LAB IX
Simulation of a quantum particle in harmonic potential

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Pseudo-code

procedure `naive-harmonic-path`
input $\{x_0, \ldots, x_{N-1}\}$
$\Delta_\tau \leftarrow \beta/N$
$k \leftarrow \texttt{nran}\,(0, N-1)$
$k_\pm \leftarrow k \pm 1$ **modulo N**

$x'_k \leftarrow x_k + \texttt{ran}\,(-\delta, \delta)$
$\pi_a \leftarrow \rho^{\text{free}}\left(x_{k_-}, x_k, \Delta_\tau\right) \rho^{\text{free}}\left(x_k, x_{k_+}, \Delta_\tau\right) \exp\left(-\frac{1}{2}\Delta_\tau x_k^2\right)$
$\pi_b \leftarrow \rho^{\text{free}}\left(x_{k_-}, x'_k, \Delta_\tau\right) \rho^{\text{free}}\left(x'_k, x_{k_+}, \Delta_\tau\right) \exp\left(-\frac{1}{2}\Delta_\tau x'^2_k\right)$
$\Upsilon \leftarrow \pi_b/\pi_a$
if $(\texttt{ran}\,(0,1) < \Upsilon) x_k \leftarrow x'_k$
output $\{x_0, \ldots, x_{N-1}\}$

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where $\rho^{\text{free}}(x, y, \Delta\tau) = e^{-(x-y)^2/2\Delta\tau}$

Task I

Simulate a string (quantum path) for the harmonic potential $V(x) = -\frac{1}{2}x^2$ by implementing our pseudo-code. Consider 1MCS when every x_k is updated once on average.

Plot average string position $< x >= \sum_k x_k/N$ and variance $< (x- < x >)^2 >$ versus simulation time (preferably panel plot). Take $N = 8$, $\beta = 4$, $\delta = 1$ and `MCS_max = 10 000`, start with a random configuration $x_k \in [-\delta, \delta]$.

Add horizontal lines to the plot, with mean (over MCS) position and mean (over MCS) variance. What are the values?

Task II

Speed up the simulation by implementing the update routine (Task I) under `numba` package. On a few trial runs estimate the acceptance ratio of Metropolis step. Update (by hand) $\delta_{\rm new} = \delta r_{\rm acc}/0.75$ untill you find a value for which $r_{\rm acc} \approx 0.75$

As before, plot average string position $< x >= \sum_k x_k/N$ and variance $< (x- < x >)^2 >$ versus simulation time (preferebly panel plot). Take $N = 40$, $\beta = 4$, and `MCS_max = 100 000`. Store positions: x_0 and $x_{N//2}$ throughout the simulation.

Make normalized histogram of the stored values of positions. Compare with the analytic solution for the harmonic oscillator:

$$\pi(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}, \quad \sigma^2 = \frac{1}{2\tanh\beta/2}.$$