SIMPLE HARMONIC OSCILLATOR IN 1D

Exercise 1: Exact Density Matrix

The simple harmonic oscillator (SHO) in 1D is modeled by the Hamiltonian

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2. \tag{1}$$

Its density matrix(DM) is given by the Bloch equation

$$-\frac{\partial \rho(x,x';\beta)}{\partial \beta} = \hat{\mathcal{H}}\rho(x,x';\beta), \tag{2}$$

with the initial condition $\rho(x,x';0) = \delta(x-x')$. The solution

$$\rho(x,x';\beta) = \sqrt{\frac{m\omega}{2\hbar\sinh(\hbar\beta\omega)}/\pi}\exp\left\{-\frac{m\omega}{2\hbar\sinh(\hbar\beta\omega)}\left[(x^2+x'^2)\cosh(\hbar\beta\omega) - 2xx'\right]\right\}. \tag{3}$$

Use atomic units ($\hbar = 1$) and define $A \equiv \frac{m\omega}{2\sinh(\beta\omega)}$, then

$$\rho(x,x';\beta) = \sqrt{A/\pi}\exp\left\{-A\left[(x^2+x'^2)\cosh(\beta\omega) - 2xx'\right]\right\}. \tag{4}$$

The SHO can be completely characterized by its mean squared fluctuation

$$\boxed{\langle x^2\rangle = \frac{\int dx x^2\rho(x,x;\beta)}{\int dx\rho(x,x;\beta)} = \frac{\hbar}{2m\omega}\coth(\frac{\hbar\beta\omega}{2})}. \tag{5}$$

The potential energy $\langle V\rangle = \frac{1}{2}m\omega^2\langle x^2\rangle$, and the total energy is given by the Virial theorem. Define action $S \equiv -\ln\rho$ and ignore the normalization of ρ, then the *exact link action*

$$S_e(x,x';\beta) = A\left[(x^2+x'^2)\cosh(\beta\omega) + 2xx'\right]. \tag{6}$$

Notice, if temperature is high $\beta = \tau \approx 0$, then eq. (6) reduces to the *primitive link action*

$$S_p(x,x';\tau) = \tau\left[\frac{1}{2}m\left(\frac{x-x'}{\tau}\right)^2\right] + \frac{\tau}{2}\left[\frac{1}{2}m\omega^2(x^2+x'^2)\right]. \tag{7}$$

An algorithm that performs eq. (5) with Monte Carlo sampling is equivalent to path integral Monte Carlo (PIMC) with one time slice. MC sampling of the diagonal of the density matrix $\rho(x,x;\beta)$ can be performed with Metropolis algorithm using acceptance probability

$$\mathcal{A} = \min\left(1, \exp -\Delta S_e\right). \tag{8}$$

Exercise 2: Path Integral Construction of the Density Matrix

The exact density matrix at low temperature β can be constructed exactly as a convolution of M high temperature $\tau = \beta/M$ density matrices

$$\rho(x, x'; \beta) = \int dx_1 \dots dx_{M-1} \; \rho(x, x_1; \tau)\rho(x_1, x_2; \tau) \dots \rho(x_{M-1}, x'; \tau). \tag{9}$$

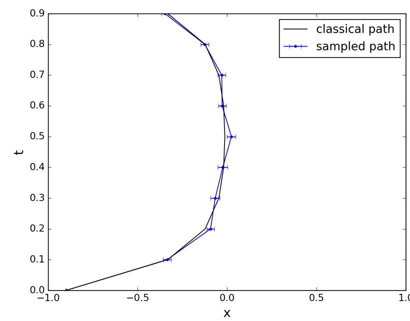

FIG. 1: Path going from $x = x' = -0.9$

The collection of *time slices* x_j can be thought of a trajectory through imaginary time $x_j \equiv x(t = j\tau)$. Then eq. (9) is a functional integral over the space of imaginary-time *paths* $x(t)$ as shown in Fig. 1. Each path has an associated *action* that determines its likelihood

$$S[\{x_j\}] = \sum_{j=0}^{M-1} S_e(x_j, x_{j+1}; \tau), \text{ where } x_0 \equiv x, x_M \equiv x'. \tag{10}$$

When $\tau \to 0$, $x_j + 1 \approx x_j$, thus eq. (6) simplifies to

$$S_e(x, \dot{x}, t = j\tau) = \tau \left[\frac{1}{2} m\dot{x}(t)^2 + \frac{1}{2} m\omega^2 x(t)^2 \right], \tag{11}$$

which is reminiscent of the Lagrangian density. The paths from x to x' can be sampled with Metropolis. The classical path, which minimizes the action, will be sampled most often.

Exercise 3: Path Integral Monte Carlo with Exact Link Action