Relativistic Path Integral Monte-Carlo

December 2023

1 Density matrix and energy

Hamiltonian

$$H = \sqrt{p^2 + m^2} + V(q). \tag{1}$$

Density matrix at small τ

$$\rho(q'', q'; \tau) = \langle q'' | e^{-\tau H} | q' \rangle. \tag{2}$$

Density matrix in coordinate representation

$$\begin{aligned}\rho(q'', q'; \tau) = & \left(\frac{m\tau}{\pi\sqrt{\tau^2 + (q'' - q')^2}} \right)^{(d+1)/2} \cdot \\ & \cdot \frac{K_{(d+1)/2}(m\sqrt{\tau^2 + (q'' - q')^2})}{(2\tau)^{(d-1)/2}} e^{-\tau V(q')},\end{aligned} \tag{3}$$

where $d = 1, 2, 3$.

Markov chain limit probability density for $d = 1$

$$\pi(q_i) = \frac{K_1\left[m\sqrt{\tau^2 + (q_i - q_{i-1})^2}\right] K_1\left[m\sqrt{\tau^2 + (q_{i+1} - q_i)^2}\right]}{\sqrt{\tau^2 + (q_i - q_{i-1})^2}\sqrt{\tau^2 + (q_{i+1} - q_i)^2}} e^{-\tau V(q_i)}. \tag{4}$$

Average value of kinetic energy for $d = 1$

$$\langle \sqrt{p^2 + m^2} \rangle = \Big\langle \frac{m\tau}{\sqrt{\tau^2 + (\Delta q)^2}} \frac{K_0(m\sqrt{\tau^2 + (\Delta q)^2})}{K_1(m\sqrt{\tau^2 + (\Delta q)^2})} + \frac{\tau^2 - (\Delta q)^2}{\tau(\tau^2 + (\Delta q)^2)} \Big\rangle. \tag{5}$$

Density matrix in coordinate representation for $d = 2$

$$\begin{aligned}\rho(q'', q'; \tau) = & \frac{m^3\tau}{2\pi} \cdot \frac{1 + m\sqrt{\tau^2 + (q'' - q')^2}}{\left(m\sqrt{\tau^2 + (q'' - q')^2}\right)^3} \cdot \\ & \cdot \exp\left[-m\sqrt{\tau^2 + (q'' - q')^2}\right] e^{-\tau V(q')}.\end{aligned} \tag{6}$$

Markov chain limit probability density for $d = 2$

$$\pi(q_i) = \frac{1 + m\sqrt{\tau^2 + (q_i - q_{i-1})^2}}{\left(m\sqrt{\tau^2 + (q_i - q_{i-1})^2}\right)^3} \cdot \frac{1 + m\sqrt{\tau^2 + (q_{i+1} - q_i)^2}}{\left(m\sqrt{\tau^2 + (q_{i+1} - q_i)^2}\right)^3} \cdot \tag{7}$$

$$\cdot \exp\left[-m\sqrt{\tau^2 + (q_i - q_{i-1})^2} - m\sqrt{\tau^2 + (q_{i+1} - q_i)^2}\right] e^{-\tau V(q_i)}. \tag{8}$$

Average value of kinetic energy for $d = 2$

$$\langle\sqrt{p^2 + m^2}\rangle = \dots \tag{9}$$

2 RPIMC calculations for oscillator model in two dimensions

Non-relativistic (NR) and ultra-relativistic (UR) limit energy

$$E_{NR} = \dots, \tag{10}$$

$$E_{UR} = \dots. \tag{11}$$

3 Neural network calculations

Oscillator potential

$$V(q) = \frac{1}{2} m\omega^2 q^2. \tag{12}$$

Let's choose parameters values

$$\begin{aligned} &m = 100, \\ &\omega = 1, \\ &N_t = 10, \\ &\tau = e/10 \approx 0.2718\dots. \end{aligned}$$