Homework #2 due May 16

1. Consider the harmonic oscillator with

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2$$

(a) Evaluate the ground state energy and plot the histogram of the ground state $|\text{wavefunction}|^2$ with the following parameters:

$m a = 1$

$\omega \cdot a = 0.15$

$N = 1000$

Recommended run parameters:

$\Delta = 3$ (~ 60% acceptance)

10^5 warmup sweeps

10^6 measurement sweeps with 100 sweep separation between measurements

~ 8 min run

Include an error calculation in the analysis

(b) Calculate first and second excited energies from the $x(0)\,x(\tau)$ and $x^2(0)\,x^2(\tau)$ correlators, respectively.

$$E_1 - E_0 = -\frac{1}{\Delta\tau} \ln\left[\frac{\langle x(0)\,x(\tau+\Delta\tau)\rangle}{\langle x(0)\,x(\tau)\rangle}\right]$$

$$\tau \to \infty$$

$$E_2 - E_0 = -\frac{1}{\Delta\tau} \ln\left[\frac{\langle x^2(0)\,x^2(\tau+\Delta\tau)\rangle}{\langle x^2(0)\,x^2(\tau)\rangle}\right]$$

$$\tau \to \infty$$

$E_1 - E_0$ in 5-12 τ range

$E_2 - E_0$ in 2-12 τ range

Include an error calculation in the analysis

2. Anharmonic Double Well Potential

$$L = \frac{1}{2} m \dot{x}^2 - \lambda (x^2 - v^2)^2$$

(a) Evaluate the ground state energy and plot the histogram of $|\Psi_0|^2$ with the following parameters:

$a \cdot m = \frac{1}{4}$

$v^2 = 2$

$\lambda = 1$

$\Delta = 2$

10^5 warmup sweeps

10^6 sweeps with 100 sweep separation between measurements

~ 10 min run

Include an error calculation in the analysis

(b) How would you determine the tunneling rate between the two minima?

$\boxed{\text{Error estimate}}$ (for energy)

$E_i \quad i = 1, 2, \ldots N_{samp}$ energy estimators of configurations while sampling

$E_i^2 \quad i = 1, 2, \cdots, N_{samp}$ useful to calculate at the same time

$$\overline{E} = \frac{1}{N_{samp}} \sum_{i=1}^{N_{samp}} E_i$$

$$\overline{E^2} = \frac{1}{N_{samp}} \sum_{i=1}^{N_{samp}} E_i^2$$

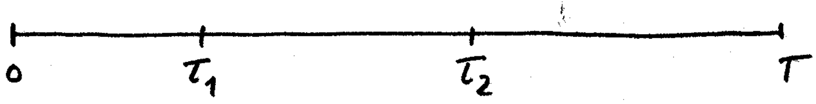
$$E_{error} = \sqrt{\frac{\overline{E^2} - \overline{E}^2}{N_{samp}}}$$

Similar for any other measured quantity

$\overline{E^2} - \overline{E}^2$ determines "intrinsic noise" (variance)

$\frac{1}{\sqrt{N_{samp}}}$ beats the noise in $N_{samp} \to \infty$ limit

Correlation Functions



$$\langle x_0 | \; x(\tau_1)\, x(\tau_2)\, e^{-HT} \; | x_T \rangle =$$

$$= \langle x_0 | \; e^{-H\tau_1} \; x(0) \; e^{H(\tau_1 - \tau_2)} \; x(0) \; e^{H(\tau_2 - T)} \; | x_T \rangle$$

$$|n_1\rangle\langle n_1| \qquad |n_2\rangle\langle n_2| \qquad |n_3\rangle\langle n_3| \qquad |n_4\rangle\langle n_4|$$

$$= \psi_0(x_0)\, e^{-E_0 \tau_1} \, \langle 0 | x(0) | 0 \rangle \, e^{E_0(\tau_1 - \tau_2)} \, \langle 0 | x(0) | 0 \rangle \, \times$$

$$\times \, \psi^*(x_T) \, e^{E_0(\tau_2 - T)} \quad +$$

$$+ \; \psi_0(x_0)\, e^{-E_0 \tau_1} \, \langle 0 | x(0) | 1 \rangle \langle 1 | x(0) | 0 \rangle \, e^{E_1(\tau_1 - \tau_2)} \, \times$$

$$\times \, e^{E_0(\tau_2 - T)} \, \psi^*(x_T) \qquad + \; \ldots\ldots$$

negligible for large T

for large T and large $\tau_2 - \tau_1$

$$\langle x_0 | \, x(\tau_1) \, x(\tau_2) \, e^{-HT} \, | x_T \rangle =$$

$$= \psi_0(x_0) \, \psi^*(x_T) \, e^{-E_0 T} \Big\{ |\langle 0 | x(0) | 0 \rangle|^2 +$$

$$+ e^{-(E_1 - E_0)(\tau_2 - \tau_1)} \langle 0 | x(0) | 1 \rangle \langle 1 | x(0) | 0 \rangle \Big\}$$

$x_T = x_0$ in our case

zero for first excited state

$$C(\tau_1, \tau_2) = \frac{\mathrm{Tr}\left(x(\tau_1) \, x(\tau_2) \, e^{-HT}\right)}{\mathrm{Tr}\, e^{-HT}} - \left(\frac{\mathrm{Tr}\, x \, e^{-HT}}{\mathrm{Tr}\, e^{-HT}} \right)^2$$

$$= e^{-(E_1 - E_0)(\tau_2 - \tau_1)} \cdot |\langle 0 | x | 1 \rangle|^2$$

Similar for second excitation

Clarification on Dimensional Analysis:

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

E_n energy eigenvalues

$$\frac{H}{m} = \frac{p^2}{2m^2} + \frac{1}{2}\frac{\omega^2}{m^2} m^2 x^2$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

$\frac{H}{m}$, $\frac{p}{m}$, $\frac{\omega}{m}$, mx are dimensionless

$$\frac{p^2}{2m^2} \rightarrow -\frac{d^2}{d\xi^2}$$

$mx = \xi$

$\frac{\omega}{m} = \Omega$

$\hbar = 1$

$$\left(-\frac{d^2}{d\xi^2} + \frac{1}{2}\Omega^2 \cdot \xi^2\right)\psi_n(\xi) = \frac{E_n}{m}\psi_n(\xi)$$

$$\frac{E_n}{m} = \Omega\left(n + \frac{1}{2}\right)$$

If we now discretize ξ, a is dimensionless

$m \cdot T$ is also dimensionless

$$e^{-E_n T} \rightarrow e^{-\frac{E_n}{m} \cdot mT}$$

$m \cdot T = \mathbb{T}$ dimensionless number

in path integral :

$$-\sum_{i=1}^{N} \frac{1}{2a}(\xi_i - \xi_{i-1})^2 - \sum_{i=0}^{N-1} a \cdot V(\xi_i)$$

$$\left.\begin{matrix} a \\ \xi_i \end{matrix}\right\} \text{dimensionless}$$

$$\mathbb{T} = N \cdot a$$

if $V(\xi_i) = \frac{1}{2}\mu^2 \xi_i^2$

Ω^2 true frequency

from path integral : $\frac{E_n}{m} = \varepsilon_n = \Omega\left(1 + \frac{a^2\mu^2}{4}\right)^{1/2}$

$\times \left(n + \frac{1}{2}\right)$