Quantum Monte Carlo methods

Many-body problems in quantum mechanics

N degrees of freedom $\qquad N \gg 1$

$$\hat{\mathcal{H}} = \underbrace{\sum_{i=1}^{N} \hat{\mathcal{H}}_i}_{\text{single-body (single-mode) term}} + \underbrace{\sum_{i<j} \hat{V}_{ij}}_{\text{two-body term}} + \dots$$

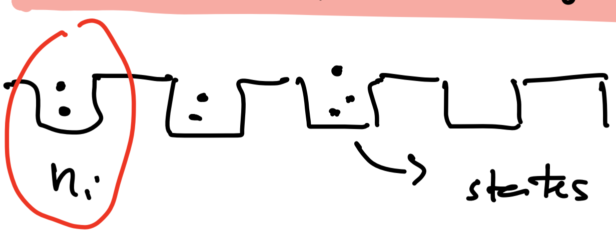
1) Particles in continuum space

$$\hat{\mathcal{H}}_i = \frac{\hat{p}_i^2}{2m_i} + U_{ext}(\hat{\vec{r}}_i)$$

$$\hat{V}_{ij} = v(|\vec{r}_i - \vec{r}_j|)$$

ex.

2) Lattice quantum gases $\longrightarrow$ ex. electrons in a solid, photons in cavities, atoms in arrays of traps, ...



states / modes for single particles

indistinguishable quantum particles

second quantization

$$\hat{H}_i = -\mu n_i + \frac{U}{2} n_i (n_i - 1) + \dots$$

\# of pairs of particles

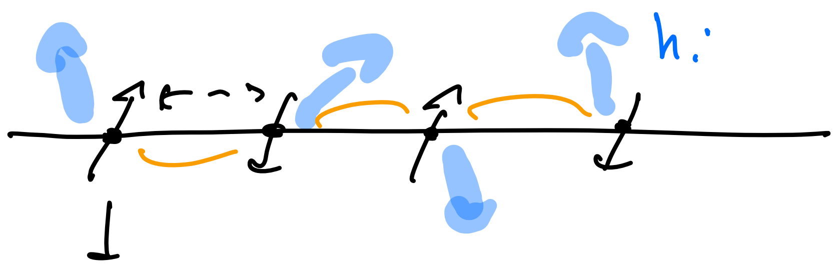
$$\hat{V}_{ij} = -t\,(c_i^{\dagger} c_j + c_j^{\dagger} c_i)$$

creates a particle @ site i

destroys a particle @ site j

$$+ \, v_{ij}\, n_i\, n_j$$

3) Lattice spin models



$s = \frac{1}{2}$ spins

$$H_i = -\vec{h}_i \cdot \hat{\vec{S}}_i$$

ex.

$$V_{ij} = \sum_{\alpha\beta = x,y,z} J_{ij}^{\alpha\beta}\, \hat{S}_i^{\alpha}\, \hat{S}_j^{\beta}$$

4) example of your choice

...

In principle $\hat{H} |\psi\rangle = E |\psi\rangle$

just too hard!

diagonaliz a matrix $D \times D$

$D \sim \mathcal{O}(\exp(N))$

lattice spin models
$S = 1/2$

$D = 2^N$

impossible when
$N \gtrsim 50$

$\langle \hat{A} \rangle_T$ observables @ thermal equilibrium

QMC

$= \mathrm{Tr}(\hat{\rho} \hat{A})$

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z}$$

$$\beta = \frac{1}{k_B T}$$

$Z = \mathrm{Tr}(e^{-\beta \hat{H}})$

$k_B =$ Boltzmann constant

Classical statistical mechanics

states $\underline{\alpha}$ ex. $\uparrow \downarrow \uparrow \uparrow \downarrow \uparrow$

$\Rightarrow E_\alpha$ energy

$\Rightarrow A_\alpha$ observable

$$\langle A \rangle_T = \sum_\alpha A_\alpha \frac{e^{-\beta E_\alpha}}{Z}$$

$$Z = \sum_\alpha e^{-\beta E_\alpha}$$

Quantum Monte Carlo

for some Hamiltonians, a solution to eq. statistical mechanics

$\rightarrow$ scalable : at polynomial cost you can tackle bigger systems

Time $\sim$ poly(N)

→ not specific to # of dimensions of space

→ fully unbiased : solution is "numerically exact"

{ path-integral MC { particles, fermions
{ Stochastic Series Expansions
{ ...

There are also "biased" QMC approaches

↓

quantum chemistry

Classical vs. quantum statistical mechanics

$$\langle A \rangle_T = \frac{\sum_\alpha A_\alpha \, e^{-\beta E_\alpha}}{Z} \Rightarrow \boxed{\text{Monte Carlo approach}}$$

A = energy
density
magnetization
...

N Ising spins : 2^N terms
↑ ↓

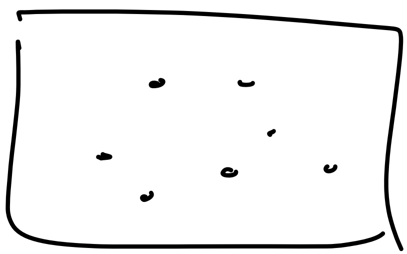
$$Z = \sum_\alpha e^{-\beta E_\alpha} \quad \Longleftarrow$$

$$F(T,\ldots) = -k_B T \log Z$$

ex. T, N, V fixed

$$U = \left.\frac{\partial(\beta F)}{\partial \beta}\right|_{N,V}$$

V



$$p = -\left.\frac{\partial F}{\partial V}\right|_{N,T}$$

...

What's special about quantum mechanics

$$\langle \hat{A} \rangle_T = \frac{\mathrm{Tr}\left(e^{-\beta \hat{H}} \hat{A}\right)}{\mathrm{Tr}\left(e^{-\beta \hat{H}}\right)}$$

$$= \frac{\sum_\alpha \langle \phi_\alpha | e^{-\beta \hat{H}} \hat{A} | \phi_\alpha \rangle}{\sum_\alpha \langle \phi_\alpha | e^{-\beta \hat{H}} | \phi_\alpha \rangle}$$

$$\boxed{\hat{H} | \phi_\alpha \rangle = E_\alpha | \phi_\alpha \rangle} \leftarrow$$

$$= \qquad =$$

unknowns

$$= \frac{\sum_\alpha A_\alpha e^{-\beta E_\alpha}}{\sum_\alpha e^{-\beta E_\alpha}}$$

$$A_\alpha = \langle \phi_\alpha | \hat{A} | \phi_\alpha \rangle$$

QMC : rewriting $\langle \hat{A} \rangle_T$ as "estimator"

$$\langle \hat{A} \rangle_T = \frac{\text{"}\sum_c\text{"} \; A_c \; e^{-S_c}}{\text{"}\sum_c\text{"} \; e^{-S_c}}$$

p_c

quantum-to-classical mapping

c : configuration

S_c : "action" associated with c

c is NOT a quantum state $|\psi_c\rangle$

A_c is NOT (necessarily) $\langle \psi_c | \hat{A} | \psi_c \rangle$

S_c is NOT $\beta \langle \psi_c | \hat{H} | \psi_c \rangle$

Efficient QMC approach :

① A_c , S_c are efficiently computable

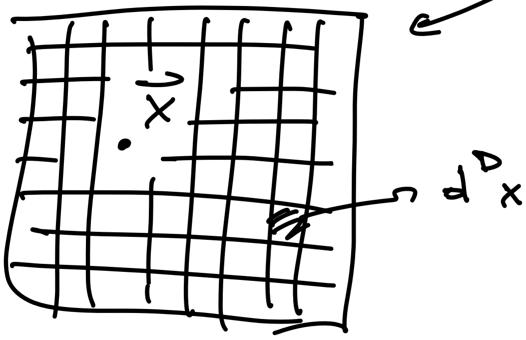
I give you c → you know A_c , S_c in a time ~ poly (N) .

② $e^{-S_c} \geq 0$ semi-positive definite statistical weights

MONTE CARLO METHOD

statistical integrals : integral in a high-dimensional space

$$I = \langle g \rangle_p = \int d^D x \; g(\vec{x}) \, \frac{p(\vec{x})}{N}$$



D dimensions

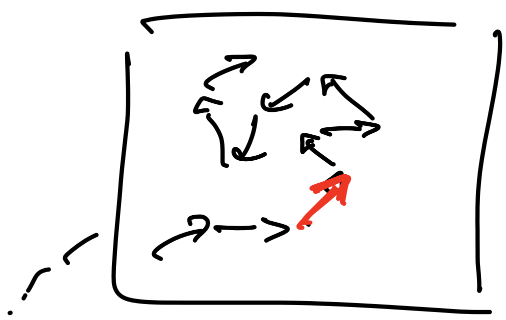
$$\int d^D x \; p(\vec{x}) = N$$

"sample" the distribution $p(\vec{x})/N$

produce a set of points $(\vec{x}_1, \vec{x}_2, \ldots \vec{x}_L)$

s.t.
$$\frac{n(\vec{x}_k)}{L} \underset{L \to \infty}{\simeq} \frac{p(\vec{x}_k)}{N} d^D x$$

Markov-chain Monte Carlo

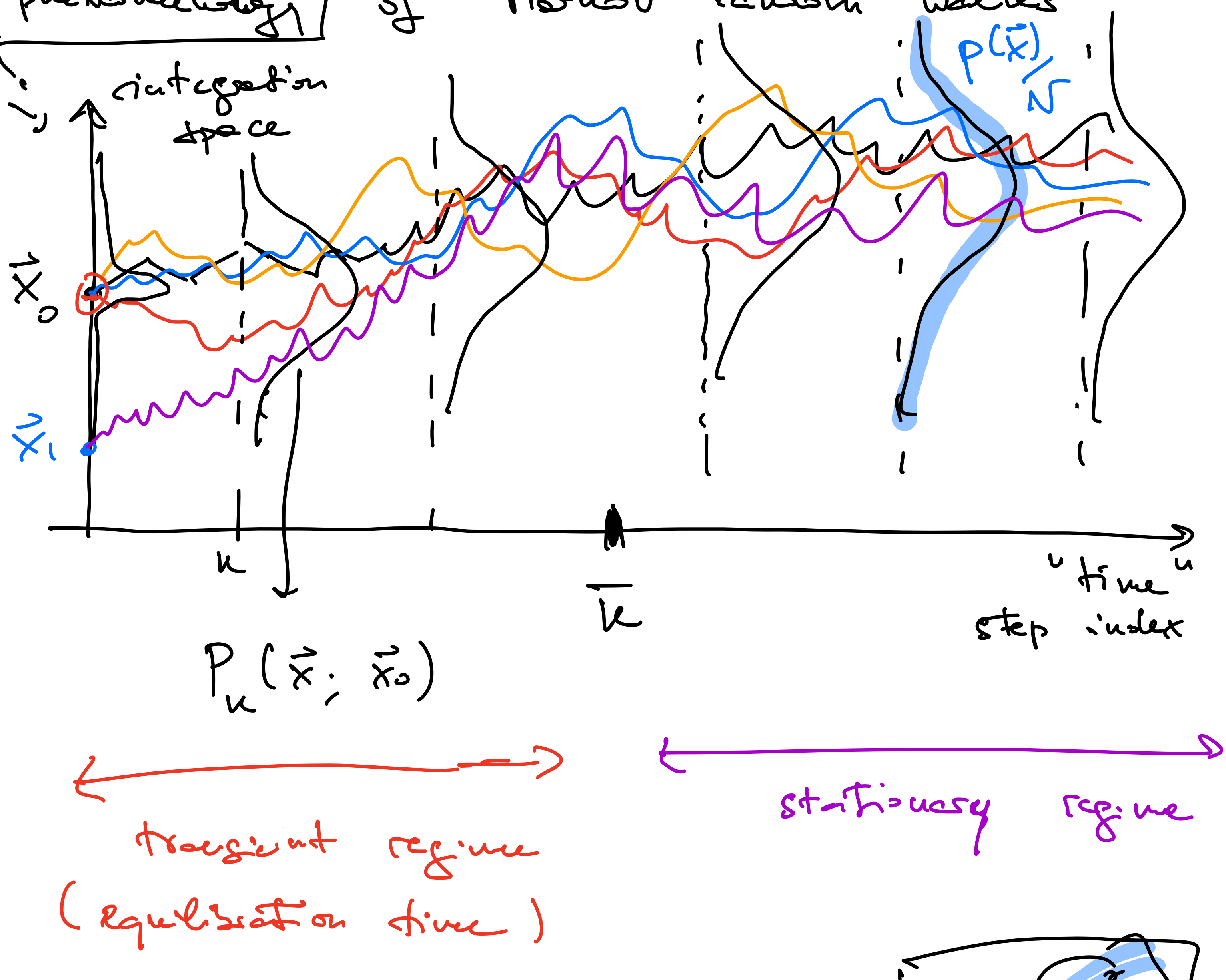


random walk : Markov process

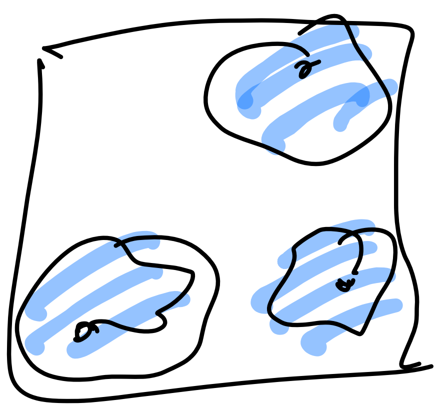
$\vec{x}_k$ is extracted by knowing $\vec{x}_{k-1}$

$T(\vec{x} \to \vec{y})$ transition probability

Phenomenology of Markov random walks



Evolution of $P_k(\vec{x}; \vec{x}_0)$



$$\frac{d P_u}{dt} = P_{u+1}(\vec{x}\,;\,\vec{x}_0) - P_u(\vec{x}\,;\,\vec{x}_0)$$

$$= \sum_{\vec{y}} \Big[P_{\cancel{u}}(\vec{y}\,;\,\cancel{\vec{x}_0})\, T(\vec{y}\to\vec{x}) - P_{\cancel{u}}(\vec{x}\,;\,\cancel{\vec{x}_0})\, T(\vec{x}\to\vec{y}) \Big] = 0$$

stationary regime

$$P_u(\vec{x}\,;\,\vec{x}_0) \hookrightarrow P(\vec{x}) = \frac{p(\vec{x})}{N}$$ forget

$$\vec{x} = (\uparrow\downarrow\uparrow\uparrow\downarrow\ldots)$$ # of configurations is 2^N

T $\quad 2^N \times 2^N$ matrix

solution :

$$\frac{p(\vec{y})}{\cancel{N}}\, T(\vec{y}\to\vec{x}) = \frac{p(\vec{x})}{\cancel{N}}\, T(\vec{x}\to\vec{y})$$

detailed balance condition

$$T(\vec{x} \to \vec{y}) = \frac{p(\vec{y})}{p(\vec{x})} \, T(\vec{y} \to \vec{x})$$

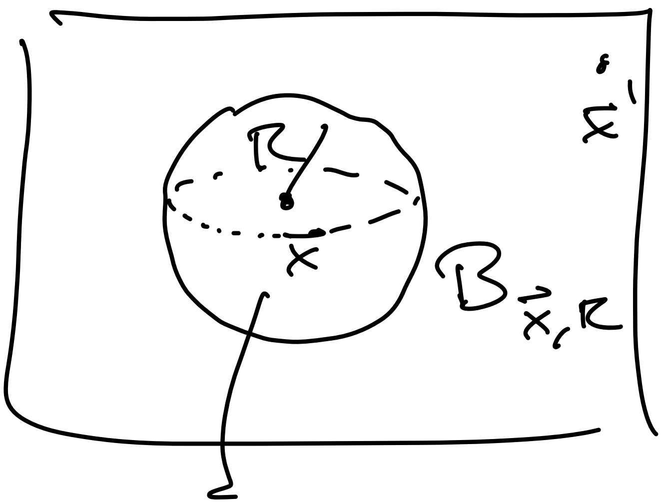
proposal probability (density)

$$T(\vec{x} \to \vec{y}) = T_{prop}(\vec{x} \to \vec{y}) \, A(\vec{x} \to \vec{y})$$

geometric

acceptance probability

ex.



$$T_{prop}(\vec{x} \to \vec{y}) = T_{prop}(\vec{y} \to \vec{x})$$

extract $\vec{y}$ at random from $B_{\vec{x},R}$

$$A(\vec{x} \to \vec{y}) = \frac{p(\vec{y})}{p(\vec{x})} \, A(\vec{y} \to \vec{x})$$

Metropolis-Hastings solution

$$A(\vec{x}\to\vec{y}) = \min\left(1, \frac{p(\vec{y})}{p(\vec{x})}\right)$$

Build a sample of $\frac{p(\vec{x})}{N}$

k-th step.

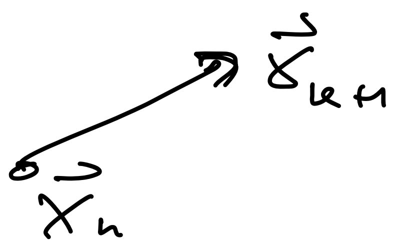
1) $\vec{X}_k \to$ propose $\vec{y}$ with $T_{prop}(\vec{x}_k\to\vec{y})$

2) extract rand. number $z\in[0,1]$

3) $z \le A(\vec{x}_k\to\vec{y}) \Rightarrow \vec{x}_{k+1}=\vec{y}$

otherwise $\Rightarrow \vec{x}_{k+1}=\vec{x}_k$

4) goto 1



$(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_L)$ sample

$$I_L = \frac{1}{L} \sum_{n=1}^{L} g(\vec{x}_n) \underset{L\to\infty}{\simeq} I$$

$$= \sum_j \frac{n(\vec{x}_j)}{L}\, g(\vec{x}_j)$$

$$\underset{L\to\infty}{\simeq} p(\vec{x}_j)\ \frac{d^D x}{N}$$