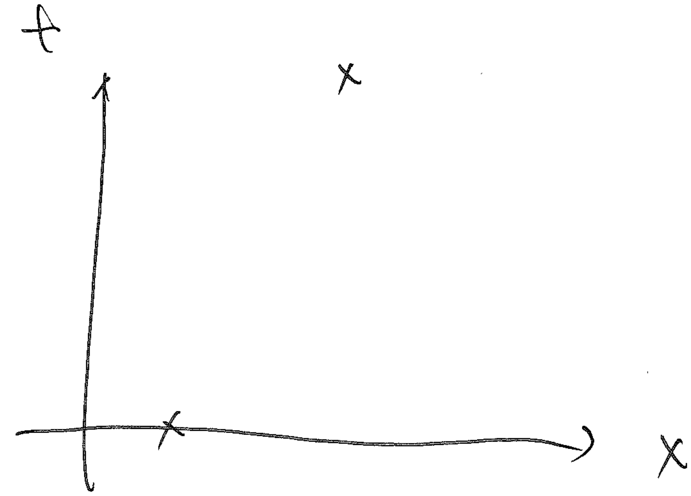
Q.M on Lattice

free $u = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} \exp\left[\frac{i m x^2}{2\hbar t}\right]$

Review of PI in QM



Propagator (Green's function) in configuration space $U(x_f, t_f, x_i, t_i)$

① Draw all possible paths connecting $x_i x_f$ that are monotonic in time,

② Evaluate classical action S_{cl} along each path, assign factor $e^{iS_{cl}/\hbar}$;

③ $U(x_f, t_f; x_i, t_i) = N \sum_{\text{All paths}} e^{iS_{cl}/\hbar} = \langle x_f, t_f | e^{-iH(t_f - t_i)} | x_i, t_i \rangle$.

Can show this is equivalent to that obtained from wave mechanics.

- S_{cl} is stationary with respect to variation in path along classical trajectory, $x_{cl}(t)$, hence nearby paths contribute coherently to the phase factor. For those deviates a lot from $x_{cl}(t)$, $e^{iS_{cl}/\hbar}$ rapidly oscillating leads to cancellation.

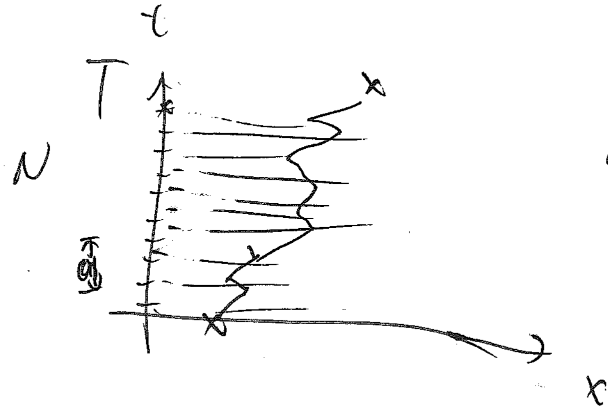
$\Rightarrow$ Only $x_{cl}(t)$ and nearby paths dominates $U(x_f, t_f, x_i, t_i)$.

PI can give analytic results for $V(x) = a + bx + cx^2 + d\dot{x} + ex\dot{x}$, H atom...!

numeric issues ① $\sum_{\text{All paths}}$ ② $e^{iS_{cl}/\hbar}$

① $\sum_{\text{All path}} e^{iS_{cl}/\hbar} = \int_{-\infty}^{\infty} \prod_i dx_i \, e^{iS_{cl}[x]/\hbar}$

$= \int \mathcal{D}x \, e^{iS_{cl}[x]/\hbar}$



$a = \frac{T}{N}$

② wick-rotation $\tau = it$

$$S_{cl} = \int \left[\frac{m}{2}\left(\frac{dx}{dt}\right)^2 - V(x)\right] dt = i \int \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)\right] d\tau = i S_E$$

$$\int \mathcal{D}x \, e^{iS_{cl}/\hbar} = \int \mathcal{D}x \, e^{-S_E/\hbar} = \langle x_f | e^{-H\Delta\tau} | x_i \rangle$$

Sanity check: Most cases $x_{cl}(t)$ minimize S, unimportant paths damped.

maximize

saddle point ~~stationary~~ ?

U is hermitian instead of unitary, $U = \sum_n \langle x_f | n \rangle \langle n | x_i \rangle e^{-E_n \Delta\tau}$

$\lim_{\Delta\tau \to \infty} U = \langle x_f | 0 \rangle \langle 0 | x_i \rangle e^{-E_0 \Delta\tau}$

All states unless orthogonal to GS will eventually evolve to GS.

→ Similar to Gibbs distribution in stat mech

$$p(E) = \frac{1}{Z} e^{-E/T}, \quad Z = \sum_n e^{-E_n/T}.$$

If take trace of $U(x_f, x_i)$ (periodic B.C.), integrate over all possible x_s,

$$Z = \int dx \sum_n \langle x | n \rangle \langle n | x \rangle e^{-E_n \delta\tau/\hbar} = \mathrm{Tr}\, e^{-H\delta\tau/\hbar}$$

Comparision with stat mech:

① Temp → 0, no thermal fluctuations

$\hbar \to 0$, $e^{-S_E/\hbar}$ dominated by classical path, no quantum fluctuations.

② Freeenergy $F_{stat} = - T_{temp} \ln Z$

$$\frac{F}{T} = -\frac{\hbar}{T} \ln Z \xrightarrow{\lim_{T\to\infty}} E_0 \quad \text{ground state energy.}$$

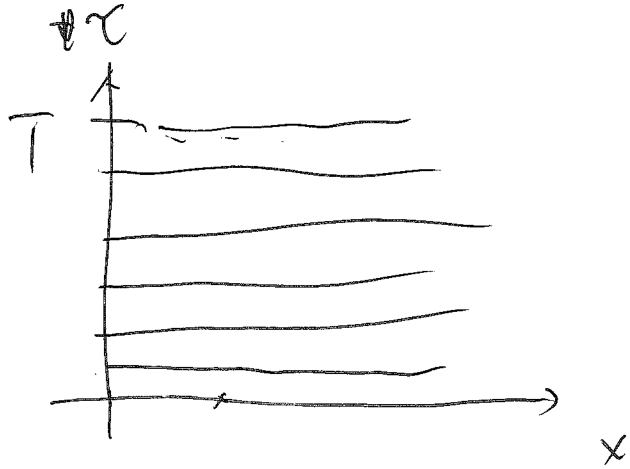
③ Expectation values

$$\langle \hat{O} \rangle = \frac{\int \mathcal{D}x(t)\, O[x]\, e^{-S_E[x]/\hbar}}{\int \mathcal{D}x(t)\, e^{-S_E[x]/\hbar}};$$

④ correlators

$$\langle \varphi_1 \varphi_2 \cdots \varphi_n \rangle = \frac{1}{Z} \int \mathcal{D}x(t) (\varphi_1 \varphi_2 \cdots \varphi_n) e^{-\frac{S_E[x]}{\hbar}}$$

Now on our 1-D lattice sites



$$Z_{S_E} = \int \mathcal{D}x(t)\; e^{-S_E[x(t)]/\hbar}$$

Discretized version of S_E: (naive version).

$$S_E = \sum_i \left[\frac{m}{2}\frac{(x_{i+1}-x_i)^2}{a} + V(x_i)a\right] \quad (1)$$

Problem: $\langle T \rangle \to \infty$ as $a \to 0$ (continuum limit)

why? Consider functional $F[x(t)]$

$$\langle F \rangle = \int \mathcal{D}x(t)\, F[x(t)]\, e^{-S_E[x(t)]/\hbar}$$

By variation can show $\left\langle \frac{\partial F}{\partial x_k} \right\rangle = \frac{1}{\hbar}\left\langle F \frac{\partial S_E}{\partial x_k} \right\rangle$

From (1) $\frac{\partial S_E}{\partial x_k} = m\left[\frac{(x_k - x_{k-1})}{a} - \frac{(x_{k+1}-x_k)}{a}\right] + aV'(x_k)$

So $\left\langle \frac{\partial F}{\partial x_k} \right\rangle = \frac{a}{\hbar}\left\langle F\left[m\left(\frac{x_k - x_{k-1}}{a^2} - \frac{x_{k+1}-x_k}{a^2}\right) + V'(x_k)\right]\right\rangle$ (2)

Take $F = x_k$, $\langle 1 \rangle = \frac{a}{\hbar}\left\langle m x_k\left(\frac{x_k - x_{k-1}}{a^2} - \frac{x_{k+1}-x_k}{a^2}\right) + V'(x_k)\right\rangle$

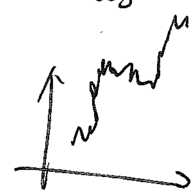
Suppose $V(x)$ is smooth

$$\langle m x_k \frac{x_k - x_{k-1}}{a} \rangle - \langle m x_k \frac{x_{k+1} - x_k}{a} \rangle = \hbar$$

up to $O(\varepsilon)$ $$\langle m x_k \frac{x_k - x_{k-1}}{a} \rangle \approx \langle m x_{k+1} \frac{x_{k+1} - x_k}{a} \rangle$$

$$\Rightarrow \langle \cancel{m} \frac{(x_{k+1} - x_k)(x_{k+1} - x_k)}{a} \rangle = \frac{\hbar}{m} \Rightarrow \langle \frac{(x_{k+1} - x_k)^2}{a^2} \rangle = \frac{\hbar}{am} + O(1)$$

Paths that are important in QM are highly irregular at fine scales



$\langle v \rangle$ is well-defined but not $\langle v^2 \rangle$

Solution: Note if $m \to m + \delta m$, $\frac{\delta \langle k \rangle}{\delta m} \sim \langle k \rangle$, $\overline{\delta m}$ / more straightforward:

$m \to m(1+\varepsilon)$ / subtract the $\frac{1}{a}$ divergence / see what's left.

1. S changes by $\frac{\varepsilon m}{2} \left[\frac{(x_{k+1} - x_k)^2}{a} \right]$

2. normalization changes by $(1 + \frac{\varepsilon}{2})$

Hence $$\delta Z = \frac{\varepsilon m}{2} \left[\frac{(x_{k+1} - x_k)^2}{a} - \frac{\varepsilon \hbar}{2} \right] \sim T = \frac{m}{2} \left[\frac{(x_{k+1} - x_k)^2}{a^2} - \frac{\hbar}{2a} \right]$$

$$= 0 + O(\tfrac{1}{a}) \qquad = ?$$

In fact this is finite.

Take $F = x_{k+1} - x_k$

$$-\langle 1 \rangle = \frac{a}{\hbar} \left\langle (x_{k+1} - x_k) \left[m \left(\frac{x_k - x_{k-1}}{a^2} - \frac{x_{k+1} - x_k}{a^2} \right) + V'(x_k) \right] \right\rangle$$

$$= \frac{ma}{\hbar} \left[\left\langle \frac{(x_{k+1} - x_k)(x_k - x_{k-1})}{a^2} \right\rangle - \left\langle \frac{(x_{k+1} - x_k)^2}{a^2} \right\rangle \right]$$

$$\Rightarrow \quad \left\langle \frac{(x_{k+1} - x_k)(x_k - x_{k-1})}{a^2} \right\rangle = \left\langle \frac{(x_{k+1} - x_k)^2}{a^2} \right\rangle - \frac{\hbar}{ma}$$

Therefore ~~can use~~ $\langle T \rangle = \frac{m}{2} \left\langle \frac{(x_{k+1} - x_k)(x_k - x_{k-1})}{a^2} \right\rangle$ is well-behaved in the continuum limit

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Another solution : viral theorem

$$\langle \tfrac{1}{2} m v^2 \rangle = \tfrac{1}{2} \langle x V'(x) \rangle$$

$$H(t) = \tfrac{1}{2} x_n V'(x_n) + V(x_n)$$

Observables:

① G.S energy: $f = \frac{F}{T} \xrightarrow[T\to\infty]{} E_0$ / $\langle H(t)\rangle = \langle T+V\rangle$

$= \cdots$ discussed above

② G.S (wave function):
probability density

\# pts fall within $(x, x+\Delta x) = \rho(x)$

If phase not important $\varphi(x) = \sqrt{\rho(x)}$

③ First excited states: Suppose $[\hat{P}, \hat{H}] = 0$.

consider

$$\langle \hat{x}_H(\tau_2)\, \hat{x}_H(\tau_1)\rangle = \cancel{\frac{1}{Z}\sum_n \langle E_n | \hat{x}\, e^{-(\hat{H}-E_k)}}$$

$$\left(= \cancel{\frac{1}{Z}\int dx_{end} \langle x_{end}| e^{-\hat{H}(t_f-t)}\, \hat{x}\, e^{-\hat{H}\Delta\tau}} \right.$$

$$= \lim_{T\to\infty} \frac{1}{Z} \int dx_{end}\, \langle x_{end} | e^{-HT}\, e^{H\tau_2}\, \hat{x}\, e^{H(\tau_1-\tau_2)}\, \hat{x}\, e^{-H\tau_1} | x_{end}\rangle$$

$$= \lim_{T\to\infty} \frac{1}{Z}\sum_n \int dx_{end}\, |\langle x_{end}|n\rangle|^2 e^{-HT} \langle n|\hat{x}\, e^{-(H-E_n)\Delta\tau}\, \hat{x}\, |n\rangle \qquad \Delta\tau = \tau_2-\tau_1$$

$$= \langle 0|\hat{x}\, e^{-(H-E_0)\Delta\tau}\, \hat{x}\,|0\rangle.$$

$|0\rangle$ is even parity (node theorem?)

$\hat{x}|0\rangle$ is odd

$$\hat{x}|0\rangle = \cancel{\sum_{\text{odd } p} C_n|2n+1\rangle}\ \sum_n C_{2n+1}|2n+1\rangle$$

$$\langle x(\tau_2)x(\tau_1)\rangle = \sum_n |C_{2n+1}|^2 e^{-(E_{2n+1}-E_1)\Delta\tau}$$

$\lim \Delta\tau \to \infty$ again $\langle x(\tau_2)x(\tau_1)\rangle \longrightarrow |C_1|^2 e^{-(E_1-E_0)\Delta\tau}$.

Define $G(n) = \langle \hat{x}(\tau_i + na)\hat{x}(\tau_i)\rangle$, $n\to\infty$

then $\lim_{n\to\infty} \frac{G(n)}{G(n+1)} = e^{+(E_1-E_0)a}$

$\Rightarrow \quad E_1 - E_0 = \frac{1}{a}\ln\left[\frac{G(n)}{G(n+1)}\right]$ gives energy split.

④ higher energy states. (again assume $[\hat{p}, \hat{n}] = 0$).

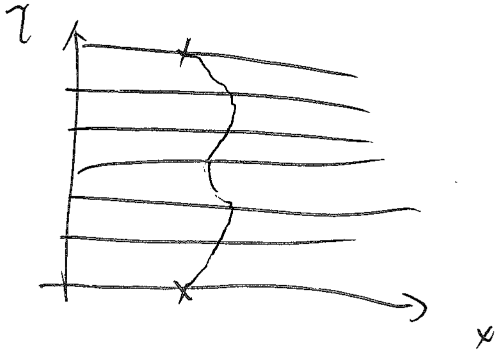
Fit $\sum_n |C_{2n+1}|^2 e^{-(E_{2n+1}-E_0)\Delta\tau}$ for higher odd parity excited states

or even correlator $\langle x^2(\tau_2)x^2(\tau_1)\rangle$ for even parity excited state.

⑤ other.

tunneling. ::

Effectively choose paths?



Metroplis algorithm ① start with an arbitrary path

calculate $S_{E,prev}$.

② Iterate through lattice $i=1,\dots,N-1$. for each site i,

i. update $x_i = x_i + y r_i$, r_i is a random # from uniform distribution $\in [-1,1]$

ii. Calculate $S_{E,new}$ after updating each site i, calculate $S_{E,new}$, $\Delta S_E = S_{E,new} - S_{E,old}$.

iii. If $\Delta S_E < 0$, accept this update at lattice site i, go to next site;

Gibbs: If $\Delta S_E > 0$, ~~pick~~ generate random # $r_i' \in (0,1)$ from uniform distribution.

Metroplis do global updates. Iff $r' < e^{-\Delta S}$, keep the update; else rejected and reverse to previous position x_i.

~~③~~ A sweep through all lattice sites is called a Monte Carlo Iteration.

③ Add this path to collection, repeat itr from step ②

Benifits: this approach generate paths obeys Boltzmann distribution

$P \propto e^{-S_E/\hbar}$. Z can be replaced by N_{itr}.

$\Rightarrow$ can be shown by using Markov chain.

Technical

~~Technical~~ details

① "Thermalization".

If initial path is far from "classical" path, it'll take some time

to arrive at a equilibrium configuration. First N_{therm} MCI throw away.

Criterion for thermalization: $\langle \hat{O} \rangle$ convergence.

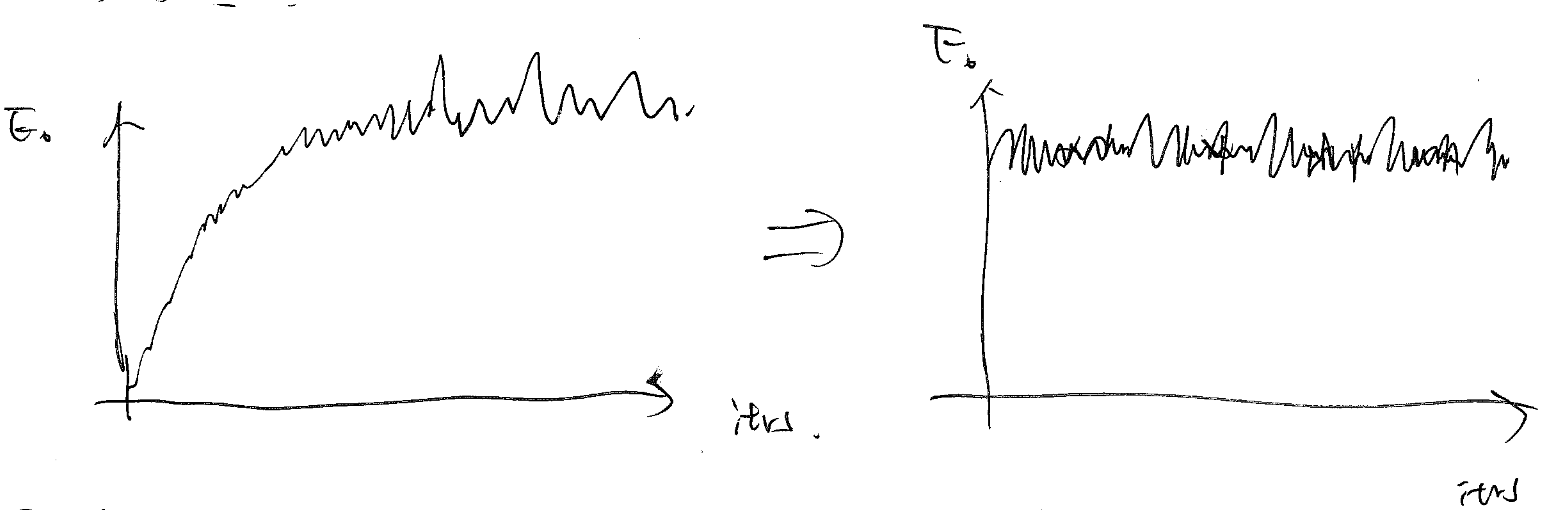
improvements: slow convergence

② "Decorrelation". — Randomness.

do multiple updates at ~~each~~ lattices in one itr)

Nearby Monte Carlo Iterations are somewhat correlated. Throw away

Ncorr iterations between ~~ea~~ every Ncorr iterations.



③ choice of η. η too small : slow convergence & / parameter space not explored enough.

η too large : many updates will be rejected. optimally rejection rate $\sim 60\% - 80\%$ $>50\%$

Example: $V(x) = \lambda(x^2 - f^2)^2$

characteristic time scale $\tau_c = 2\pi\hbar/E_0$.

choose parameter $N \sim 10^2 - 10^3$

$$a/\tau_c \sim \left[\frac{1}{20}, \frac{1}{10}\right]$$

$$Na/\tau_c \sim [3, 10].$$

$N_{therm} \sim 10 - 50$

$N_{corr} \sim 3 - 5$

$$\Delta\hat{O} \sim \frac{1}{\sqrt{N}} = \frac{\sqrt{\overline{\Delta O^2}}}{|\bar{O}|}$$

~~En~~ typical paths. $\lambda = 1$ tunneling probability decrease $\longrightarrow$