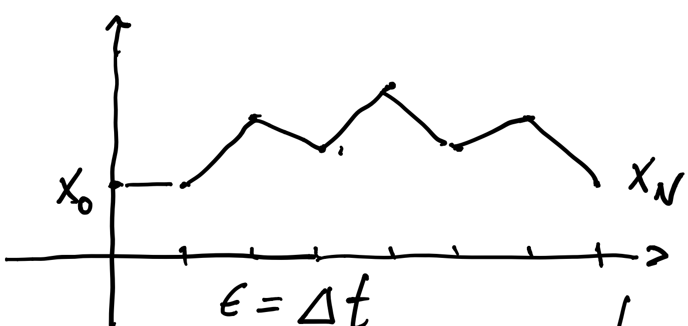
Lecture 17: Markov Chain MC in QM

road map to MCMC in QM following Feynman's picture of path summation:

$$\int K(x,t;x,0)\,dx = \sum_n e^{-\frac{i}{\hbar}E_n t}$$

Trace K



zig-zag paths

continuum limit

$t = N\cdot\epsilon$ t fixed, $\epsilon \to 0$

$x(t) = x(0)$ all closed paths

$x_0 = x_N$ after discretization

K described the return probability amplitude for QM observations but prob. amplitudes cannot be sampled as probabilities in importance sampling therefore we mathematically continued t to imaginary axis on both sides of the propagator trace:

$$t = -i\tau$$

$$\underbrace{\int K(x,\tau;x,0)\,dx}_{Z(\tau)\ \text{notation}} = \sum_n e^{-\frac{E_n \tau}{\hbar}}$$

looks like formal trick

but then:

electron in heat bath (θ temperature)

$$P_n = \frac{e^{-\frac{E_n}{k\theta}}}{Z}$$ prob. of n^{th} energy eigenstate

$$Z = \sum e^{-\frac{E_n}{k\theta}} \rightarrow \sum_n P_n = 1$$

$$\rho_\theta(x) = \sum_n P_n(\theta)|\psi_n(x)|^2$$ probability density of observations

$$\rho_\theta(x) \xrightarrow[\theta \to 0]{} |\Psi_0|^2$$

knowing the energy spectrum and the wave functions we can calculate $\rho_\theta(x)$ at any temp θ

Feynman: let us reverse and calculate $\rho_\theta(x)$ from path integral

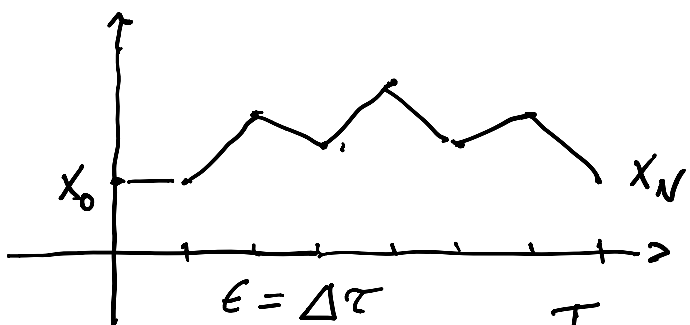
$$\rho_\theta(x) \longleftrightarrow E_n \text{ and } |\Psi_n(x)|^2$$

basic idea: approximate $Z(\tau)$ using probability theory (importance sampling)
Can be made arbitrarily accurate!

We will be able to use then classical MCMC methods (like for a polymer chain) to simulate the quantum electron

Wil quantum computing lead to a revolution?

We needed to cast P_n prob. distribution into continuum distribution of closed paths (loops) equivalent to thermal response of the election to all observations:



zig-zag paths

$T = N \cdot \epsilon$

$x(T) = x(0)$ all closed paths

$x_0 = x_N$ after discretization

$$Z = \lim_{\to 0} \int dx_0 \cdots \int dx_{N-1} \left(\frac{m}{2\pi\hbar\epsilon} \right)^{\frac{N}{2}} \times$$

$$\times \exp\left\{ -\frac{m}{2\hbar\epsilon} \sum_{i=1}^{N} (x_i - x_{i-1})^2 - \frac{\epsilon}{\hbar} \sum_{i=1}^{N} V(x_i) \right\}$$

discretized for computer

discretized form of integrated energy over the closed loop:

$$\mathcal{E} = \frac{1}{T} \int_0^T \left(\frac{1}{2} m \dot{x}^2 + V(x(\tau))\right) d\tau$$

average over path

$$Z = \int \mathcal{D}[x(\tau)]\, e^{-\frac{1}{\hbar} \int_0^T \left[\frac{1}{2} m \left(\frac{dx}{d\tau}\right)^2 + V(x(\tau))\right] d\tau}$$

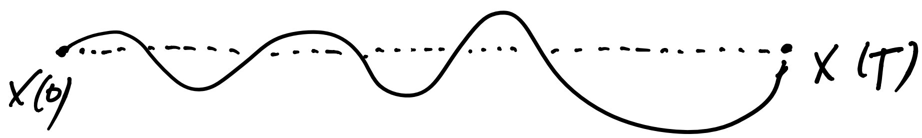
$$Z = \int \mathcal{D}[x(\tau)] \cdot e^{-\frac{\mathcal{E} \cdot T}{\hbar}}$$

$\mathcal{D}[x(\tau)]$ is just the measure

$dx_0 \cdots dx_{N-1} \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{\frac{N}{2}}$ in continuum limit

$$p[x(\tau)] \cdot \mathcal{D}[x(\tau)] = \frac{e^{-\frac{\mathcal{E} \cdot T}{\hbar}}}{Z} \mathcal{D}[x(\tau)]$$

problem is mapped into one-dimensional classical problem of elastic chain of length T



polymer

elastic deformation energy:

$$\int_0^T \left(\frac{1}{2} m \left(\frac{dx}{d\tau} \right)^2 + V(x(\tau)) \right) d\tau = \mathcal{E} \cdot T$$

classical problem solved with classical simulation mapped into physics of quantum electron!

future: Q-bits and quantum computing instead

Boltzmann maps the problem at finite temperature for the elastic chain:

time travel

$$\frac{T}{\hbar} = \frac{1}{k\theta} \qquad Z = \int \mathcal{D}[x(\tau)] \cdot e^{-\frac{\mathcal{E}[x(\tau)]}{k\theta}}$$

temp

$$P_\theta[X[\tau]] = \frac{e^{-\frac{\mathcal{E}[X(\tau)]}{k\theta}}}{Z}$$

↑

probability density of chain at deformation $X(\tau)$

$E[X(\tau)]$ chain deformation energy

θ temperature of heat bath

if we know how to generate $p[X(\tau)]$ we can calculate the physics of the chain at temperature θ

But we proved that the same Z for the electron is given by

$$Z = \sum_n e^{-\frac{E_n}{k\theta}}$$ if f.eg. confining potential with discrete spectrum E_n

$$\langle \mathcal{E}[x(\tau)] \rangle_\theta = \int \mathcal{D}[x(\tau)] \cdot \mathcal{E}[x(\tau)] \cdot p_\theta[x(\tau)]$$

thermal av. energy of elastic continuum chain

$$\frac{dE(\theta)}{d\theta} \rightarrow \text{heat capacity of chain}$$

$$\langle E \rangle_\theta = \sum_n P_n(\theta) \cdot E_n$$

thermal energy of quantum electron

$$\frac{d\mathcal{E}(\theta)}{d\theta} \rightarrow \text{heat capacity of quantum electron}$$

knowing all thermal averages, we can extract full quantum theory of the electron

This is the Feynman idea

although late in his life he basically established the idea (desire) for quantum computing we have Q-bits now and quantum computing is beginning to show results

$\rightarrow$ long way to go

back to the ground: how to simulate classically the probability distribution of all shapes of the elastic chain (polymer)

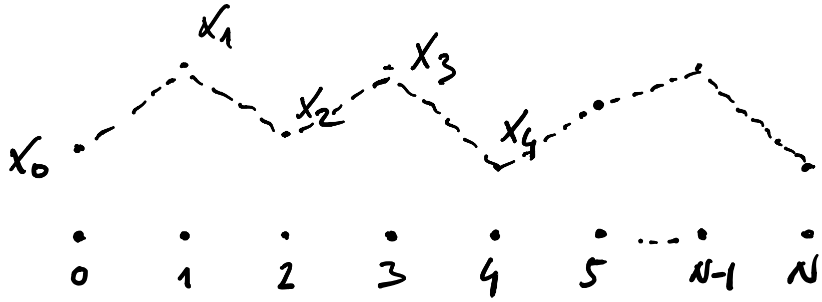
We first discretize the chain and generate $p(x_0, x_1, \dots, x_{N-1})$ for arbitrary $x_0, x_1, \dots, x_{N-1}$ configurations

MCMC will be capable of doing this

$$X \leftrightarrow \{x_0, x_1 \dots, x_{N-1}\} \qquad x_N \equiv x_0$$

state of the chain

$$p(X) \sim e^{-\frac{\mathcal{E}(X)}{k\theta}}$$



$T(X \to X')$ along Markov chain

$= \omega(X, X')\, A_{XX'}$

$\omega(X, X')$ symmetric $\quad \Delta\{[\cdot]\quad X_i \to X_i'$

in Δ interval

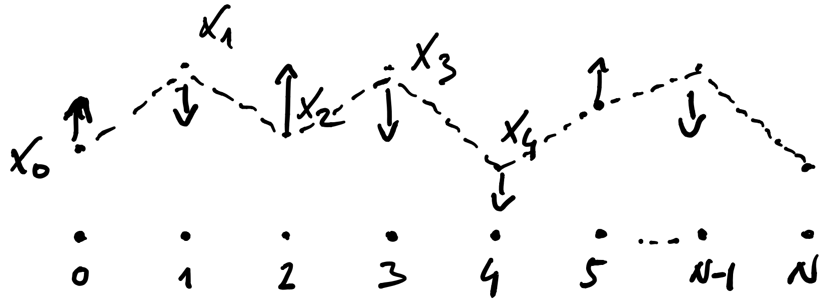
acceptance:

$$A_{XX'} = \begin{cases} 1 & \text{if } E_i < E_i' \\ \dfrac{e^{-\frac{E_i}{kT}}}{e^{-\frac{E_i'}{kT}}} & \text{if } E_i > E_i' \end{cases}$$

we attempt a local change on each site i

cycling through the chain will complete

the $T(X \to X')$ move along the chain



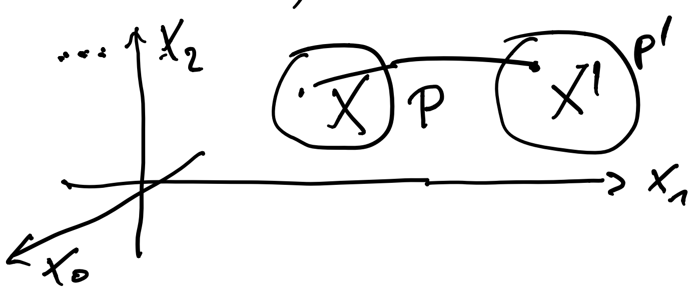
sweeping through the Metropolis update of each site will generate the $T(X \to X')$ MCMC transition

interpretation:

$X = \{x_0, x_1, \ldots, x_{N-1}\}$ chain state is represented by point in N-dim state space

was drawn from $P(X)$ distribution

new $P'(X')$ distribution generated



after finite number of steps original $P(X)$ distribution will converge to target distribution:

$$\frac{T}{\hbar} = \frac{1}{k\theta} \qquad Z = \int D[X(\tau)] \cdot e^{-\frac{E[X(\tau)]}{k\theta}}$$

$$P_\theta[X[\tau]] = \frac{e^{-\frac{E[X(\tau)]}{k\theta}}}{Z}$$

physics: taking measurements on distribution

One can simply follow a single walker along MCMC evolution. Walker will find the right distribution and walking in it will fill the right density function practical considerations:

(1) equilibration time (needed for walker to reach target distribution)

(2) autocorrelation time

(3) tuning of selection Δ

(4) histogram in X-space $[X(\tau)]$ will build the thermal spatial distribution of electron

Sophisticated "measurements" on $P([X(\tau)])$ will extract full quantum physics of electron from simulating the equivalent classical system one dimension higher ($0+1$ or $d+1$)