I. RING POLYMER MOLECULAR DYNAMICS - I. FUNDAMENTALS

Text Reference:

Code Reference: ./ExampleCode/tps_integrator.f90

i) **[Observing the quantum effects]**

1. We now turn to a quantum harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 \tag{1}$$

living in a heat bath with $\beta = 1$. In ring polymer molecular dynamics (RPMD), quantum mechanical effects can be captured by running dynamics with a classical isomorphic system

(2)

2. (Static quantity)

3. (Dynamical quantity)

4. Given , devise a symplectic integrator