PHYS 142/242

Lecture 16: Path Integral & MCMC

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Path integral

We've studied the path integral to evaluate the propagator, which represents the probability amplitude of a particle at spacetime point (x_a, t_a) reaching spacetime point (x_b, t_b)

$$K(x_b, t_b; x_a, t_a) = \int \mathscr{D}x(t) \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} L(x(t))dt\right]$$

where $L(x(t)) = \frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x)$ is the classical Lagrangian, $\mathscr{D}x(t)$ denotes the integral over all spacetime paths between (x_a, t_a) and (x_b, t_b)

Imaginary-time path integral

An alternative formulation uses imaginary time, where t is replaced by $-i\tau$

$$\tilde{\rho}(x_b, \tau_b; x_a, \tau_a) = \int \mathscr{D}x(\tau) \exp\left[-\frac{1}{\hbar}\int_{\tau_a}^{\tau_b} L_E(x(\tau))d\tau\right]$$

where $L_E(x(\tau)) = \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x(\tau))$ is the "Euclidean Lagrangian"

Just as for real times, the path integral is over all paths between (x_a, τ_a) and (x_b, τ_b)

Connection to quantum stat. mech.

If we set $x_b = x_a = x$ and integrate over $x(\tau)$ (i.e. take the trace), $\tau_a = 0$, and $\tau_b = \hbar\beta$ where $\beta = 1/(k_{\mathrm{B}}T)$, we get partition function

$$Z = \int \mathscr{D}x(\tau) \exp\left[-\frac{1}{\hbar}\oint_0^{\hbar\beta} L_E(x(\tau))d\tau\right]$$

which alternatively can be calculated from the Boltzmann distribution

$$Z = \sum_{n=0}^{\infty} e^{-\beta E_n}$$

Calculating the ground state

Note, as we approach $T \to 0$, i.e. $\tau_b = \hbar\beta \to \infty$,

$Z = \sum_{n=0}^{\infty} e^{-\beta E_n} \sim e^{-\beta E_0}$ (i.e. only the first eigenvalue dominates the sum)

and

$$\tilde{\rho}(x, \hbar\beta; x, 0) = \sum_{n}^{\infty} p_n \, |\, \phi_n(x) \,|^2 \sim |\, \phi_0(x) \,|^2$$

So if we run with a long enough τ_f, our probability distribution should converge to the ground state.

We can use the path integral (with imaginary time) to directly calculate the ground state!

Imaginary-time path

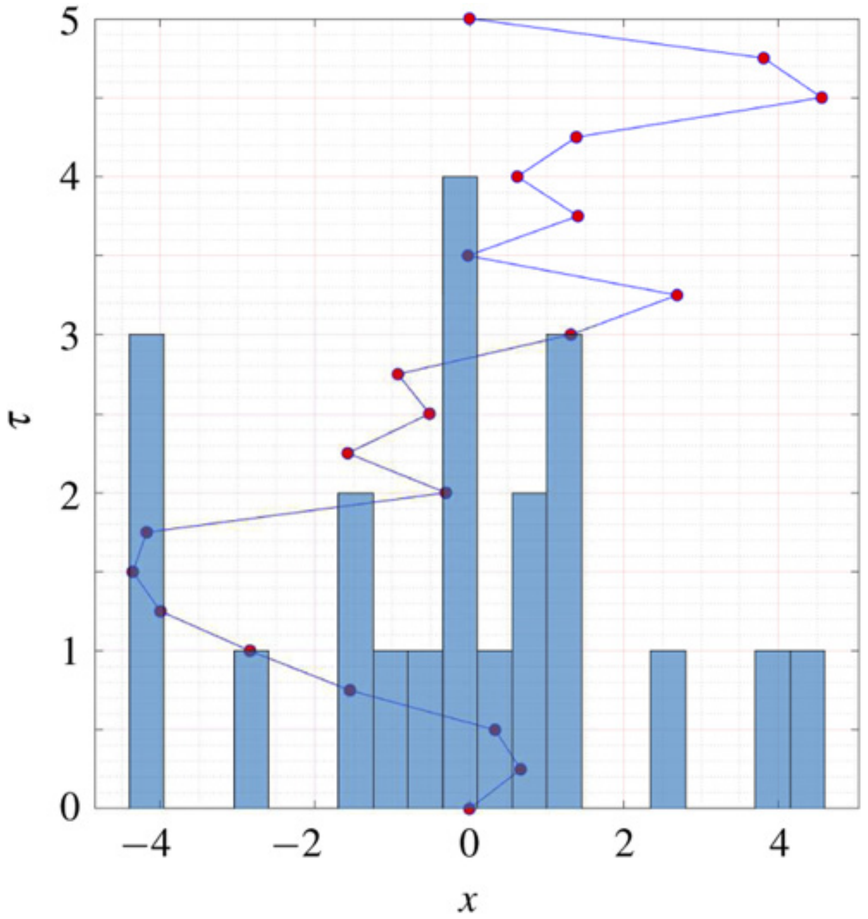
Discretize “time” with N increments, $\tau_a = 0$, and $\tau_b = N\eta$

Each vector $(x_0, x_1, \ldots, x_{N-1})$ in N-dimensional space represents an imaginary-time path

The probability density over this N-dimensional space is

$$p(x_0, \ldots, x_{N-1}) = \frac{1}{Z}\left(\frac{2\pi\hbar\eta}{m}\right)^{-\frac{N}{2}} \exp\left[-\frac{1}{\hbar}\left(\sum_{i=1}^{N}\frac{m(x_i - x_{i-1})^2}{2\eta} + \eta V\left(\frac{x_{i-1}+x_i}{2}\right)\right)\right]$$

Calculating the ground state



S. Mittal et al., “Path integral Monte Carlo method for the quantum anharmonic oscillator”, Eur. J. Phys. 41 055401 (2020)

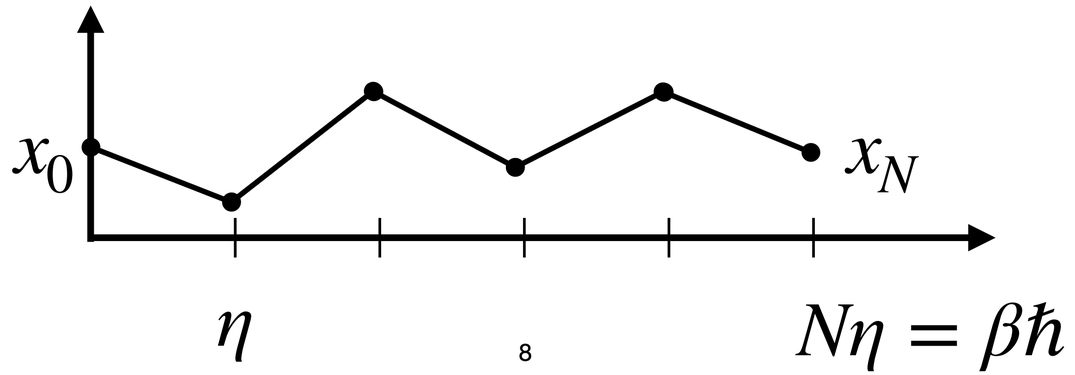
A discrete imaginary time path ⇒ histogram of the probability density by summing up the number of times a particle is in a bin

Figure 1. A discrete imaginary-time path between $(0, 0)$ and $(0, 5)$. The histogram indicates the number of times the particle crosses the corresponding spatial region.

Markov chain Monte Carlo method

Markov chain Monte Carlo simulations are carried out in discrete “time” with N increments, $\tau_a = 0$, and $\tau_b = N\eta$

$$Z = \lim_{\eta \to 0} \int \cdots \int dx_0 \cdots dx_{N-1} \left(\frac{2\pi\hbar\eta}{m} \right)^{-\frac{N}{2}} \exp \left[-\frac{1}{\hbar} \left(\sum_{i=1}^{N} \frac{m(x_i - x_{i-1})^2}{2\eta} + \eta V \left(\frac{x_{i-1} + x_i}{2} \right) \right) \right]$$



MCMC steps

Begin with an initial path, which may be an array of random numbers (‘hot’ start) or zeros (‘cold’ start).

Update the path by applying Metropolis-Hastings algorithm to each element x_i of the path in random order (called a ‘sweep’)

(a) Generate a uniform random number $u \in [-h, h]$

(b) Propose the new value $x_i' = x_i + u$ of the path element and calculate the resulting change ΔS in the action.

If $\Delta S \leq 0$, accept the new path element.

If $\Delta S > 0$, accept with probability $\exp(-\Delta S/\hbar)$

MCMC considerations

One sweep produces the next path from the previous one

Each path is determined only by the immediately preceding path, so the complete sequence of paths forms a Markov chain, but the paths are correlated

The initial path ‘thermalizes’, that is, attains equilibrium after N_{therm} sweeps

To counteract the inherent autocorrelation in a Markov chain, a number N_{sep} of paths between successive paths used for measurements (i.e. representative of the equilibrium distribution) can be discarded

Probability density calculation

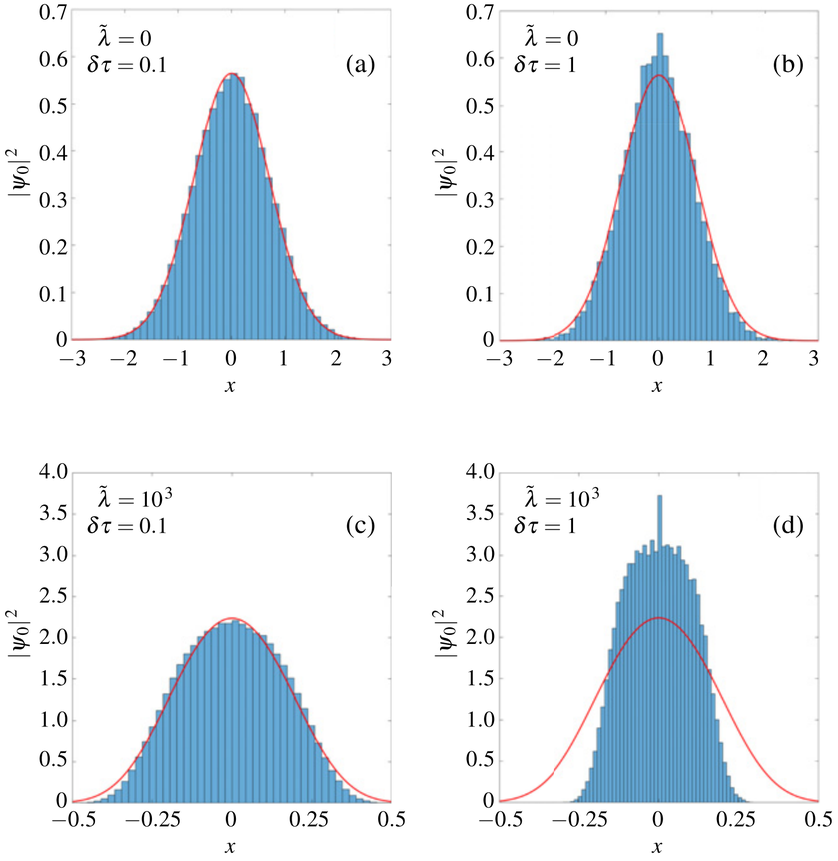


Figure 5. The probability densities $|\psi_0(x)|^2$ of the ground-state wave functions for the harmonic oscillator (a), (b) and the strong quartic limit (c), (d) in the Schrödinger equation with Hamiltonian (32) for $\delta\tau = 1$ (b), (d) and $\delta\tau = 0.1$ (a), (c). The histograms were obtained according to the procedure shown in figure 1, with 200 paths (every 100th from a chain of 20 000) used for determining the probability density. The red curves superimposed on these histograms are numerical solutions to Schrödinger's equations with the corresponding Hamiltonians (32) obtained by using the `bvp4c` solver of MATLAB (reference [44, 45]).[4]

Better approximation to the ground state for smaller time step ($\epsilon = 0.1$ vs. $\epsilon = 1$)

Probability density calculation

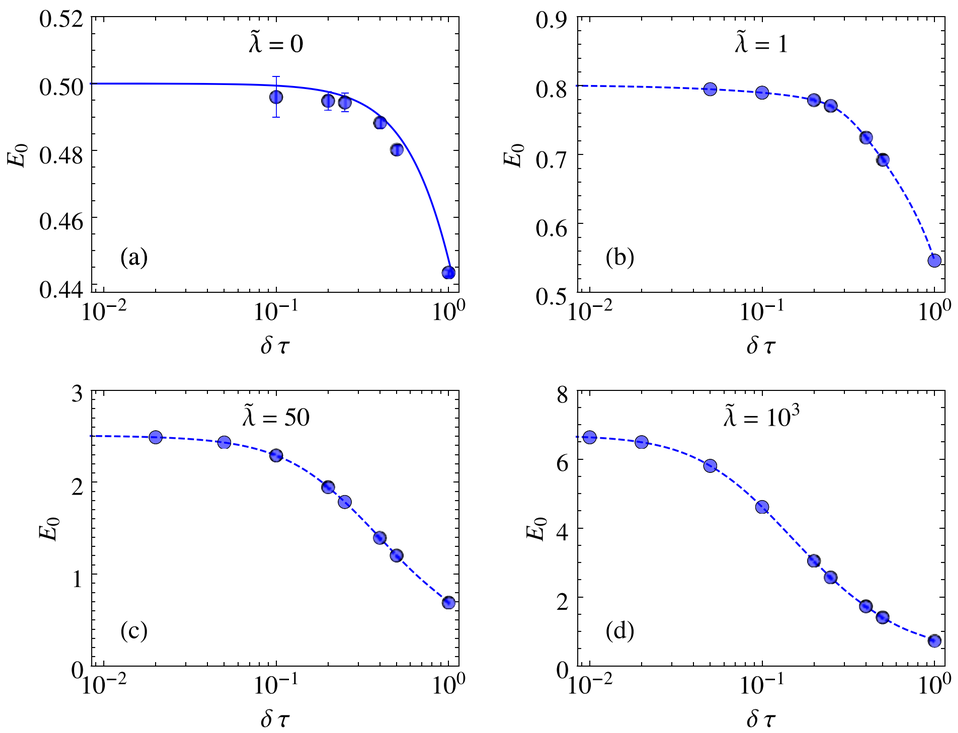


Figure 6. Calculation of the ground-state energy of the anharmonic oscillator with quartic couplings (a) $\tilde{\lambda} = 0$, (b) $\tilde{\lambda} = 1$, (c) $\tilde{\lambda} = 50$, and (d) $\tilde{\lambda} = 10^3$. The filled circles represent values calculated from the MCMC method. In (a), the solid line is the exact result calculated in reference [24, 30], while in (b)–(d), the broken curve is a (not-a-knot) cubic spline fit carried out on linear axes. The logarithmic axis for $\delta\tau$ is for presentation purposes only. Where error bars are not indicated, the errors are of the same size or smaller than the symbol.

Better approximation to the ground state for smaller time step ($\epsilon = 0.1$ vs. $\epsilon = 1$)