Markov-Chain Monte Carlo

$M \to P$

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

$\vec{x}_n : \quad \vec{x}_1 \to \vec{x}_2 \to \dots \to \vec{x}_M$

$$\frac{n(\vec{x}_n)}{M} \xrightarrow[M \to \infty]{} \frac{p(\vec{x}_n) \, d^D x}{N}$$

$$I_M = \frac{1}{M} \sum_{n=1}^{M} g(\vec{x}_n) = \text{"}\sum_{\vec{x}}\text{"} \frac{n(\vec{x})}{M} g(\vec{x})$$

$$\underset{M \to \infty}{\simeq} I$$

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

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

$|I_M - I| \xrightarrow[M \to \infty]{} 0$ How ?

I_M is a sum of random variables

$g(\vec{x}_n)$ are random variables

$\vec{x}_n$ are distributed according to $p(\vec{x})$

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

$$\Rightarrow \overline{I_M} = I$$

$$\sigma^2_{I_M} \sim |I - I_M|^2$$

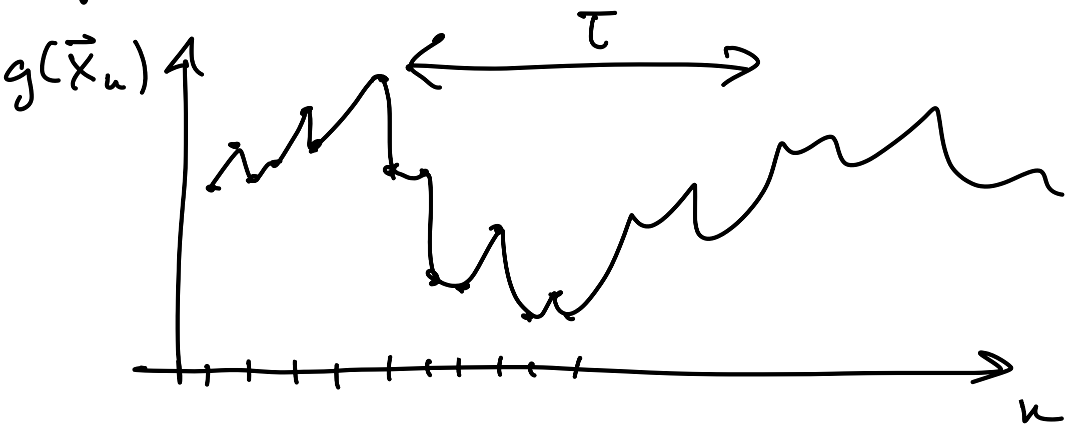
$g(\vec{x}_n)$ is a random variable

$\overline{g} = I$, σ_g^2 variance

$$\sigma^2_{I_M} \stackrel{?}{=} \frac{M \sigma_g^2}{M^2} = \frac{\sigma_g^2}{M}$$

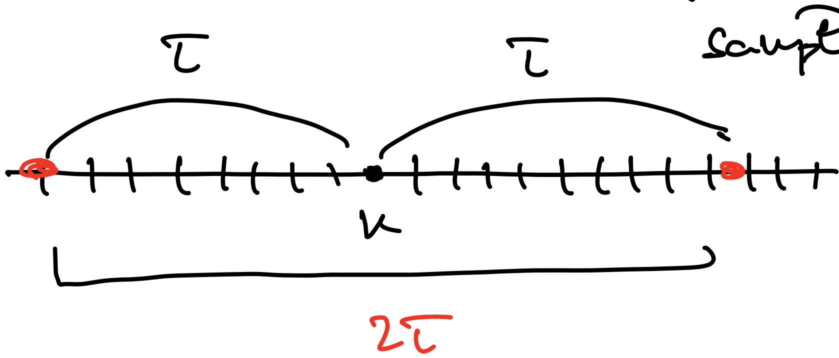
true if $g(\vec{x}_n)$ are independent random variables

equilibration time / autocorrelation time τ



M samples of $g(\vec{x}_n)$ $\to$ $M_{eff} = \frac{M}{2\tau}$

of effectively independent samples

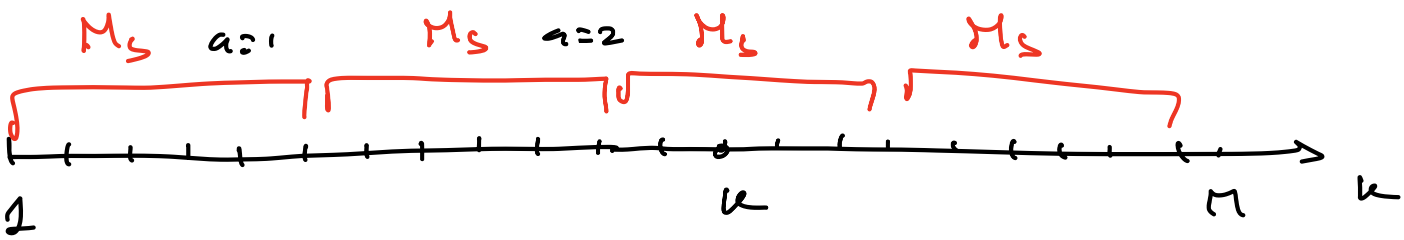


$$\sigma^2_{I_M} = \frac{\sigma_g^2}{M_{\text{eff}}} = \frac{2\tau}{M}\,\sigma_g^2$$

| central limit theorem

How to <u>estimate τ</u> ?

An independent estimate of $\sigma^2_{I_M}$:



$$n_b = \frac{M}{M_s} \qquad M_s \gtrsim \tau$$

$$I_M = \frac{1}{M}\sum_{k=\bar{k}+1}^{\bar{k}+M} g(\vec{x}_k) = \frac{1}{n_b}\sum_{a=1}^{n_b} \underbrace{\frac{1}{M_s}\sum_{j=1}^{M_s} g(\vec{x}_{\underset{\downarrow\, k}{(a-1)M_s+j}})}_{\bar{g}_a}$$

after having visited $\bar{k}$ configurations

<u>block average</u>

$M_s > \tau \rightarrow \bar{g}_a$ block averages are <u>independent</u>

$$I_M = \frac{1}{n_b} \sum_a \bar{g}_a$$

$\Rightarrow$ central limit theorem

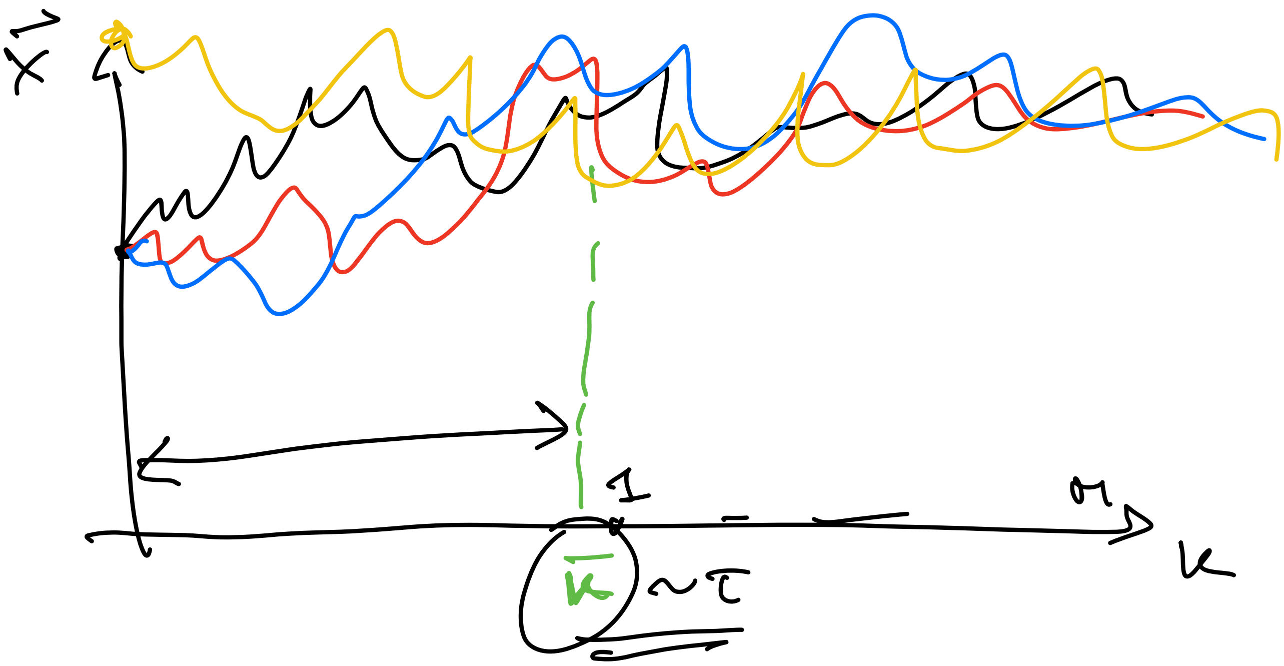
$$\sigma^2_{I_M} = \frac{\sigma^2_{\bar{g}}}{n_b}$$

$\sigma^2_{\bar{g}}$ variance of the fluctuations of $\bar{g}_a$

$$= \frac{2\tau}{M} \sigma_g^2$$

$\hookrightarrow$ variance of the fluctuations of $g(\vec{x}_k)$

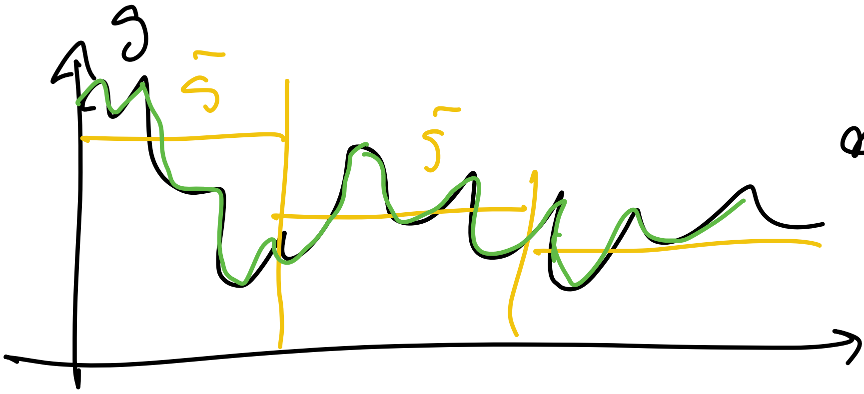
$$\boxed{\tau = \frac{1}{2} \frac{\sigma^2_{\bar{g}}}{\sigma_g^2} M_b}$$



__In practice__ : __guess__ $\bar{n}$ (thermalization time) ($\gtrsim \tau$)

__guess__ M_b ($\gtrsim \tau$)

estimate $\tau = \frac{1}{2} M_b \frac{\sigma_{\bar{g}}^2}{\sigma_g^2}$



$\Rightarrow$ if $\tau \lesssim M_b, \bar{n}$

✓ $$\sigma_{I_M}^2 = \frac{\sigma_{\bar{g}}^2}{n_b}$$

$$|I - I_M| \underset{M \to \infty}{\sim} \sqrt{\frac{2\tau}{M}} \, \sigma_g$$

$$\sim \sqrt{\frac{\tau}{M}}$$

$$\boxed{I = \int_V d^D x \, \frac{p(\vec{x})}{N} \, g(\vec{x})}$$

$\underline{V} = \underline{\underline{L}}^{D}$

$\tau = \tau(D, L)$?

luckily : $\boxed{\underline{\tau} \simeq A \, D \, \underline{L}^{z}}$ ←

$z \sim O(1)$ typically

→ z = dynamical exponent

typically $\underline{z = 2}$

⇒ Efficient estimate of $\underline{\tau}$

M → P

Path-integral formulation of quantum statistical mechanics

→ path-integral Monte Carlo (PIMC)

Single particle in continuum space

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

$$Z = \mathrm{Tr}\left(e^{-\beta\hat{\mathcal{H}}}\right) \qquad \beta = \frac{1}{k_B T}$$

$$\langle \hat{A} \rangle = \frac{\mathrm{Tr}\left(\hat{A}\, e^{-\beta\hat{\mathcal{H}}}\right)}{\mathrm{Tr}\left(e^{-\beta\hat{\mathcal{H}}}\right)} \qquad \vec{x} = (x_1, x_2, \dots, x_d)$$

$$Z = \sum_\alpha \langle\alpha|\, e^{-\beta\hat{\mathcal{H}}}\, |\alpha\rangle$$

$|\alpha\rangle \to |\vec{x}\rangle$ basis of the position operator(s) $\hat{x}_1, \hat{x}_2, \dots, \hat{x}_d$

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

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

$it = \beta$ imaginary-time propagator

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

(propagates)

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

Trotter-Lie decomposition

$$e^{-\beta\left(\frac{\hat{\vec{p}}^2}{2m}+U(\hat{\vec{x}})\right)} = \lim_{M\to\infty}\Big(\underbrace{e^{-\frac{\beta}{M}\left(\frac{\vec{p}^2}{2m}+U(\vec{x})\right)}}\Big)^M$$

$$e^{A} = \left(e^{A/M}\right)^M$$

$$= \lim_{M\to\infty}\left(e^{-\beta/M\,\frac{p^2}{2m}}\ e^{-\beta/M\,U(\vec{x})}\right)^M$$

diagonal on $|\vec{x}\rangle$

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

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

completeness relations

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

$$= \lim_{M\to\infty} \left[\int \left(\prod_{k=1}^{M-1} d^d x_k \right) \langle \vec{x} | \, e^{-\frac{\beta}{M}\frac{p^2}{2m}} \, \cancel{e^{-\frac{\beta}{M}U}} \, | \vec{x}_1 \rangle \langle \vec{x}_1 | \, e^{-\frac{\beta}{M}\frac{\vec{p}^2}{2m} - \frac{\beta}{M}U} \, | \vec{x}_2 \rangle \right.$$

$$\left. \cdots \langle \vec{x}_{M-1} | \, e^{-\frac{\beta}{M}\vec{p}^2/2m} \, | \vec{x}' \rangle \; e^{-\frac{\beta}{M}\left[U(\vec{x}_1) + U(\vec{x}_2) + \cdots + U(\vec{x}_{M-1}) + U(\vec{x}')\right]} \right]$$

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

evaluate the "free propagator"

$$\langle \vec{x}_k | \, e^{-\frac{\beta}{M}\frac{\hat{\vec{p}}^2}{2m}} \, | \vec{x}_{k+1} \rangle$$

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

$$= \int d^d p \, \underbrace{\langle \vec{x}_k | \vec{p} \rangle}\underbrace{\langle \vec{p} | \vec{x}_{k+1} \rangle} \, e^{-\frac{\beta}{M}\frac{\vec{p}^2}{2m}}$$

$$\frac{e^{\frac{i}{\hbar}\vec{p}\cdot(\vec{x}_k - \vec{x}_{k+1})}}{(2\pi\hbar)^d}$$

$$= \prod_{j=1}^{d} g\left(x_u^{(j)} - x_{u+1}^{(j)}\right)$$

$$g\left(x_u^{(j)} - x_{u+1}^{(j)}\right) = \int \frac{dp}{2\pi\hbar} e^{i p (x_u^{(j)} - x_{u+1}^{(j)})} e^{-\frac{\beta}{2Mm} p^2}$$

$$\dashrightarrow \frac{1}{2\pi\hbar}\sqrt{\frac{2\pi m M}{\beta}}\; e^{-\frac{mM}{2\beta\hbar^2}\left(x_u^{(j)} - x_{u+1}^{(j)}\right)^2}$$

$$\frac{\sqrt{M}}{\lambda}$$

$$\sim \ell^{-2}$$

de Broglie thermal wavelength

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

$$\langle \vec{x} |\, e^{-\beta \mathcal{H}} \,| \vec{x}' \rangle$$

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

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

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

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

$$= \lim_{M \to \infty} \left(\frac{M}{\Lambda} \right)^{\frac{1}{2} dM} \int \left(\prod_{n=1}^{M-1} d^d x_n \right) e^{-S[\{\vec{x}_n\}]}$$

$$\vec{x}_0 \quad \vec{x}_1 \quad \vec{x}_2 \quad \cdots \quad \vec{x}_{M-1} \quad \vec{x}_M = \vec{x}$$

$\frac{1}{2} \bar{K}$

$$S[\{x_n\}] = \beta \left[\frac{\pi M}{\beta \Lambda^2} \sum_{n=0}^{M-1} (\vec{x}_n - \vec{x}_{n+1})^2 + \frac{1}{M} \sum_{n=1}^{M} U(\vec{x}_n) \right]$$

effective action

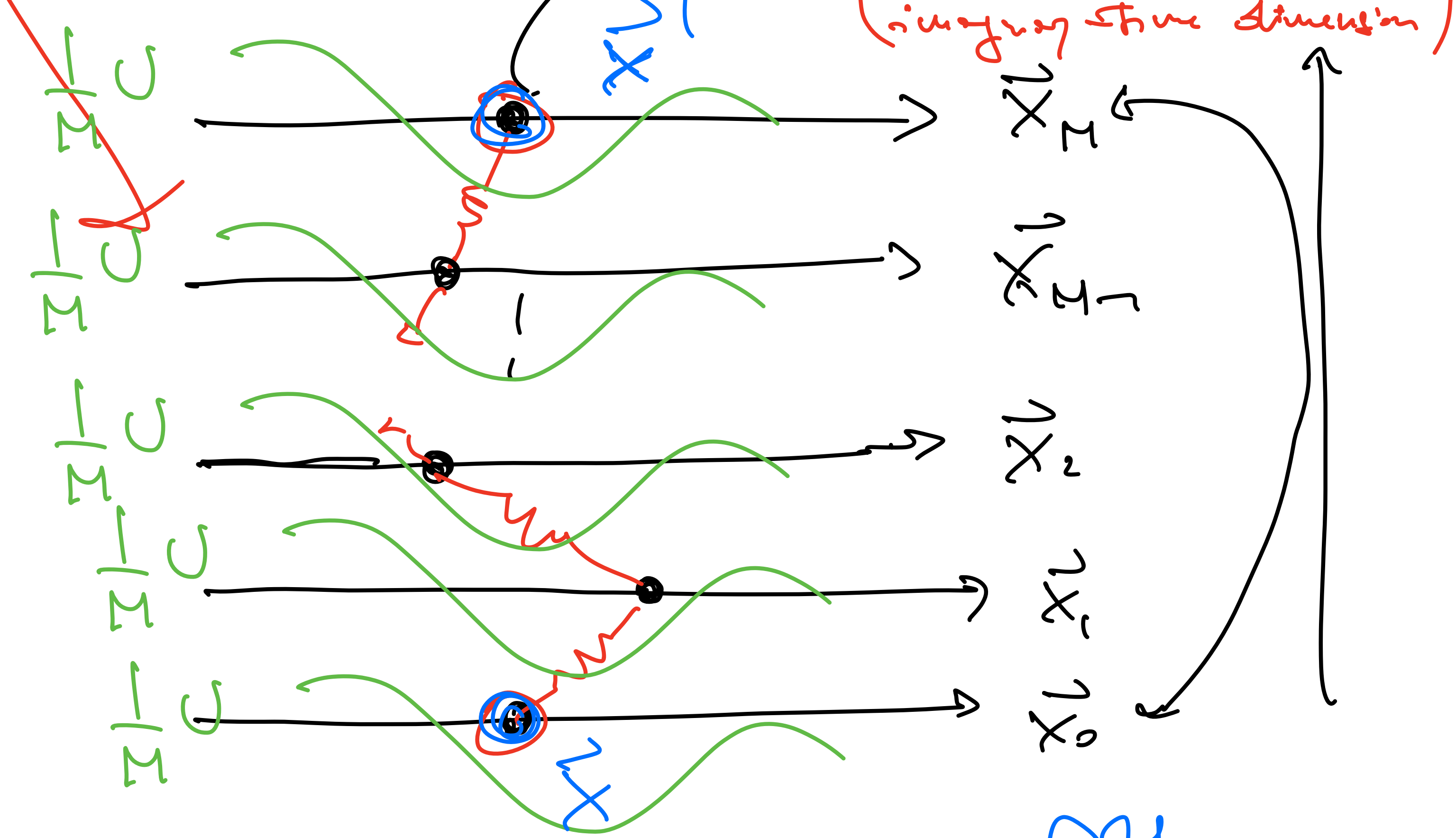
$$= \beta \, \mathcal{H}_{eff}(\{\vec{x}_n\})$$

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

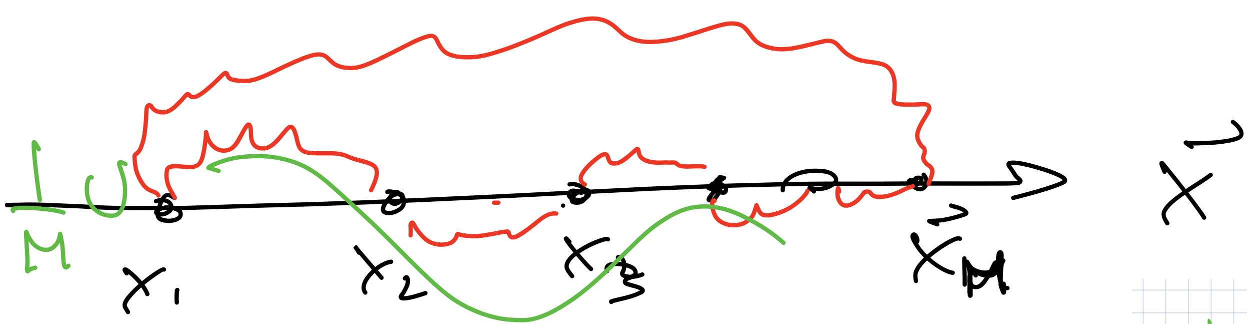
spring constant

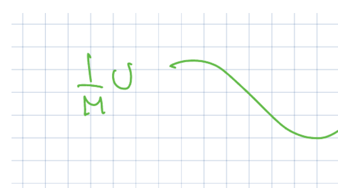
"beads"

(Trotter dimension)



$$\langle \vec{x} | e^{-\beta H} | \vec{x}' \rangle$$





Ring elastic polymer

$Z = (\quad) \times \lim_{M \to \infty}$ partition function of a ring polymer of M beads

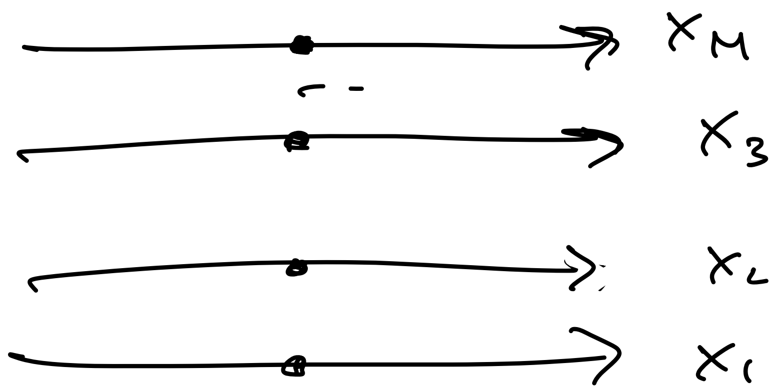
Spring constant $\quad \tilde{k} = \dfrac{2\pi M}{\beta \Lambda^2}$

$$\Lambda = \frac{h}{\sqrt{2\pi m k_B T}}$$

$$= \frac{2\pi M}{h} \, 2\pi m \, (k_B T)^2$$

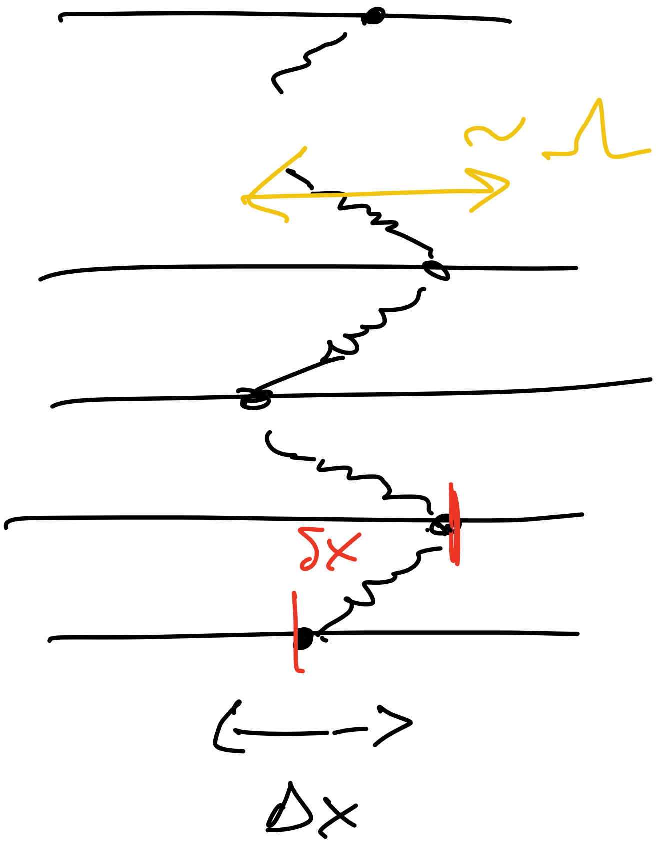
$$= \begin{cases} \to 0 & T \to 0 \\ \to \infty & T \to \infty \end{cases}$$

ring polymer becomes infinitely stiff



$$Z \sim \int d^d x \, e^{-\beta U(\vec{x})} \int d^d p \, e^{-\beta \frac{p^2}{2m}}$$

$T \to 0$



$$\delta x = x_n - x_{n+1}$$

Gaussian variables $\sim e^{-\overbrace{\frac{\pi M}{\Lambda^2}}^{\frac{1}{2\sigma^2}}(\delta x)^2}$

$$\to \quad \sigma^2 = \frac{\Lambda^2}{2\pi M}$$

$$(\Delta x)^2 = M\,\sigma^2 = \frac{\Lambda^2}{2\pi}$$

$$\Delta x = \frac{\Lambda}{\sqrt{2\pi}}$$

$\vec{x}_1 \to \vec{x}_2 \to \cdots \quad \vec{x}_M$

"path" in imaginary time

$Z =$ "integral over paths" =

" over ring polymer configurations