4x_k^4$ where g is a coupling constant. The configuration space path integral (13) can be rewritten as

$$\Omega(x,x',E)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}dt\,e^{Et}t^{-\nu-1}\int [dx_n]e^{-(1/t)A_F-tV}, \tag{30}$$

where the integral representation for $J_\nu(z)$ has been used, the t variable rescaled. The potential can be split $V=V_0+V_{\rm int}$ where V_0 is the harmonic potential and $V_{\rm int}$ contains higher order terms. The exponential is expanded

$$\Omega(x,x',E)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}dt\,e^{Et}t^{-\nu-1}\times\int [dx_n]e^{-(1/t)A_F-tV_0}\sum_{k=0}^{\infty}\frac{(-)^kV_{\rm int}^kt^k}{k!} \tag{31}$$

and the Bessel function reconstituted to give the following perturbative series:

$$\Omega(x,x',E)=\sum_{k=0}^{\infty}\frac{(-)^k}{k!}\int [dx_n](V_{\rm int})^k\sqrt{\frac{(E-V_0)}{A_F}}^{\nu-k}\times J_{\nu-k}[2\sqrt{A_F(E-V_0)}]\theta(E-V_0). \tag{32}$$

If $V_{\rm int}$ is small, we can keep only the leading terms. Note that the $k=0$ term gives the harmonic oscillator.

We now calculate the first order correction to $\omega(E)$ for the anharmonic oscillator. The integral to evaluate is

$$\omega^{(1)}=-\int d\overline{x}\int [dx_n]V_{\rm int}(E-V_0)^{\nu-1}\times\frac{J_{\nu-1}[2\sqrt{A_F(E-V_0)}]}{\sqrt{A_F(E-V_0)}^{\nu-1}}\theta(E-V_0), \tag{33}$$

where again the end points have been identified and integrated. Using the integral for the Bessel function, and simplifying, we obtain

$$\omega^{(1)}=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}dt\,e^{Et}t^{-\nu-1}\frac{g}{4}\times\int_{-\infty}^{\infty}d\overline{xx^4}\int [dx_n]e^{-(1/t)A_F-tV_0}. \tag{34}$$

The quantity under the path integral again has the form of a propagator for a Euclidian harmonic oscillator. Its result is well known

$$\int [dx_n]e^{-(1/t)A_F-tV_0}=\left(\frac{m\omega_0t}{2\pi\sinh(\omega_0t)}\right)^{1/2}\times e^{[-m\omega_0/\sinh(\omega_0t)]2\sinh^2[(\omega_0/2)t]\overline{x^2}}. \tag{35}$$

Inserting this expression, performing the integral, and expanding the hyperbolic functions in terms of exponentials gives

$$\omega^{(1)}=-\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}dt\,e^{Et}\sum_{n=0}^{\infty}[1+2n(n+1)]\times\beta te^{-(n+1/2)\omega_0t} \tag{36}$$

where $\beta=3/16g(1/m\omega_0)^2$. We combine this quantity with the zeroth order result and perform the t integration which amounts to an inverse Laplace transform to get our final result

$$\omega(E)=\sum_{n=0}^{\infty}\delta(E-\widetilde{E}), \tag{37}$$

where $\widetilde{E}=(n+\frac{1}{2})\omega_0+[1+2n(n+1)]\beta$ for $n=0,1,2,\ldots,$ are the perturbative eigenvalues for the anharmonic oscillator. This expression agrees identically with first order results obtained through Rayleigh-Ritz perturbation theory [5].

VII. ANHARMONIC OSCILLATOR: NUMERICAL INTEGRATION

To obtain nonperturbative results, numerical evaluations will generally be needed. To illustrate this and the generality of the exact integral expression, direct numerical integration of the integrals were performed for a small number of time slices $N=2$. Notice that changing the form of the potential means only trivial adjustments to the numerical scheme.

We consider again the anharmonic oscillator, but for nonperturbative values of the coupling $g=1.0$. The results for $N=2$ are shown in Fig. 1. Because only a small number of time slices are used, only a crude estimate of the eigenvalue spectrum is obtained. The first peak occurs at $E_o^{N=2}\approx 0.7$. The current estimate for the ground state energy is $E_o\approx 0.6$ [6]. Recall that in the continuum limit, $\omega(E)$ is a series of delta function spikes. For small N, the peaks are rounded and shifted. The discrepancy between finite N and the continuum is due to using the Trotter formula for finite N.

In this paper, we have presented path integral representations for matrix elements of the number operator and density operator for the microcanonical ensemble. Previous work has focused mainly on path integral expressions for the density of states $\omega(E)$. Early work relied heavily on semiclassical expansions of the Feynman path integral [7]. More recently, Doll and Freeman have developed a Fourier path integral for $\omega(E)$ using a Hubbard-Stratonovich transformation [8]. This path integral requires integration over a set of auxiliary variables as well as the Fourier path variables. Fixed energy and Gaussian ensembles have also been discussed in the context of lattice gauge theory [9].

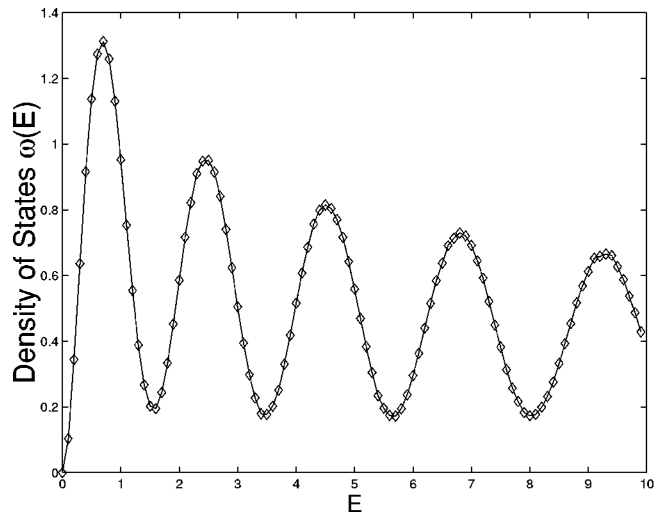

FIG. 1. Numerical evaluation of the density of states $\omega(E)$ path integral for the anharmonic oscillator for $N=2$ (two-time slices) and parameter values $m=\omega_0=g=1.0$. Each peak corresponds to an energy eigenvalue.

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