

Path Integral Monte Carlo on Oscillators

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Path integral Monte Carlo is implemented and applied to oscillators trapped by a central potential.

CONTEXT

In the context of continuum-space path integral Monte Carlo (PIMC), the physical system to be studied is a collection of non-relativistic particles in three spatial dimensions each contributing a kinetic operator to the Hamiltonian $\hat{T}_j = \lambda_j (i\nabla_{\vec{r}_j})^2$, where $j = 1, \dots, N$ label the particles, and \vec{r}_i is the position of particle j . Often $\lambda_j = \frac{1}{2m_j}$, where m_j is the mass of the j^{th} particle. Let the $3N$ -vector $R = \{\vec{r}_j\}$ contain all $3N$ coordinates of the N particles. Let the position basis that spans the Hilbert space of these particles be $|R\rangle$.

THEORY

The Density Matrix

The thermal density matrix in operator notation is

$$\hat{\rho} = e^{-\beta\hat{H}}, \quad (1)$$

where \hat{H} is the Hamiltonian and $\beta = \frac{1}{kT}$ is inverse temperature. It can be written in the position basis $|R\rangle$ and have the factorization property

$$\rho(R_0, R_M; \beta) = \int [\prod_{t=1}^{M-1} dR_t] \prod_{t=1}^M \langle R_{t-1} | e^{-\tau\hat{H}} | R_t \rangle, \quad (2)$$

where M is an integer and $\tau = \beta/M$. If ρ is to be viewed as a time evolution operator, then β is the imaginary time of propagation. In this context, (2) can be viewed as a discretization of the total propagation path of length β into M segments of length τ . In the thermal dynamics context, the low temperature (quantum) behavior of the system is expressed as a convolution of high temperature (classical) behavior.

If τ is small enough and the Hamiltonian has separable kinetic and potential pieces $\hat{H} = \hat{T} + \hat{V}$, then each segment in (2) can be separated using the Trotter formula

$$\begin{aligned} \rho(R_{t-1}, R_t; \tau) &\equiv \langle R_{t-1} | e^{-\tau\hat{H}} | R_t \rangle \approx \langle R_{t-1} | e^{-\tau\hat{T}} e^{-\tau\hat{V}} | R_t \rangle \\ &= \int dR' \langle R_{t-1} | e^{-\tau\hat{T}} | R' \rangle \langle R' | e^{-\tau\hat{V}} | R_t \rangle, \end{aligned} \quad (3)$$

which is exact in the limit $\tau \rightarrow 0$ [1]. Assuming the potential is local, then $\langle R' | e^{-\tau\hat{V}} | R_t \rangle = e^{-\tau V(R_t)} \delta^{(3N)}(R' - R_t)$

and

$$\rho(R_{t-1}, R_t; \tau) = \langle R_{t-1} | e^{-\tau\hat{T}} | R_t \rangle e^{-\tau V(R_t)}. \quad (4)$$

Recall each particle contributes a term $\hat{T}_j = \lambda_j (i\nabla_{\vec{r}_j})^2$ to the kinetic operator. To proceed, I will break up the particles into species, where all particles in a species have the same λ . Unless specified otherwise, I will only consider a single species in the rest of this document. Contributions from different species can be added together at the end. Assuming the particles are held in a 3D box with side length L , the kinetic piece can be evaluated by inserting a complete set of momentum states

$$\begin{aligned} \langle R_{t-1} | e^{-\tau\hat{T}} | R_t \rangle &= \int dP \langle R_{t-1} | P \rangle \langle P | e^{-\tau\hat{T}} | R_t \rangle \\ &= \sum_n L^{-3N} \exp \{ -\tau \lambda 4\pi^2 n \cdot n / L^2 - 2i\pi n \cdot (R_{t-1} - R_t) / L \} \\ &\approx \frac{1}{(4\pi\lambda\tau)^{3N/2}} \exp \left(-\frac{(R_{t-1} - R_t)^2}{4\lambda\tau} \right). \end{aligned} \quad (5)$$

The last line is valid in the limit when the “size” of a particle is much smaller than the size of the box $\tau\lambda \ll L^2$, or when periodic boundary condition is used. Plugging (3)-(5) back into (2) and we arrive at a practical expression for the thermal density matrix

$$\begin{aligned} \rho(R_0, R_M; \beta) &= \int [\prod_{t=1}^{M-1} dR_t] \prod_{t=1}^M \frac{1}{(4\pi\lambda\tau)^{3N/2}} \times \\ &\quad \exp \left(-\tau \left(\frac{(R_{t-1} - R_t)^2}{4\lambda\tau^2} + V(R_t) \right) \right) \\ &= \frac{1}{(4\pi\lambda\tau)^{3MN/2}} \int [\prod_{t=1}^{M-1} dR_t] \\ &\quad \exp \left(-\tau \sum_{t=1}^M \left(\frac{(R_{t-1} - R_t)^2}{4\lambda\tau^2} + V(R_t) \right) \right) \\ &\propto \int \mathcal{D}R \exp \left(-\sum_{t=1}^M \tau L_{cl} \right), \end{aligned} \quad (6)$$

where $\int \mathcal{D}R \equiv \int [\prod_{t=1}^{M-1} dR_t]$ and the Classical Lagrangian [2, 3]

$$L_{cl}(R_{t-1}, R_t; \tau) \equiv \sum_{t=1}^M \frac{1}{4\lambda} \left(\frac{R_{t-1} - R_t}{\tau} \right)^2 + V(R_t). \quad (7)$$

The Classical Lagrangian is sufficient for later sampling, but for an exact expression for the density matrix, a con-

stant term needs to be added in the *primitive Lagrangian*

$$L_{cl}^P(R_{t-1}, R_t; \tau) \equiv -\frac{1}{\tau} \ln \rho(R_{t-1}, R_t; \tau) \\ \approx \frac{3N}{2\tau} \ln(4\pi\lambda\tau) + \frac{1}{4\lambda} \left(\frac{R_{t-1} - R_t}{\tau} \right)^2 + V(R_t). \quad (8)$$

It is worth noting that the classical Lagrangian (7) has a spring-like term and a potential term. This allows a classical interpretation of the quantum problem through an isomorphism with classical ring polymers.

Classical Isomorphism

To see a classical picture of the path integral formulation of the density matrix, we can break down the $3N$ vector R into visualizable particle positions $r_j^{(i)}$. [1] Now

$$\sum_{t=1}^M (R_{t-1} - R_t)^2 = \sum_{t=1}^M \sum_{j=1}^N (r_{t-1}^{(i)} - r_t^{(i)})^2 \\ = \sum_{j=1}^N \left(\sum_{t=1}^M (r_{t-1}^{(i)} - r_t^{(i)})^2 \right). \quad (9)$$

That is, each particle can be visualized as a collection of beads, one at each imaginary time slice. In this context, the kinetic contribution (5) to the classical action can be considered particle-by-particle

$$\left(\sum_{t=1}^M \frac{(R_{t-1} - R_t)^2}{4\lambda\tau} \right)_i = \sum_{t=1}^M \frac{(r_{t-1}^{(i)} - r_t^{(i)})^2}{4\lambda\tau}. \quad (10)$$

This term can be interpreted as series of a spring potentials coupling beads belonging to the same particle i at adjacent time slices.

The Partition Function and Observables

The partition function can be evaluated as a trace of the density matrix

$$Z(\beta) = \int dR \rho(R, R; \beta) \\ = \lim_{M \rightarrow \infty} \int \mathcal{D}R \exp \left(- \sum_{t=1}^M \tau L_{cl}^P(R_{t-1}, R_t; \tau) \right) \\ \equiv \int \mathcal{D}R \exp(-S_{cl}^P(R, R; \beta)), \quad (11)$$

which is of path integral form. The expectation value of any operator \hat{O} can be formally written as an operator insertion in the path integral

$$\langle \hat{O} \rangle = \text{tr}(\hat{O}\hat{\rho}) = \int \mathcal{D}R \hat{O} \exp(-S_{cl}^P). \quad (12)$$

Due to the cyclic nature of trace, \hat{O} can be inserted between any two segments (time slices) in a discretized path integral. If the operator is local in space, then \hat{O}_l can be evaluated at a single time slice

$$\langle \hat{O}_l \rangle = \frac{1}{Z} \int \mathcal{D}R \mathcal{O}_l(R_t) \exp(-S_{cl}^P), \quad (13)$$

for any $t = 1, \dots, M$. Although in practice, one may choose to average over all M time slices to obtain better statistics

$$\langle \hat{O}_l \rangle \leftarrow \frac{1}{N} \sum_{t=1}^M \mathcal{O}_l(R_t) \quad (14)$$

The expectation value of the kinetic operator can be evaluated by a derivative against imaginary time. Notice

$$\langle R_{t-1} | \hat{T} e^{-\tau \hat{T}} | R_t \rangle = -\frac{\partial}{\partial \tau} \langle R_{t-1} | e^{-\tau \hat{T}} | R_t \rangle \\ \approx -\frac{\partial}{\partial \tau} \frac{1}{(4\pi\lambda\tau)^{3N/2}} \exp \left(-\frac{(R_{t-1} - R_t)^2}{4\lambda\tau} \right) \\ = \left(\frac{3N}{2\tau} - \frac{1}{4\lambda} \left(\frac{R_{t-1} - R_t}{\tau} \right)^2 \right) \frac{\exp \left(-\frac{(R_{t-1} - R_t)^2}{4\lambda\tau} \right)}{(4\pi\lambda\tau)^{3N/2}} \\ \approx \left(\frac{3N}{2\tau} - \frac{1}{4\lambda} \left(\frac{R_{t-1} - R_t}{\tau} \right)^2 \right) \langle R_{t-1} | e^{-\tau \hat{T}} | R_t \rangle. \quad (15)$$

Therefore the kinetic energy evaluation involves two adjacent time slices. Again, for better statistics

$$\langle \hat{T} \rangle \leftarrow \frac{3N}{2\tau} - \frac{1}{4\lambda\tau^2} \frac{1}{M} \sum_{t=1}^M (R_{t-1} - R_t)^2. \quad (16)$$

Now we can simulate the classical system of $M \times N$ particles according to the classical action (7), record observables according to formulae such as (14) and (16) to solve the quantum system of N particles.

IMPLEMENTATION

The classical isomorphism makes the implementation of PIMC fairly straight forward. In particular, I will use the Metropolis algorithm to sample classical ring polymer configurations according to the classical action. Each configuration is defined by a 3-dimensional array R_{ti} of size $(M, N, 3)$, which contains the spatial locations of the $M \times N$ classical beads or equivalently, a *path*.

From an initial path, p_1 , some move will be proposed with probability $T(p_1 \rightarrow p_2)$ and accepted with the Metropolis acceptance rate

$$A = \min \left\{ \frac{\exp(-S_{cl}(p_2))}{\exp(-S_{cl}(p_1))} \frac{T(p_2 \rightarrow p_1)}{T(p_1 \rightarrow p_2)} \right\}, \quad (17)$$

and observables will be accumulated. Different forms of the transfer matrix $T(p_1 \rightarrow p_2)$ can be explored for an efficient sampling algorithm.

A Single Oscillator Trapped by a Central Potential

For the simplest case, I will consider a single harmonic oscillator of mass m trapped by a harmonic potential [4]

$$V(\vec{r}) = \frac{1}{2}m\omega^2 r^2, \quad (18)$$

where \vec{r} is the position of the oscillator. The Hamiltonian

$$H = \lambda(i\vec{\nabla})^2 + \frac{1}{2}m\omega^2 r^2, \quad (19)$$

in three spatial dimensions has eigenvalues

$$E(n_x, n_y, n_z) = \hbar\omega(n_x + n_y + n_z + \frac{3}{2}). \quad (20)$$

The partition function

$$\begin{aligned} Z &= \sum_{n_x=0}^{\infty} \sum_{n_y=0}^{\infty} \sum_{n_z=0}^{\infty} \exp(-\beta E(n_x, n_y, n_z)) \\ &= \frac{1}{8} \text{csch}^3\left(\frac{1}{2}\beta\hbar\omega\right). \end{aligned} \quad (21)$$

The expectation energy can then be calculated as

$$\langle E \rangle = -\partial_{\beta} \ln Z = \frac{3}{2}\hbar\omega \coth\left(\frac{1}{2}\beta\hbar\omega\right). \quad (22)$$

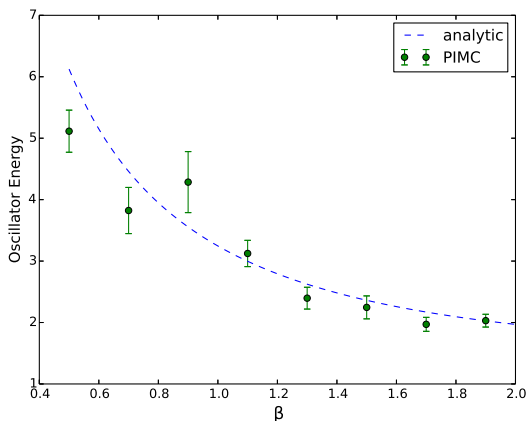


FIG. 1. Energy of a single harmonic oscillator calculated with PIMC and analytically.

PIMC simulation was performed for a single harmonic oscillator with unit mass and unit frequency in atomic units $m = \omega = \hbar = 1$. The PIMC results matches the analytical solution as shown in Figure 1. Single bead moves are used, but displacement moves and bisection moves can be implemented and integrated with the main code in a straight forward manner. Pair potential can be added as a subtype of the potential type. Please see details of the implementation in the jupyter notebook inside my GitHub folder “algorithmic-perspective/PIMC/pimc.ipynb”.

APPENDIX

The kinetic integral can be performed by completing the square

$$\int dp e^{ip \cdot (R_{t-1} - R_t) + \lambda \tau p} = \frac{1}{(4\pi\lambda\tau)^{3N/2}} \times \exp\left\{-\frac{(R_{t-1} - R_t)^2}{4\lambda\tau}\right\}$$

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