

Homework # 2

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:

$$\Delta = 3 \quad (\sim 60\% \text{ acceptance})$$

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.

$$E_1 - E_0 = - \lim_{\tau \rightarrow \infty} \frac{1}{\Delta\tau} \ln \left[\frac{\langle X(0)X(\tau + \Delta\tau) \rangle}{\langle X(0)X(\tau) \rangle} \right]$$

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

$E_1 - E_0$ 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:

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

$$v^2 = 2$$

$$\lambda = 1$$

$$\Delta = 2$$

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?

Error estimate (for energy)

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

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

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

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

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

Similar for any other measured quantity

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

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

Correlation Functions

5.



$$\begin{aligned} & \langle x_0 | x(\tau_1) x(\tau_2) e^{-HT} | x_T \rangle = \\ & = \langle x_0 | e^{-H\tau_1} x(0) e^{H(\tau_1 - \tau_2)} x(0) e^{H(\tau_2 - T)} | x_T \rangle \\ & \quad \uparrow \quad \quad \uparrow \quad \quad \uparrow \quad \quad \uparrow \\ & \quad |n_1\rangle \langle n_1| \quad |n_2\rangle \langle n_2| \quad |n_3\rangle \langle n_3| \quad |n_4\rangle \langle n_4| \end{aligned}$$

$$\begin{aligned} & = \psi_0(x_0) e^{-E_0 \tau_1} \langle 0 | x(0) | 0 \rangle e^{E_0(\tau_1 - \tau_2)} \langle 0 | x(0) | 0 \rangle \times \\ & \quad \times \psi^*(x_T) e^{E_0(\tau_2 - T)} + \\ & + \psi_0(x_0) e^{-E_0 \tau_1} \langle 0 | x(0) | 1 \rangle \langle 1 | x(0) | 0 \rangle e^{E_1(\tau_1 - \tau_2)} \times \\ & \quad \times e^{E_0(\tau_2 - T)} \psi^*(x_T) + \dots \\ & \quad \text{negligible for large } T \end{aligned}$$

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

$$\begin{aligned} \langle x_0 | x(\tau_1) x(\tau_2) e^{-HT} | x_T \rangle &= \\ &= \psi_0(x_0) \psi^*(x_T) e^{-E_0 T} \left\{ |\langle 0 | x(\tau) | 0 \rangle|^2 + \right. \\ &\quad \left. + e^{-(E_1 - E_0)(\tau_2 - \tau_1)} \langle 0 | x(\tau) | 1 \rangle \langle 1 | x(\tau) | 0 \rangle \right\} \end{aligned}$$

$x_T = x_0$ in our case

$$\begin{aligned} C(\tau_1, \tau_2) &= \frac{\text{Tr} \left(x(\tau_1) x(\tau_2) e^{-HT} \right)}{\text{Tr} e^{-HT}} - \left(\frac{\text{Tr} x e^{-HT}}{\text{Tr} e^{-HT}} \right)^2 \\ &= e^{-(E_1 - E_0)(\tau_2 - \tau_1)} \cdot |\langle 0 | x | 1 \rangle|^2 \end{aligned}$$

zero for first excited state
↓

Similar for second excitation

Clarification on Dimensional Analysis:

7.

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \quad E_n \text{ energy eigenvalues}$$

$$\frac{H}{m} = \frac{p^2}{2m^2} + \frac{1}{2} \frac{\omega^2}{m^2} m^2 x^2 \quad E_n = \hbar \omega \left(n + \frac{1}{2}\right)$$

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

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

$$m x = \xi$$

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

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

$$\frac{\hbar}{\hbar} = 1$$

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

If we now discretize ξ , a is dimensionless

$m \cdot T$ is also dimensionless

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

$m \cdot T = \mathbb{T}$ dimensionless number
in path integral :

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

a } dimensionless
 ξ_i }

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

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

Ω^2 true frequency

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