

Homework # 2

Due: May 10

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

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

Clarification on Dimensional Analysis:

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

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

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

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

$$m x = \xi$$

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

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

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

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

If we now discretize ξ , a is dimensionless

$m \cdot T$ is also dimensionless

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

$m \cdot T = \Pi$ 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 }

$$\Pi = N \cdot a$$

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

Ω^2 true frequency

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