Quantum Monte Carlo for quantum many-body systems

N quantum particles

$$\hat{\mathcal{H}} = \underbrace{\sum_{i=1}^{N} \hat{\mathcal{H}}_i}_{\text{one-body term}} + \underbrace{\sum_{i<j} \hat{V}_{ij}}_{\text{two-body term}} \left(+ \sum_{i<j<k} \hat{W}_{ijk} + \dots \right)$$

→ particles in continuum space

$\hat{\vec{x}}_i$, $\hat{\vec{p}}_i$

$$\hat{\mathcal{H}}_i = \frac{\vec{p}_i^{\,2}}{2m_i} + \underbrace{V(\hat{\vec{r}}_i)}_{\text{scalar potential}} \qquad \text{(first quantization)}$$

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

→ lattice gas of indistinguishable particles

$\hat{c}_{i\sigma}$, $\hat{c}^{\dagger}_{i\sigma}$ $\qquad$ $i =$ "mode index" $\qquad$ $i = 1, \dots$ position, momentum, ...

$$\boxed{\begin{array}{ll} [\hat{c}_{i\sigma}, \hat{c}^{\dagger}_{j\sigma'}] = \delta_{ij}\delta_{\sigma\sigma'} & \text{BOSONS} \\ \{\hat{c}_{i\sigma}, \hat{c}^{\dagger}_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'} & \text{FERMIONS} \end{array}}$$

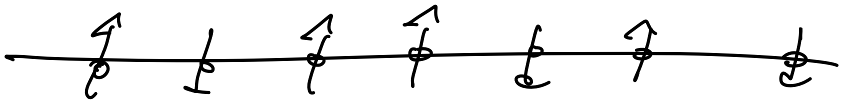
$$\hat{\mathcal{H}}_i = -\sum_{\sigma} \mu_{i\sigma} \hat{n}_{i\sigma} + \cancel{\sum_{\sigma} \frac{U_\sigma}{2} \hat{n}_{i\sigma}(\hat{n}_{i\sigma} - 1)} + \underbrace{\sum_{\sigma\sigma'} V_{\sigma\sigma'} n_{i\sigma} n_{i\sigma'}}_{+\dots}$$

$\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}$

$$\hat{V}_{ij} = -J_{ij\sigma\sigma'} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma'} + c^{\dagger}_{j\sigma'} c_{i\sigma} \right) + U_{i\sigma;j\sigma'} \hat{n}_{i\sigma} \hat{n}_{j\sigma'} + \dots$$

(Hubbard models)

→ lattice spin models



$$\hat{\vec{S}}_i = \left(\hat{S}_i^x, \hat{S}_i^y, \hat{S}_i^z\right)$$

$$\left[\hat{S}_i^\alpha, \hat{S}_j^\beta\right] = i\,\epsilon_{\alpha\beta\gamma}\,\hat{S}_i^\gamma\,\delta_{ij}$$

$$\epsilon_{\alpha\beta\gamma} = \begin{cases} 1 & \alpha\beta\gamma \text{ is an even permut. of } xyz \\ -1 & \text{" " odd "} \\ 0 & \text{otherwise} \end{cases}$$

$$\hat{H}_i = -\vec{h}_i \cdot \hat{\vec{S}}_i + \sum_\alpha B_i^\alpha \left(\hat{S}_i^\alpha\right)^2 + \dots$$

$$\hat{U}_{ij} = -\sum_{\alpha\beta} J_{ij}^{\alpha\beta}\,\hat{S}_i^\alpha\,\hat{S}_j^\beta$$

<u>other examples</u> : quantum field theory

etc...

QMC: equilibrium physics of quantum many-body systems

Temperature T

$$, \; N, \; \mu, \; \ldots, \; P, \; V, \; \ldots$$

$$\langle \hat{A} \rangle_{T, \ldots} = \frac{\mathrm{Tr}\left[\hat{A} \, e^{-\beta \hat{H}} \right]}{\mathrm{Tr}\left[e^{-\beta \hat{H}} \right]} \qquad \beta = \frac{1}{k_B T}$$

$\uparrow$ observable

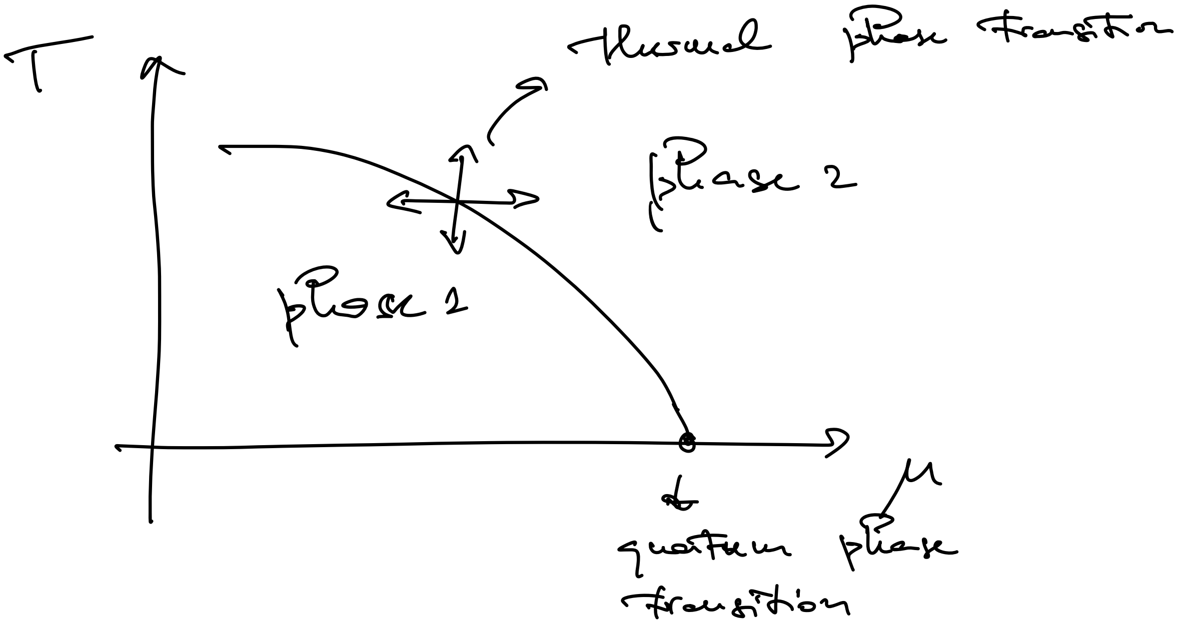
$\mathrm{Tr}\left[e^{-\beta \hat{H}} \right] \to Z$

$$\hat{H} = \hat{H}_0 - \mu \hat{N}$$

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

$$= \mathrm{Tr}\left[\hat{\rho} \, \hat{A} \right]$$

$\to$ phase diagrams



→ <u>low-energy spectrum</u>

$|\psi\rangle$ $\qquad\qquad$ $\hat{H}|\psi\rangle = E|\psi\rangle$

$$\downarrow$$

$$\langle \phi_\alpha|\hat{H}|\phi_\beta\rangle = H_{\alpha\beta}$$

$$\downarrow$$

$$\text{Dim}(H) \sim O(\exp(N))$$

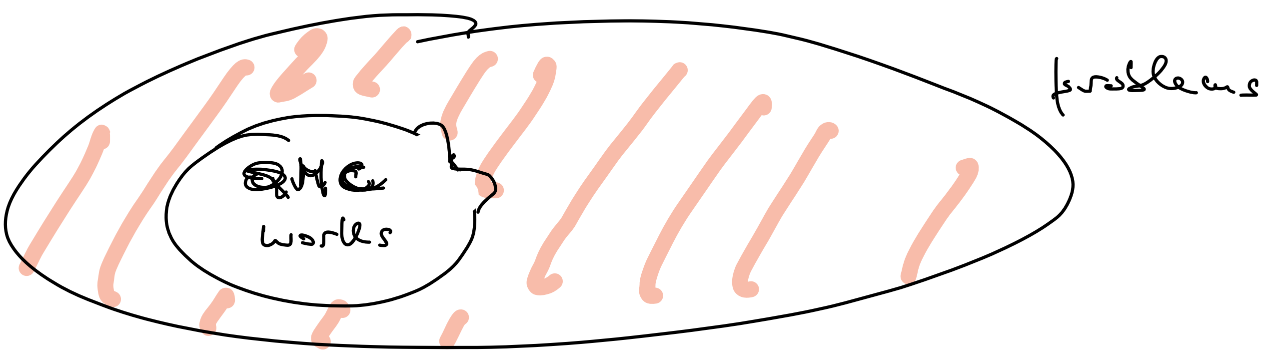
<u>Hard problem</u>

QMC <u>when it works</u> it gives

1) unbiased (numerically exact) prediction for $\underline{\langle \hat{A}\rangle_T}$, ...

2) prediction in polynomial time

$$t \sim O(N^\alpha)$$



Feynman (1982)

"Can quantum systems be probabilistically simulated by a classical computer?"

NO

in general

Monte Carlo method for numerical integration

$$\boxed{I = \frac{\sum_{\alpha} f_\alpha \, w_\alpha}{\sum_\alpha w_\alpha} = \langle f \rangle_w}$$

state, configuration in phase space

(statistical)

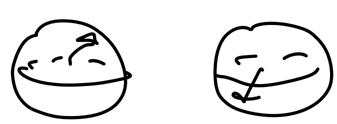
w_α = weights ≥ 0

$$p_\alpha = \frac{w_\alpha}{\sum_\beta w_\beta} \quad \text{probabilities}$$

classical d.o.f.

$$\alpha = \{\vec{x}_i, \vec{p}_i\} \qquad \sum_\alpha \longleftrightarrow \int \prod_{i=1}^{N} d^d x_i \, d^d p_i$$

$$\alpha = \{\vec{S}_i\}$$



$\{\sigma_i\}$ $\uparrow$ $\downarrow$ $\uparrow$ $\downarrow$

...

$$Z = \sum_\alpha w_\alpha$$ partition function

$$Z = Z(T, V, N, \dots)$$

$$F = -k_B T \log Z$$

$$\frac{\partial(\beta F)}{\partial \beta} = U$$ internal energy

$$= \langle \mathcal{H} \rangle$$

$$-\frac{\partial F}{\partial T} = S$$ entropy

$$-\frac{\partial F}{\partial V} = P$$

etc...

Even though # of α configurations is $O(\exp(N))$

ex. $\uparrow \quad \downarrow \quad \uparrow \quad \uparrow \quad \cdots \quad \uparrow$

$\sigma_1 \quad \sigma_2 \quad \cdots \quad \sigma_N$

2^N possible α configurations

MC gives you a result in $O(\text{poly}(N))$ time

<u>Our problem</u> :

$$\langle \hat{A} \rangle_T = \frac{\text{Tr}\left[e^{-\beta \hat{H}} \hat{A}\right]}{Z}$$

$\{|\phi_\alpha\rangle\}$ basis of H

$f_\alpha w_\alpha$

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

$|\phi_\alpha\rangle$ eigenbasis of $\hat{H}$

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

$$= \frac{\sum_\alpha e^{-\beta E_\alpha} \underbrace{\langle \phi_\alpha | \hat{A} | \phi_\alpha \rangle}_{\to f_\alpha}}{\sum_\alpha e^{-\beta E_\alpha}} \qquad e^{-\beta E_\alpha} \to w_\alpha$$

PMC is not about sampling this sum

Quantum-to-classical mapping

$$\langle \hat{A} \rangle_T =: \frac{\sum_c A_c \, e^{-S_c}}{\sum_c e^{-S_c}} \qquad e^{-S_c} \rightarrow w_c$$

c is not a quantum state

it is a "configuration" in some space

A_c is not $\langle \psi | \hat{A} | \psi \rangle$

is "estimator"

S_c is not $\langle \psi | \hat{H} | \psi \rangle$

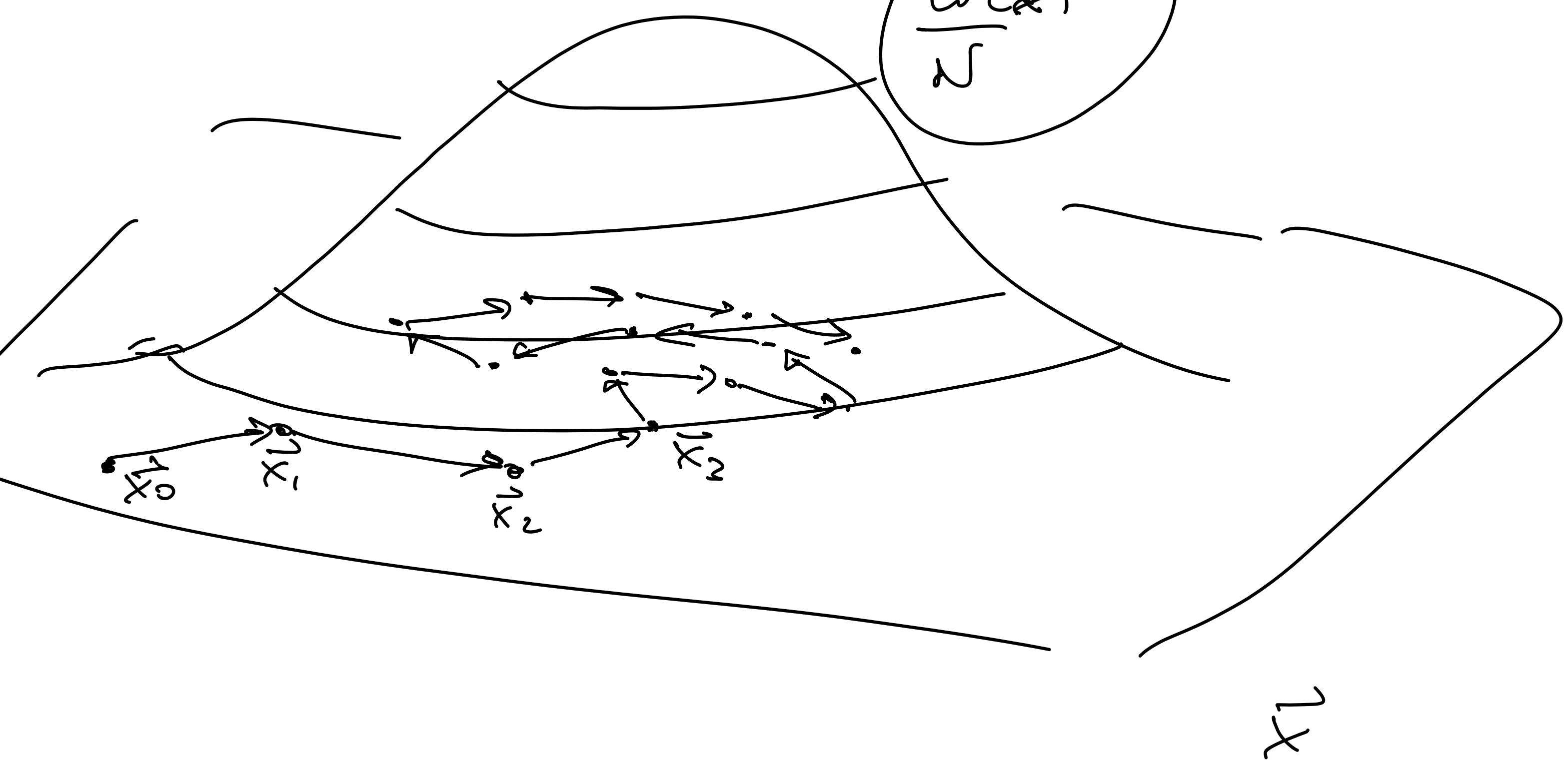
Monte Carlo method

$$I = \int d^D x \; f(\vec{x}) \, \frac{w(\vec{x})}{N} = \langle f \rangle_w$$

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

$$\vec{x} = (x_1, x_2, \ldots, x_D)$$

$$\frac{w(\vec{x})}{N}$$



Markov chain (random walk)

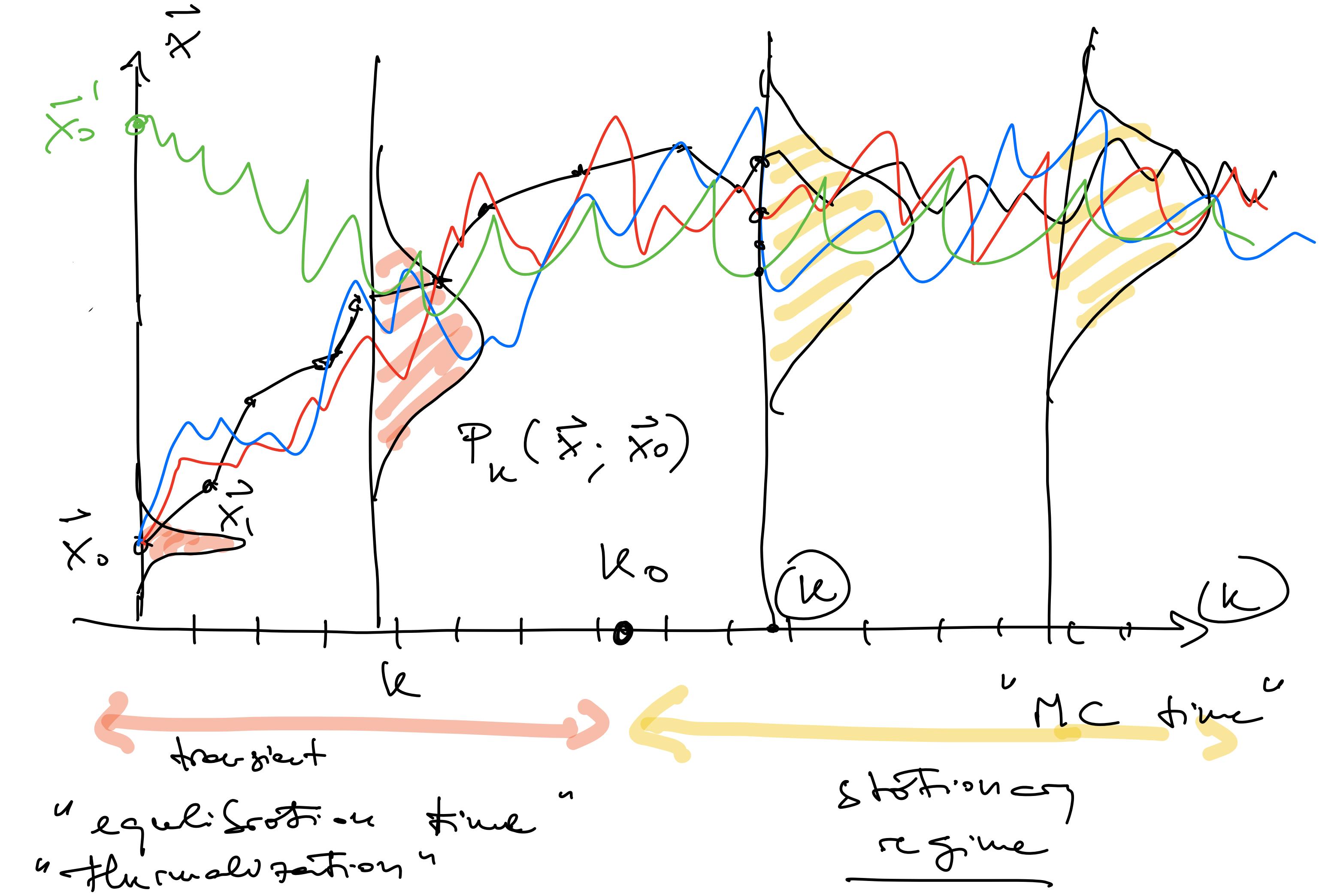
$$\vec{x}_0 \to \vec{x}_1 \to \vec{x}_2 \to \cdots \to \vec{x}_t$$

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

$$I_L = \frac{1}{L}\sum_{k=1}^{L} f(\vec{x}_k) \xrightarrow[L\to\infty]{} I$$

→ How do you build $T(\vec{x} \to \vec{y})$?

→ How does I_L converge to I ?



$$\boxed{T(\vec{x} \to \vec{y})}$$

$$P_0(\vec{x};\vec{x}_0) = \delta(\vec{x} - \vec{x}_0)$$

$$P_k(\vec{x};\vec{x}_0) \underset{k \gtrsim k_0}{=} P(\vec{x}) = \frac{w(\vec{x})}{N}$$

we want it to coincide $\frac{w(\vec{x})}{N}$

=

$$\boxed{I_L = \frac{1}{L}\sum_{k=k_0}^{k_0+L} f(\vec{x}_k)} \xrightarrow[L\to\infty]{} I$$

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

$$\frac{dP_k(\vec{x},\vec{x}_0)}{dt} = P_{k+1}(\vec{x};\vec{x}_0) - P_k(\vec{x};\vec{x}_0)$$

$$= \sum_{\vec{q}} P_k(\vec{q};\vec{x}_0)\, T(\vec{q}\to\vec{x}) - \sum_{\vec{q}} P_k(\vec{x};\vec{x}_0)\, T(\vec{x}\to\vec{q})$$

$$= 0$$

stationary regime

$P(\vec{x})$

$$\sum_{\vec q}\left[\frac{w(\vec q)}{\cancel{\Delta f}}\, T(\vec q \to \vec x) - \frac{w(\vec x)}{\cancel{\Delta f}}\, \underbrace{T(\vec x \to \vec q)}_{=0}\right]$$

$=$

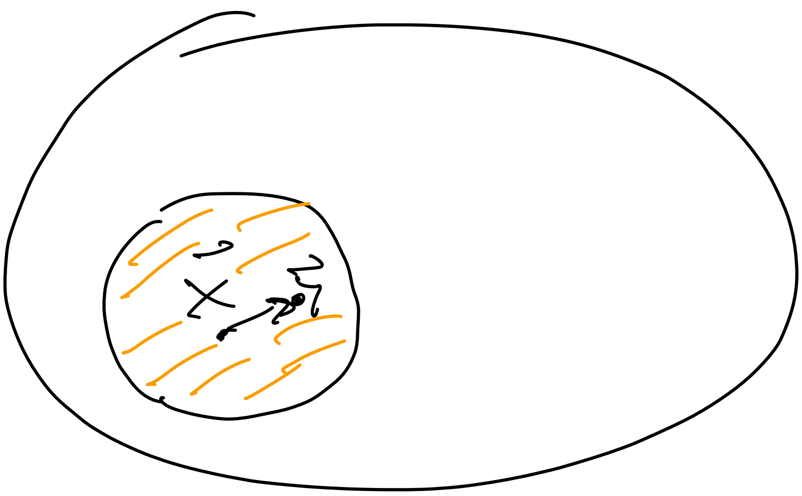
special solution

$$w(\vec q)\, T(\vec q \to \vec x) - w(\vec x)\, T(\vec x \to \vec q) = 0$$

"detailed balance condition"

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

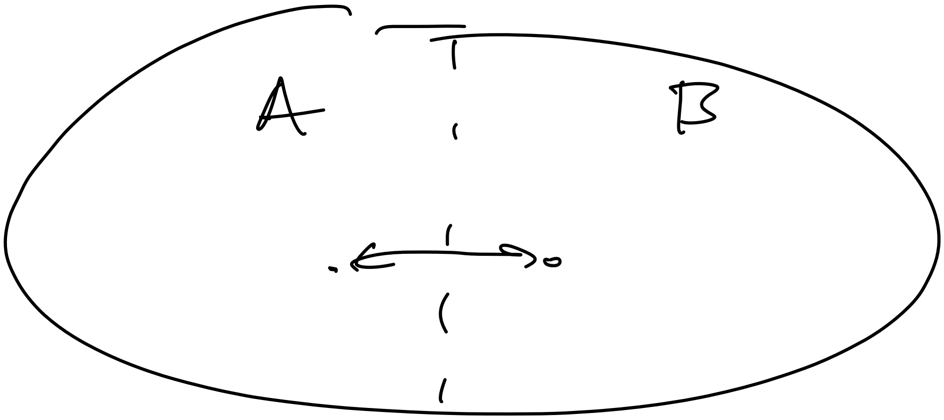
proposal probability — acceptance probability



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

"ergodicity"

bad
choice



any configuration $\vec{x}$ should be reachable from any conf. $\vec{y}$ in a finite # of steps.

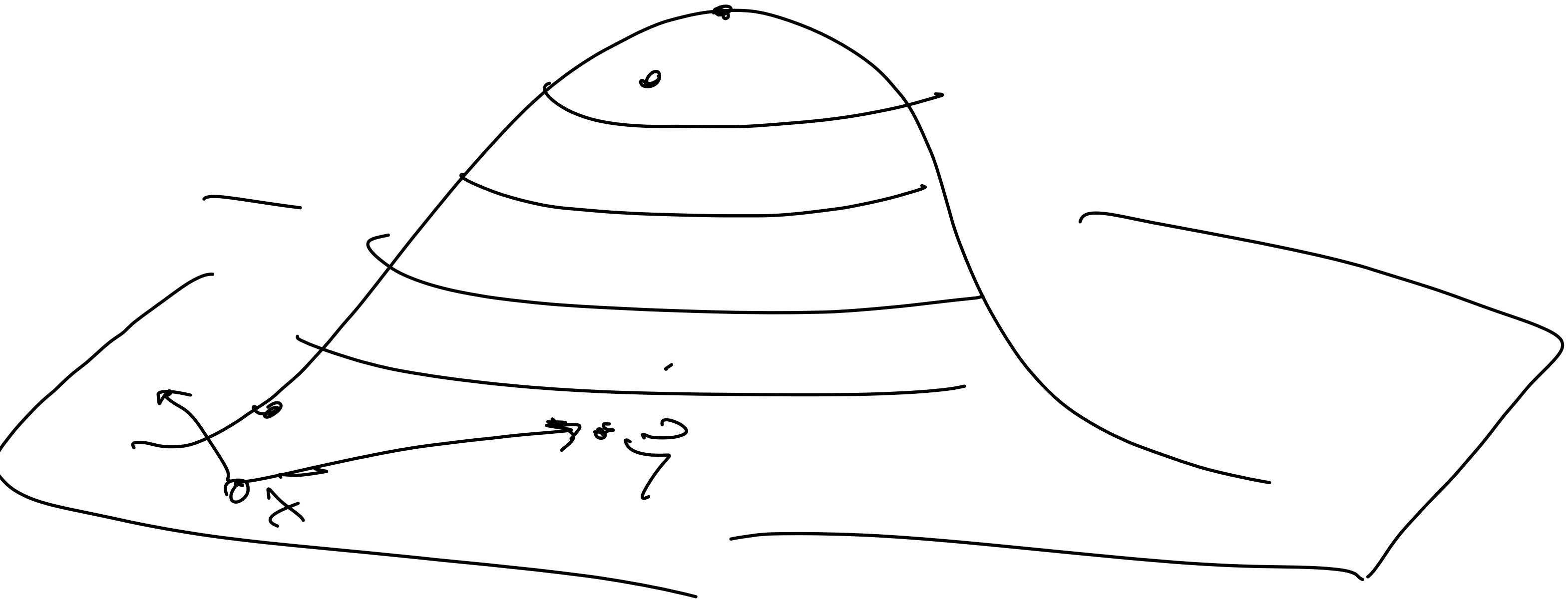
$$w(\vec{x})\, \cancel{T_{prop}(\vec{x} \to \vec{y})}\, A(\vec{x} \to \vec{y})$$

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

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

Metropolis - Hastings solution

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



Algorithm (Metropolis - Hastings)

→ pick $\vec{x}_0$ at random

→ propose $\vec{y}$ with $T_{prop}(\vec{x}_0 \to \vec{y})$

→ extract $z \in [0, 1]$

→ if $z < A(\vec{x}_0 \to \vec{y})$

$\vec{x}_1 = \vec{y}$

otherwise $\vec{x}_1 = \vec{x}_0$

$$I_L = \frac{1}{L} \sum_{k=k_0}^{k_0+L} f(\vec{x}_k) \xrightarrow[L \to \infty]{} I \quad ?$$

how fast

&

$f(\vec{x}_k)$ random variables

$$\int d^{d}x \; f(\vec{x}_k) \left(\frac{w(\vec{x})}{N}\right) = \bar{f} = I$$

$$\to \sigma_f^2 = \overline{f^2} - \bar{f}^2$$

$$\overline{I_L} = \frac{1}{L} \sum_{k=k_0}^{k_0+L} f(\vec{x}_k) = I \to I$$

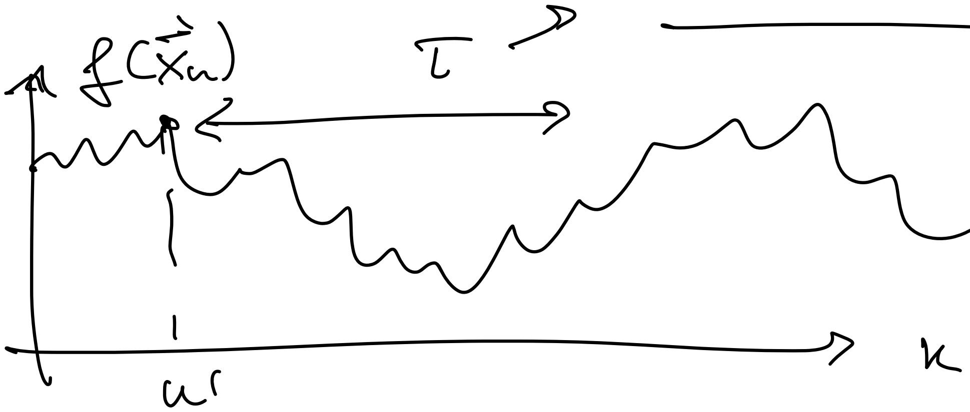
$$\sigma_{I_L}^2 \overset{?}{=} \frac{L\,\sigma_f^2}{L^2} = \frac{\sigma_f^2}{L}$$

central limit Theorem (applies to sums of independent random variables)

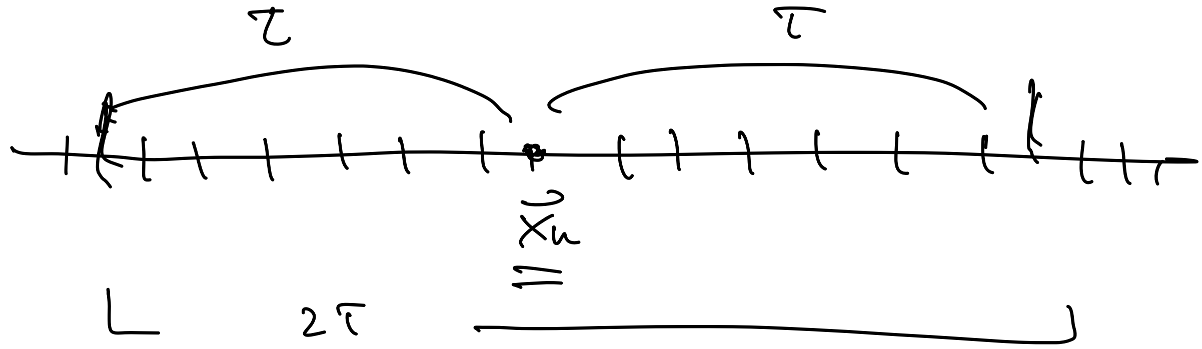
$$|I_L - I| \simeq \sigma_{I_L} \sim O\left(\frac{1}{\sqrt{L}}\right)$$

$$\sigma_{I_L}^2 \sim \frac{1}{L}$$

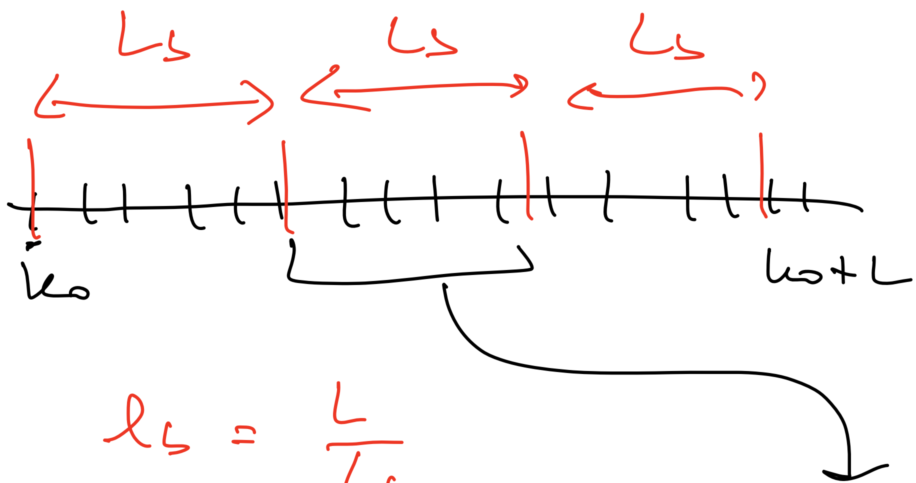
auto-correlation time



$$\sigma_{I_L}^2 = \frac{\sigma_f^2}{L_{eff}} \qquad L_{eff} = \frac{L}{2\tau}$$



$$I_L = \frac{1}{L} \sum_{n=k_0}^{k_0+L} f(\vec{x}_n)$$

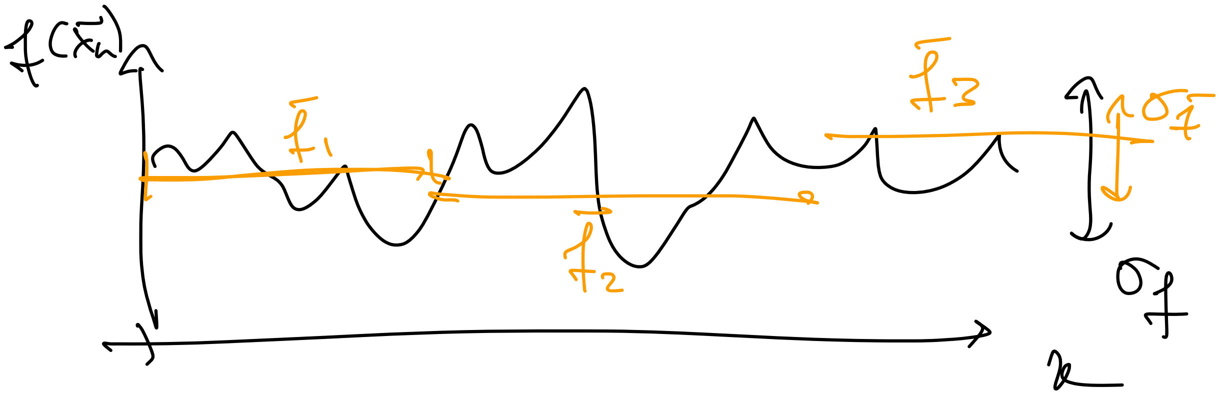


$$l_b = \frac{L}{L_b}$$

$$I_L = \frac{1}{l_b} \sum_{a=1}^{l_b} \underbrace{\frac{1}{L_b} \sum_{j=1}^{L_b} f(\vec{x}_{(a-1)L_b+j})}_{\bar{f}_a \text{ block averages}}$$

if $\underline{L_b \gg \tau}$ $\quad \{\bar{f}_a\}$ are statistically independent

$$\sigma^2_{I_L} = \frac{\sigma^2_{\bar{f}_a}}{l_b} = \frac{\sigma^2_f}{(L/2\tau)}$$



$$\boxed{\tau = \frac{1}{2}\left(\frac{L}{\ell_b}\right)\frac{\sigma_{\bar{f}}^2}{\sigma_f^2}}$$

$L_b \gtrsim \tau$

$\tau \sim$ ko

$$\underline{|I_L - I|} \simeq \sigma_{I_L} = \sqrt{\frac{2\tau}{L}}\,\sigma_f$$

How does τ scale with N ?
(D)

$\tau \sim N^{z/d}$ $d =$ # of physical dimension

$z =$ dynamical exponent

$z \sim O(1)$

Quantum-to-classical mapping

⟹ Single particle in an external potential

↪ path-integral formulation of quantum statistical mechanics

$$\hat{H} = \frac{\hat{\vec{p}}^{\,2}}{2m} + U(\hat{\vec{x}})$$

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right]$$

basis of $\hat{\vec{x}}$: $|\vec{x}\rangle$

$$= \int d^d x \, \langle \vec{x} | e^{-\beta H} | \vec{x} \rangle$$

$$\langle \vec{x} | e^{-\beta H} | \vec{x}\,' \rangle = \rho(\vec{x}, \vec{x}\,'; \beta)$$

imaginary-time propagator

$$\int \rho(\vec{x}, \vec{x}; \beta) \, d^d x = Z$$

$$\langle \vec{x} | e^{-i\frac{t}{\hbar} H} | \vec{x}\,' \rangle = \text{amplitude of going in time } t \text{ from } |\vec{x}\,'\rangle \text{ to } |\vec{x}\rangle$$

$\frac{t}{\hbar} \leftrightarrow \beta$

t: time

$\hbar$

= propagator

$$\beta = \frac{it}{\hbar} \qquad (\text{"imaginary time"})$$

$$\langle \vec{x} | e^{-\beta H} | \vec{x}' \rangle = \rho(\vec{x}, \vec{x}'; \beta)$$

$$= \langle \vec{x} | e^{-\beta\left(\frac{\vec{p}^2}{2m} + U(\vec{x})\right)} | \vec{x}' \rangle$$

$$\underbrace{e^{-\beta\left[\frac{p^2}{2m} + U(\vec{x})\right]} = e^{-\frac{\beta}{2m}\vec{p}^2}\, e^{-\beta U}\, e^{c}}$$

$$[U, \vec{p}^2] \neq 0$$

$$\left[e^{-\frac{\beta}{M}\left(\frac{p^2}{2m} + U(\vec{x})\right)}\right]^M$$

$$= \left[e^{-\beta/M \frac{p^2}{2m}}\, e^{-\frac{\beta}{M} U}\, \underbrace{e^{O\left(\frac{\beta^2}{M^2}\right)}}_{\left(1 + O\left(\frac{\beta}{M^2}\right)\right)}\right]^{M}$$

$$= \underbrace{\left[e^{-\frac{\beta}{M}\frac{p^2}{2m}} \, e^{-\frac{\beta}{M} U(\vec{x})} \right]^M}_{\downarrow} + O\left(\frac{p^2}{M}\right)$$

$\xrightarrow[M \to \infty]{}$ Lie - Trotter - Suzuki formula

$$\rho(\vec{x}, \vec{x}'; \beta) =$$

$$\lim_{M \to \infty} \langle \vec{x} | \left[e^{-\frac{\beta}{M}\left[\frac{\hat{\vec{p}}^2}{2m} + \hat{U}(\vec{x})\right]} \right]^M | \vec{x}' \rangle$$

$$= \lim_{M \to \infty} \langle \vec{x} | \underbrace{\left[e^{-\frac{\beta}{M}\frac{\hat{\vec{p}}^2}{2m}} \, e^{-\frac{\beta}{M}\underline{\underline{\hat{U}(\vec{x})}}} \right]^M}_{} \underline{\underline{| \vec{x}' \rangle}}$$

$$\int d^d x \, | \vec{x} \rangle \underline{\underline{\langle \vec{x} |}} = \underline{\mathbb{1}}$$

$$= \lim_{M \to \infty} \int \left(\prod_{k=1}^{M-1} d^d x_k \right)$$

$$\langle \vec{x} | e^{-\beta/M \frac{p^2}{2m}} | \vec{x}_1 \rangle \, e^{-\frac{\beta}{M} U(\vec{x}_1)}$$

$$\langle \underline{\underline{\vec{x}_1}} | e^{-\beta/M \frac{\vec{p}^2}{2m}} | \vec{x}_2 \rangle \, e^{-\beta/M \, U(\vec{x}_2)}$$

$$\cdots \langle \vec{x}_{M-1} | e^{-\beta/M \frac{p^2}{2m}} | \vec{x}' \rangle \, e^{-\beta/M \, U(\vec{x}')}$$

$$\underline{\vec{x}'' = \vec{x}_M}$$

$$= \lim_{M\to\infty} \int \left(\prod_{n=1}^{M-1} d^d x_n \right) \underline{\langle \vec{x} | e^{-\frac{\beta}{M} \frac{p^2}{2m}} | \vec{x}_1 \rangle}$$

$\vec{x}_0$

$$\underline{\langle \vec{x}_1 | e^{-\frac{\beta}{M} \frac{\vec{p}^2}{2m}} | \vec{x}_2 \rangle} \cdots \langle \vec{x}_{M-1} | e^{-\frac{\beta}{M} \frac{\vec{p}^2}{2m}} | \vec{x}_M \rangle$$

$$\underline{e^{-\frac{\beta}{M} \sum_{n=1}^{M} U(\vec{x}_n)}}$$

$$\langle \vec{x} | \vec{x}' \rangle = \delta(\vec{x} - \vec{x}')$$

$$\langle \vec{x} | e^{-\frac{\beta}{M} \frac{\vec{p}^2}{2m}} | \vec{x}' \rangle$$

free propagator

$$\int |\vec{p}\rangle\langle\vec{p}| \, d^d p = \mathbb{1}$$

$$= \int \frac{d^d p}{(2\pi\hbar)^d} \, \underline{e^{-\frac{\beta}{M} \frac{p^2}{2m}} \, e^{i/\hbar \, \vec{p}\cdot(\vec{x} - \vec{x}')}}$$

$$\langle \vec{x} | \vec{p} \rangle = \frac{e^{\frac{i}{\hbar} \vec{p} \cdot \vec{x}}}{(2\pi\hbar)^{d/2}}$$

$$= \prod_{j=1}^{d} \underbrace{\int_{-\infty}^{+\infty} \frac{dp_j}{2\pi\hbar} \, e^{-\frac{\beta}{M} \frac{p_j^2}{2m} - \frac{i}{\hbar} p_j (x_j - x_j')}}_{}$$

$$\int_{-\infty}^{+\infty} dx \, e^{-x^2} = \sqrt{\pi}$$

$$= \left(\frac{2\pi m M}{\beta} \right)^{\frac{d}{2}} \frac{1}{(2\pi\hbar)^d} \, e^{-\frac{m M}{2\beta\hbar^2} |\vec{x} - \vec{x}'|^2}$$

$$\lambda = \frac{h}{\sqrt{2\pi m k_B T}} = \sqrt{\frac{2\pi \hbar^2 \beta}{m}}$$

$$\frac{m}{2\beta\hbar^2} = \frac{\pi}{\lambda^2}$$

$$= \frac{M^{d/2}}{\lambda^d} \, \underbrace{e^{-\frac{\pi M}{\lambda^2} |\vec{x} - \vec{x}'|^2}}_{}$$

$$\vec{x}_0 = \vec{x}$$

$$\rho(\vec{x}, \vec{x}'; \beta)$$

$$= \lim_{M\to\infty} \int \left(\prod_{n=1}^{M-1} d^d x_n\right) \frac{M^{d/2}}{\lambda^d}\, e^{-\frac{\pi M}{\lambda^2}\sum_{n=0}^{M-1}(\vec{x}_n - \vec{x}_{n+1})^2}\, e^{-\frac{\beta}{M}\sum_{n=1}^{M} U(\vec{x}_n)}$$

$d \quad 1$

$$Z = \int d^d x \; \rho(\vec{x}, \vec{x}; \beta)$$

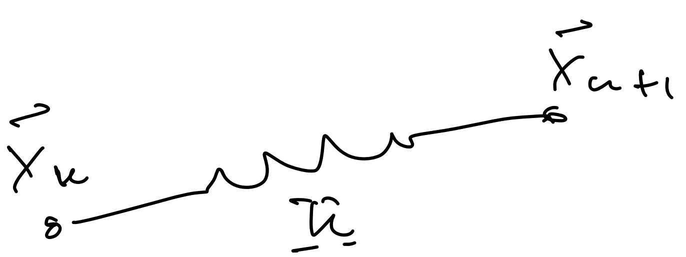
$$= \lim_{M\to\infty} \int \left(\prod_{n=1}^{M} d^d x_n\right) e^{-\beta \mathcal{H}_{eff}(\{\vec{x}_n\})} \left(\frac{M^{d/2}}{\lambda^d}\right)^M$$

$\frac{1}{2\sigma^2\beta}$ $\qquad K\beta = \frac{1}{\sigma^2}$

$d \quad 1$

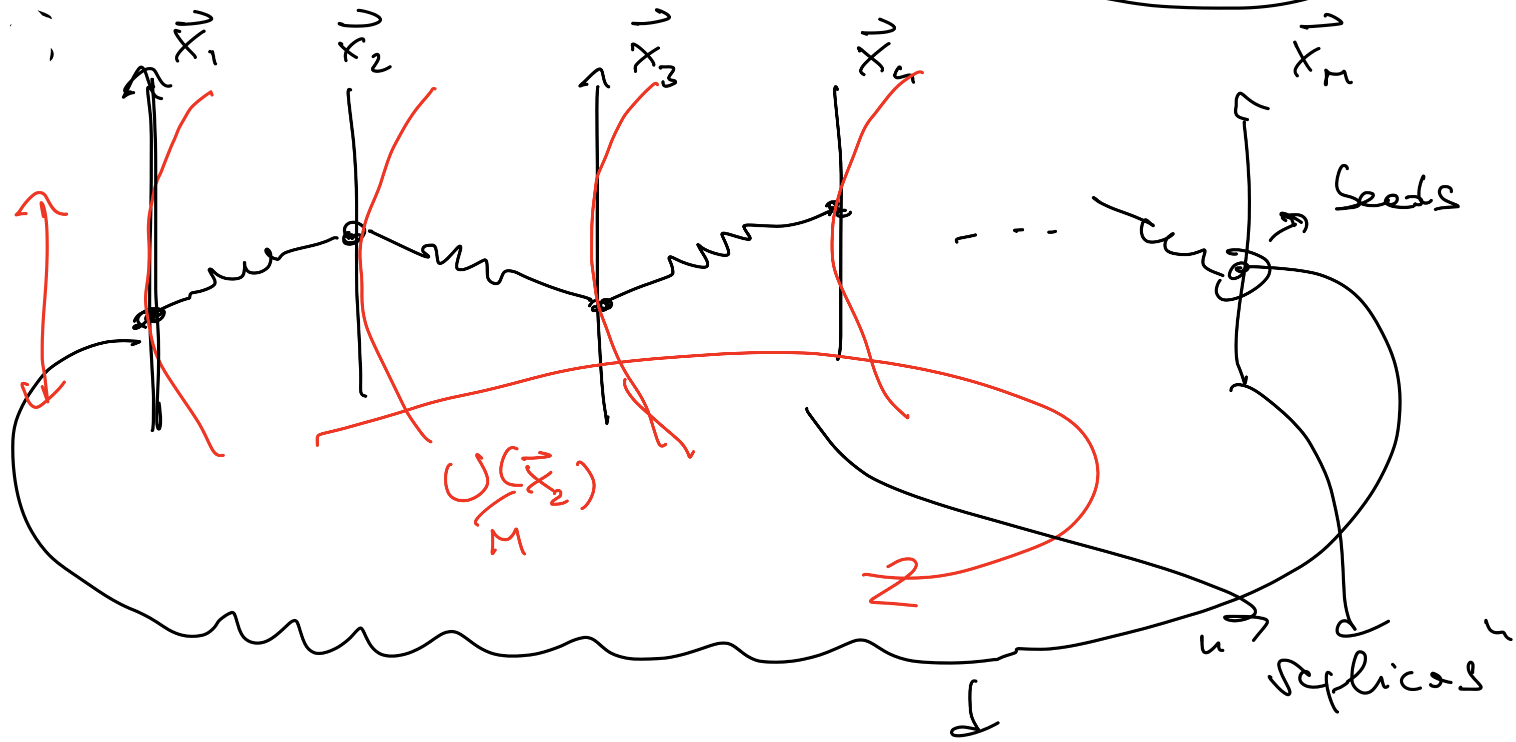
$$\mathcal{H}_{eff}(\{\vec{x}_n\}) = \sum_{n=0}^{M-1} \overbrace{\frac{\pi M}{\beta\lambda^2}}^{\frac{1}{2}K} (\vec{x}_n - \vec{x}_{n+1})^2 + \frac{1}{M}\sum_{n=1}^{M} U(\vec{x}_n)$$

$$\vec{x}_0 = \vec{x}_M$$



$$K = \frac{2\pi M}{\beta\lambda^2}$$

$$\sigma^2 = \frac{\lambda^2}{2\pi M}$$



$(d+1)$ "polymer"
dimensional

"Feynman path"

extra-dimension : $\Rightarrow$ imaginary time dimension
$\Rightarrow$ Trotter dimension

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$$\bar{\mu}_{=} = \frac{2\pi M}{\beta \Lambda^2} \sim \frac{(k_B T)^2}{\hbar^2} m$$

$\Lambda \sim \sqrt{\beta}$

$\Lambda \sim \frac{1}{\sqrt{m}}$

<u>classical limit</u>

$\hbar \to 0$

$T \to \infty$

$m \to \infty$

$\bar{\mu} \to \infty$

polymer → rigid

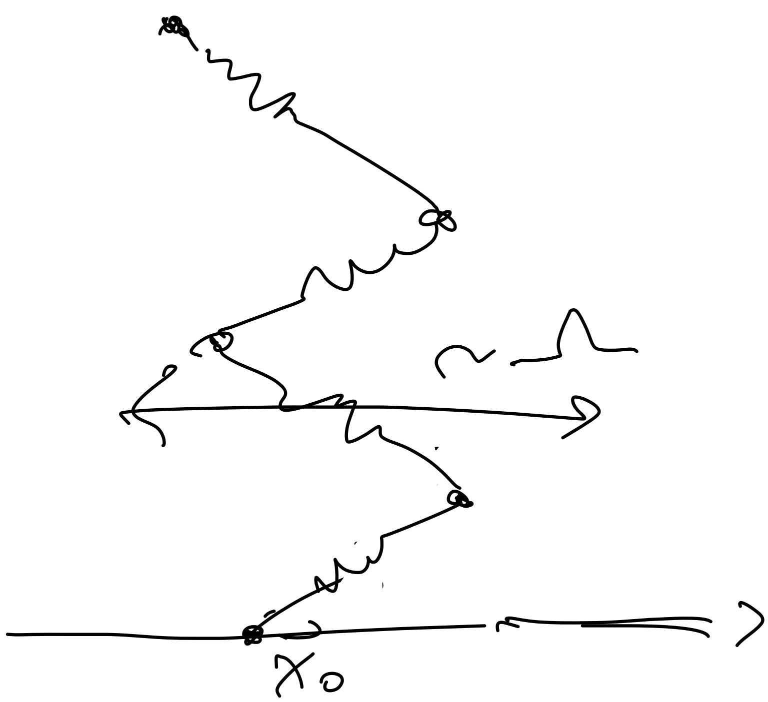
$$Z \sim \int d^d x \; e^{-\beta U(\vec{x})}$$

<u>quantum limit</u> $\quad \hbar \to 0$

$T \to 0$

"$\hbar \to \infty$"

$m \to 0$



$$x_n - x_0 = (x_1 - x_0) + (x_2 - x_1) + \ldots$$

$n \sim M$

Gaussian random var.

$\sigma^2 = \lambda^2 / 2\pi M$

$$|x_n - x_0| \sim \sqrt{M\sigma} \sim \Lambda$$

$$\langle U(\vec{x}) \rangle = \int d^d x \langle \vec{x} | U(\vec{x}) e^{-\beta H} | \vec{x}_M \rangle$$

$$= \lim_{M\to\infty} \frac{\int \left(\prod_{n=1}^{M} d^d x_n \right) U(\vec{x}_M)\, e^{-\beta H_{eff}(\{\vec{x}_n\})}}{\int \left(\prod_{n=1}^{M} d^d x \right) e^{-\beta H_{eff}(\{\vec{x}_n\})}}$$

$$\simeq \langle U(\vec{x}) \rangle_M + O\left(\frac{\beta^2}{M}\right) \rightarrow \text{Trotter error}$$

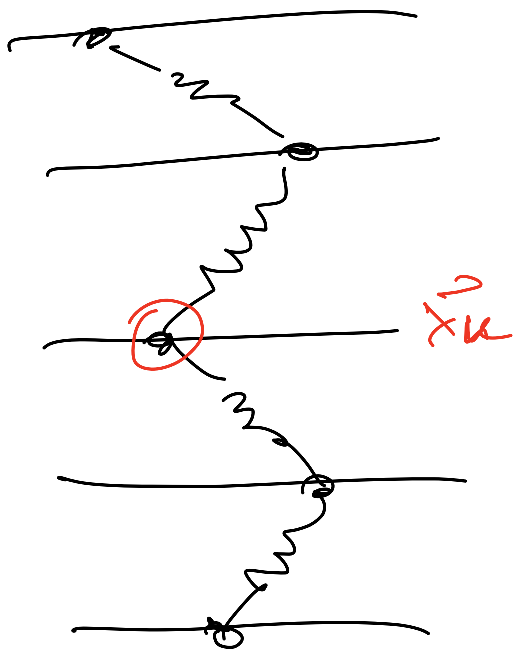
$$\downarrow$$

$$\sim \text{Good} \qquad O\left(\frac{\beta^3}{M^2}\right)$$

$$\left[e^{-\frac{\beta}{M}\left(\frac{p^2}{2m} + U(x)\right)} \right]^M \simeq \left[e^{-\frac{\beta}{2M} U(x)}\, e^{-\frac{\beta}{M}\frac{p^2}{2m}}\, e^{-\frac{\beta}{2M} U(x)} + O\left(\frac{\beta^3}{M^3}\right) \right]^M$$

$$= \; \dot{\alpha} + \underbrace{O\left(\frac{P^3}{M^2}\right)}_{\text{Trotter error}}$$

$\vec{x} \to \vec{\eta}$



1) pick a bead at random

2) move its position from $\vec{x}_k$ to $\vec{x}_k + \delta\vec{x}$

$\delta\vec{x}$ is extracted

$\delta\vec{x}$

$$\mathcal{H}_{eff} \rightarrow \mathcal{H}'_{eff} = \mathcal{H}_{eff}(\ldots, \vec{x}_n + \delta\vec{x}, \ldots)$$

$$A(\vec{x}_n \rightarrow \vec{x}_n + \delta\vec{x}) = \min\left(1, e^{-\beta(\mathcal{H}'_{eff} - \mathcal{H}_{eff})}\right)$$