Variational MC

$$|\Psi^{(\vec{\alpha})}\rangle =: \sum_x f(x;\vec{\alpha})\,|x\rangle$$

$$\min_{\vec{\alpha}} E(\vec{\alpha}) = \min_{\vec{\alpha}} \frac{\langle \Psi(\vec{\alpha})|\hat{H}|\Psi(\vec{\alpha})\rangle}{\langle \Psi(\vec{\alpha})|\Psi(\vec{\alpha})\rangle}$$

Improvement : Projector Monte Carlo

$$\lim_{\tau\to\infty} \frac{e^{-\tau H}|\Psi_T\rangle}{\| e^{-\tau H}|\Psi_T\rangle\|} = |\Phi_0\rangle$$

$|\Psi_T\rangle = |\Psi(\vec{\alpha})\rangle$
trial wave functions

$$\hat{H}|\Phi_0\rangle = E_0|\Phi_0\rangle$$

if $\langle \Psi_T|\Phi_0\rangle \neq 0$

imaginary-time "projection"

[Last time: how to approximate

$$e^{-\tau H}|\Psi(\vec{\alpha})\rangle \quad \text{with} \quad |\Psi(\vec{\alpha}')\rangle$$]

Today : reconstruct properties of $e^{-\tau H}|\Psi(\vec{\alpha})\rangle$ with minimal assumption $\neq$

$|\Psi_T\rangle$

$$e^{-\tau \mathcal{H}} = \left(e^{-\tau/n \hat{\mathcal{H}}}\right)^n \underset{n\to\infty}{=} \left(e^{-\delta\tau \hat{\mathcal{H}}}\right)^n \simeq$$

$$\delta\tau = \tau/n \qquad \left(\mathbb{1} - \delta\tau \hat{\mathcal{H}}\right)^n$$

$$\underline{\langle x | \Psi_n \rangle} = \langle x | e^{-\tau \mathcal{H}} | \Psi_T \rangle$$

$$\Psi_n(x) \simeq \langle x | \underbrace{(\mathbb{1} - \delta\tau \mathcal{H})}^n | \Psi_T \rangle$$

probability

$\mathbb{1} - \delta\tau \mathcal{H}$ = infinitesimal imaginary-time evolution operator

$$= \sum_{x_1 x_2 \dots x_n} \langle x | (\mathbb{1} - \delta\tau \mathcal{H}) | x_1 \rangle \langle x_1 | (\mathbb{1} - \delta\tau \mathcal{H}) | x_2 \rangle \dots$$

$$\dots \langle x_{n-1} | (\mathbb{1} - \delta\tau \mathcal{H}) | x_n \rangle \underline{\Psi_T(x_n)}$$

probability

$\Psi_T(x) > 0$ [true for the ground state of $\underline{\underline{\text{bosonic}}}$ systems in the absence of gauge fields. (Feynman's "no-node" theorem)]

regard Ψ_T as a probability distribution

$\Psi_n(x) > 0$

$$G_{xx'} = \langle x | (\mathbb{1} - \delta\tau \mathcal{H}) | x' \rangle$$

Green's function / infinitesimal imaginary time propagator

$$\left(\rho(x, x'; \tau) = \langle x | e^{-\tau \mathcal{H}} | x' \rangle \right)$$

If $G_{xx'} \geq 0$

$x \neq x'$ $\quad \langle x | -\delta\tau \mathcal{H} | x' \rangle \geq 0$

$\langle x | \mathcal{H} | x' \rangle \leq 0$ (true for bosonic systems without gauge fields)

$$\Rightarrow \quad \underset{\uparrow \tau}{G_{xx'}} = b_{x'} \, p(x' \to x)$$

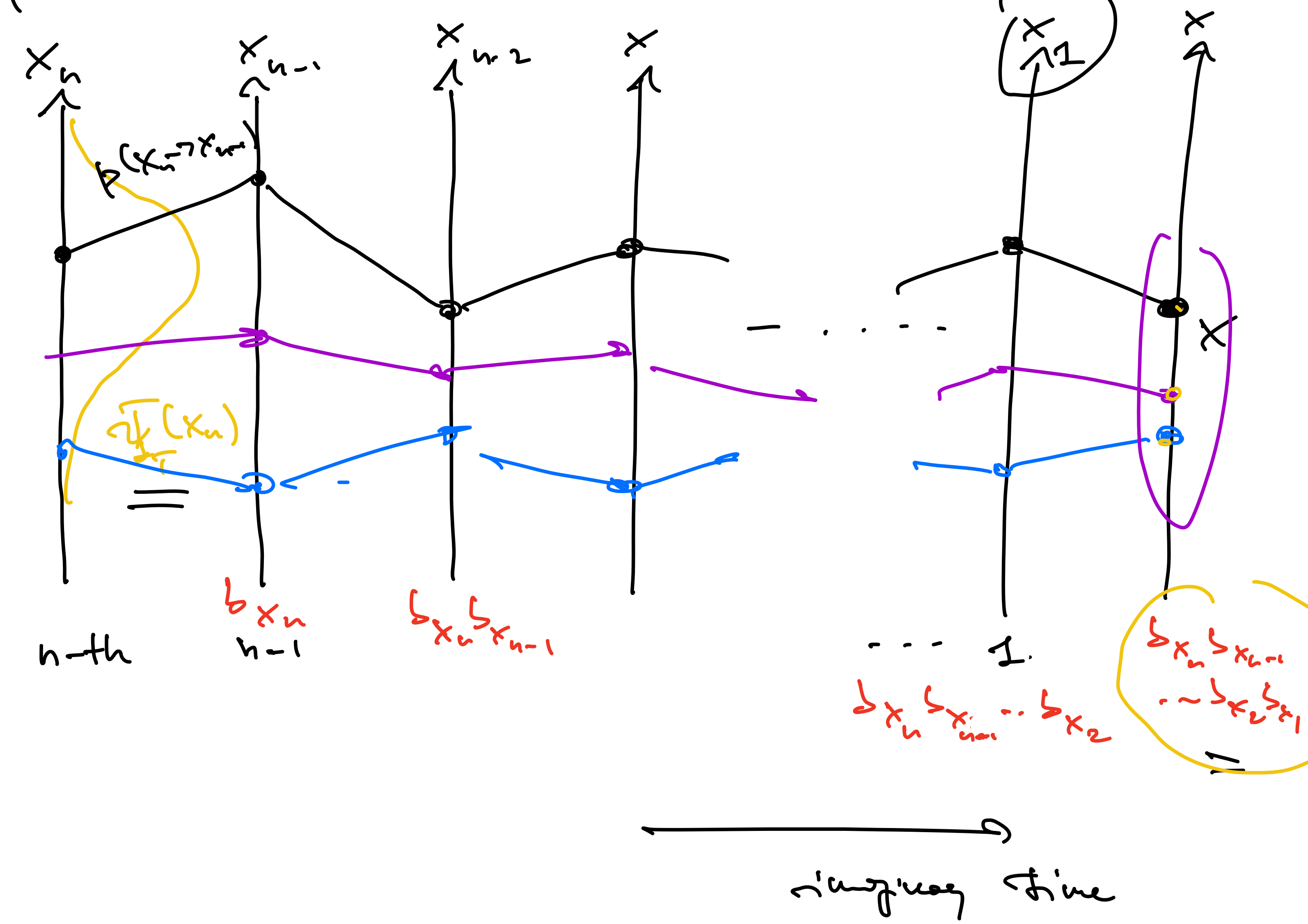
$$\underset{=}{\sum_x} \underset{=}{p(x' \to x)} = 1$$

$$b_{x'} = \sum_x G_{xx'}$$

$$\Psi_n(x) = \sum_{x_1 x_2 \dots x_n} b_{x_1} b_{x_2} \cdots b_{x_n} \, p(x_2 \to x_1) \, p(x_3 \to x_2) \cdots p(x_n \to x_{n-1})$$

$$\Psi_T(x_n)$$

$p(x \to x')$ describes a Markov random walk



The final points are distributed according to

$$\frac{\Psi_n(x)}{W_n}$$

$$W_n = \prod_{p=1}^{n} b_{x_p}$$

Estimate the ground-state energy

$$\sum_x \langle x| \hat{H} \underbrace{(\mathbb{1} - \delta\tau \hat{H})^n |\Psi_T\rangle}_{\underset{n\to\infty}{\sim} |\Phi_0\rangle} \underset{n\to\infty}{\simeq} E_0 \sum_x \langle x| (\mathbb{1} - \delta\tau \hat{H})^n |\Psi_T\rangle$$

$$E_0 \underset{n\to\infty}{\simeq} \frac{\sum_x \langle x| \hat{H} (\mathbb{1} - \delta\tau \hat{H})^n |\Psi_T\rangle}{\sum_x \underbrace{\langle x| (\mathbb{1} - \delta\tau H)^n |\Psi_T\rangle}_{\Psi_n(x)}}$$

$$= \frac{\sum_{xx'} \langle x'| H |x\rangle \Psi_n(x)}{\sum_x \Psi_n(x)}$$

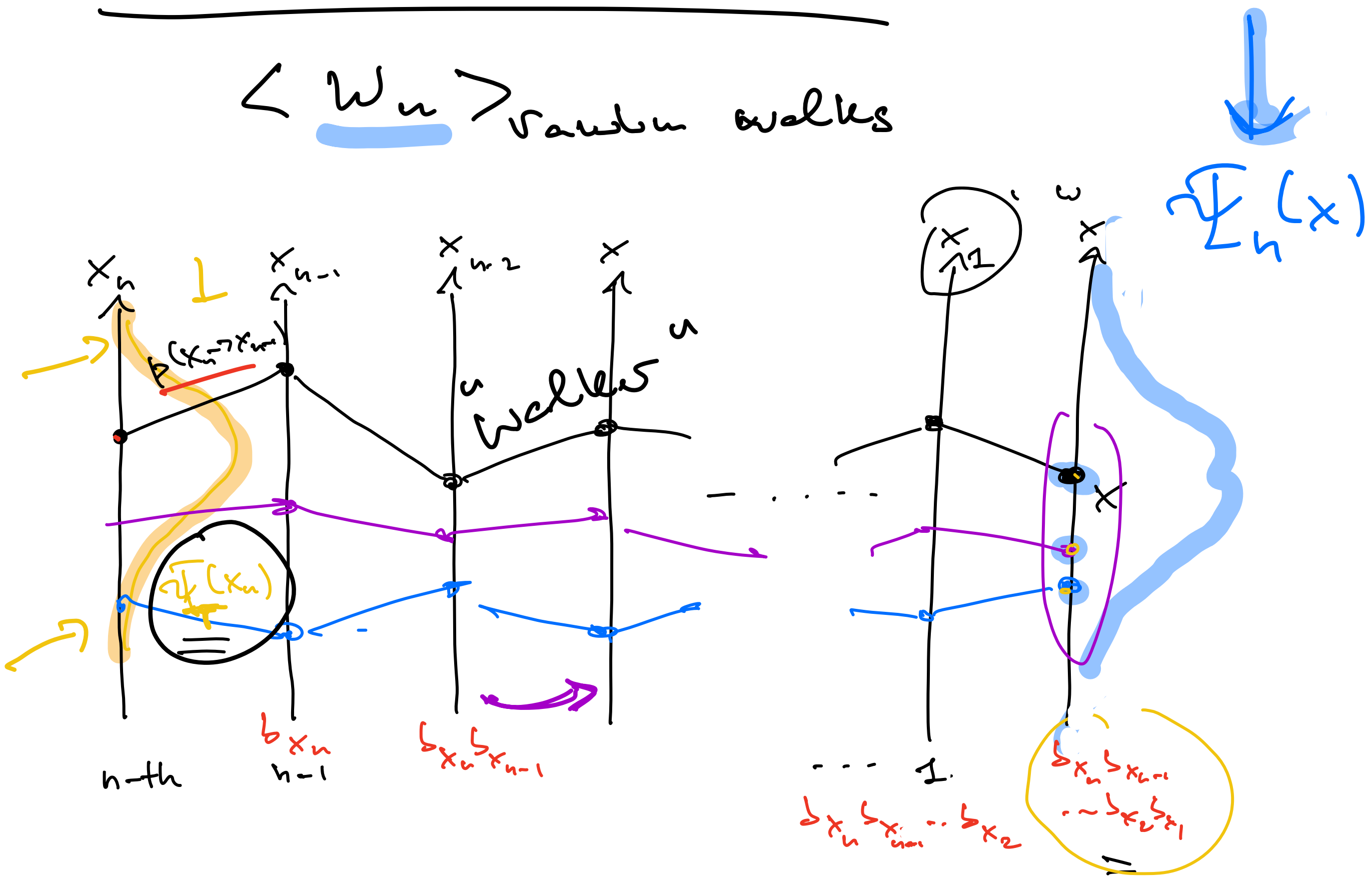
$$\approx \frac{\frac{1}{M}\sum_k \left(\sum_{x'} \langle x'|H|\underset{=n}{x}\rangle\right) e_L(x)_n \, w_n^{(k)}}{\frac{1}{M}\sum_k w_n^{(k)}}$$

k : random walk index

x : arrival point of the random walk

$$w_n^{(k)} = \prod_{p=1}^{n} b_{x_p}$$

$$= \frac{\langle e_L(x)\, W_n \rangle_{\text{random walks}}}{\langle W_n \rangle_{\text{random walks}}}$$



"Single-walker" Green's function Monte Carlo (GFMC)

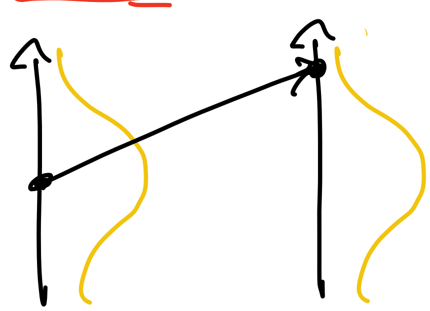
Reweighting

"Importance sampling" for GFMC

Use the trial wavefunction $\Psi_T(x)$ to guide the walkers

$$\underbrace{\Psi_T(x)\,\Psi_n(x)}_{\tilde{\Psi}_n(x)} = \sum_{x'} \frac{\Psi_T(x)}{\Psi_T(x')} G_{xx'} \underbrace{\Psi_T(x')\,\Psi_{n-1}(x')}_{\tilde{\Psi}_{n-1}(x')}$$

$$\tilde{G}_{xx'} = \underbrace{s_{x'} \frac{\Psi_T(x)}{\Psi_T(x')} p(x' \to x)}$$



reweighting of the transition probabilities

Application to systems in continuous space:

Diffusion Monte Carlo (DMC)

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

$$|x\rangle \to |\vec{R}\rangle = |\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N\rangle$$

$$\hat{H} = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + U(\vec{R})$$

$[\,,\,] \neq 0$

external potentials + particle-particle interactions

$$\hat{H} \to \hat{H} - E_T$$

$$G_{xx'} \to \langle \vec{R} | e^{-\tau(\hat{H} - E_T)} | \vec{R}' \rangle \quad (= \rho(\vec{R}, \vec{R}'; \tau))$$

$\tau \to 0$

$\frac{1}{2}$ $\hat{K}$ β

$$\simeq \left(\frac{m}{2\pi\hbar^2 \tau} \right)^{\frac{dN}{2}} e^{-\frac{m}{2\tau\hbar^2}(\vec{R} - \vec{R}')^2} \, e^{-\frac{\tau}{2}[U(\vec{R}) + U(\vec{R}') - 2E_T]}$$

$$+ \mathcal{O}(\tau^3)$$

$$e^{-\tau(\hat{H} - E_T)} |\Psi_T\rangle = e^{-\tau(E_0 - E_T)} \langle \Phi_0 | \Psi_T \rangle |\Phi_0\rangle$$

$\simeq 1$

$$+ \sum_{\alpha \neq 0} e^{-\tau(E_\alpha - E_T)} \langle \Phi_\alpha | \Psi_T \rangle |\Phi_\alpha\rangle$$

$E_T \simeq E_0$

$$\Psi_T(\vec R) \xrightarrow{\text{imaginary-time propagate}} \Psi_n(\vec R) =$$

$$\int d\vec R_1 \, d\vec R_2 \dots d\vec R_n \, \langle \vec R | e^{-\tau(H-E_T)} | \vec R_1\rangle \langle \vec R_1 | e^{-\tau(H-E_T)} | \vec R_2 \rangle \dots \Psi_T(\vec R_n)$$

Elementary step of propagation

$$\frac{1}{2\sigma^2}$$

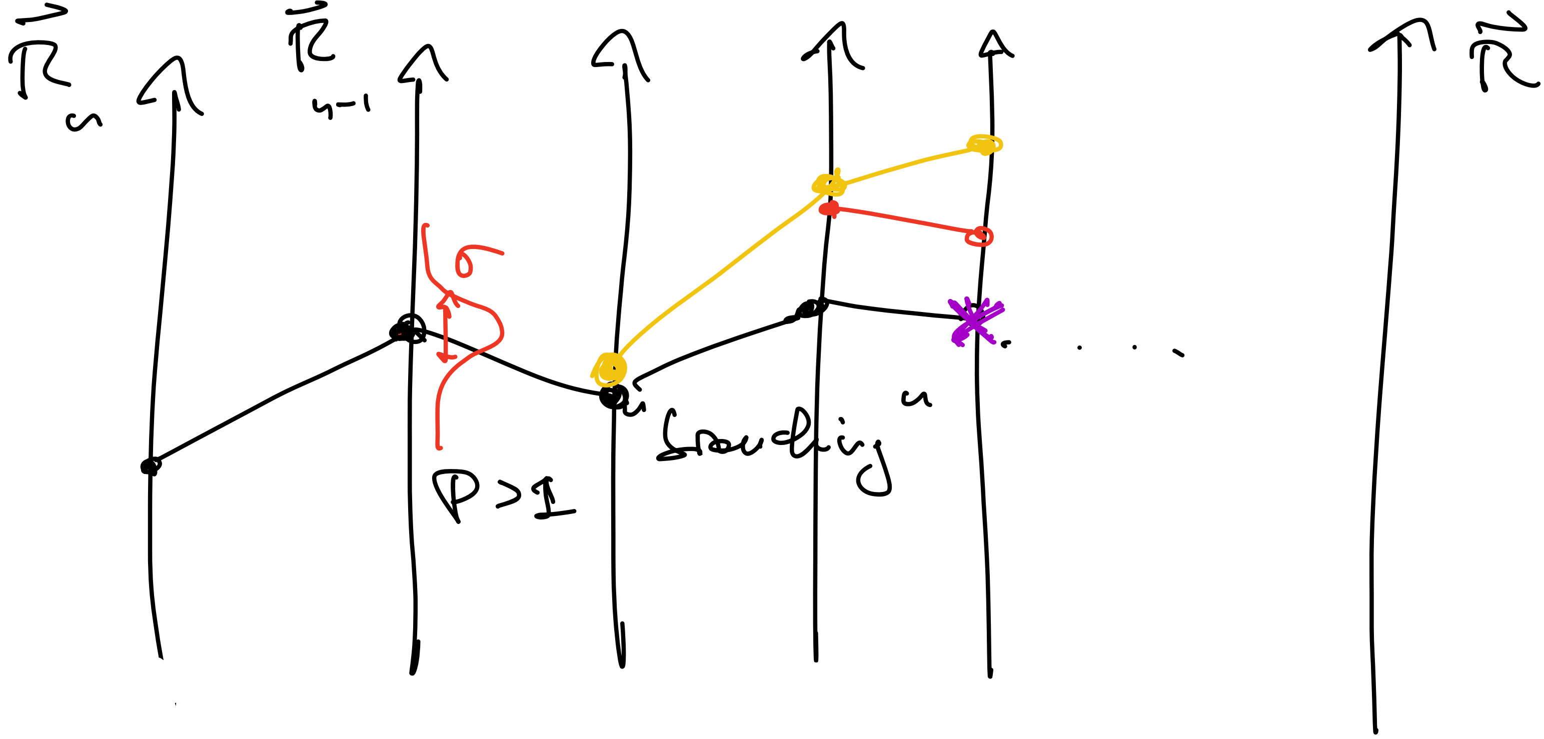
$$\underset{>0}{\Psi_n(\vec R)} = \int d\vec R \underbrace{\left(\frac{m}{2\pi\hbar^2\tau}\right)^{\frac{dN}{2}} e^{-\frac{m}{2\tau\hbar^2}(\vec R-\vec R')^2}}_{\text{Gaussian distribution for } \vec R - \vec R'} \boxed{e^{-\frac{\tau}{2}\left[U(\vec R)+U(\vec R')-2E_T\right]}} \underset{>0}{\Psi_{n-1}(\vec R')}$$

P

transition

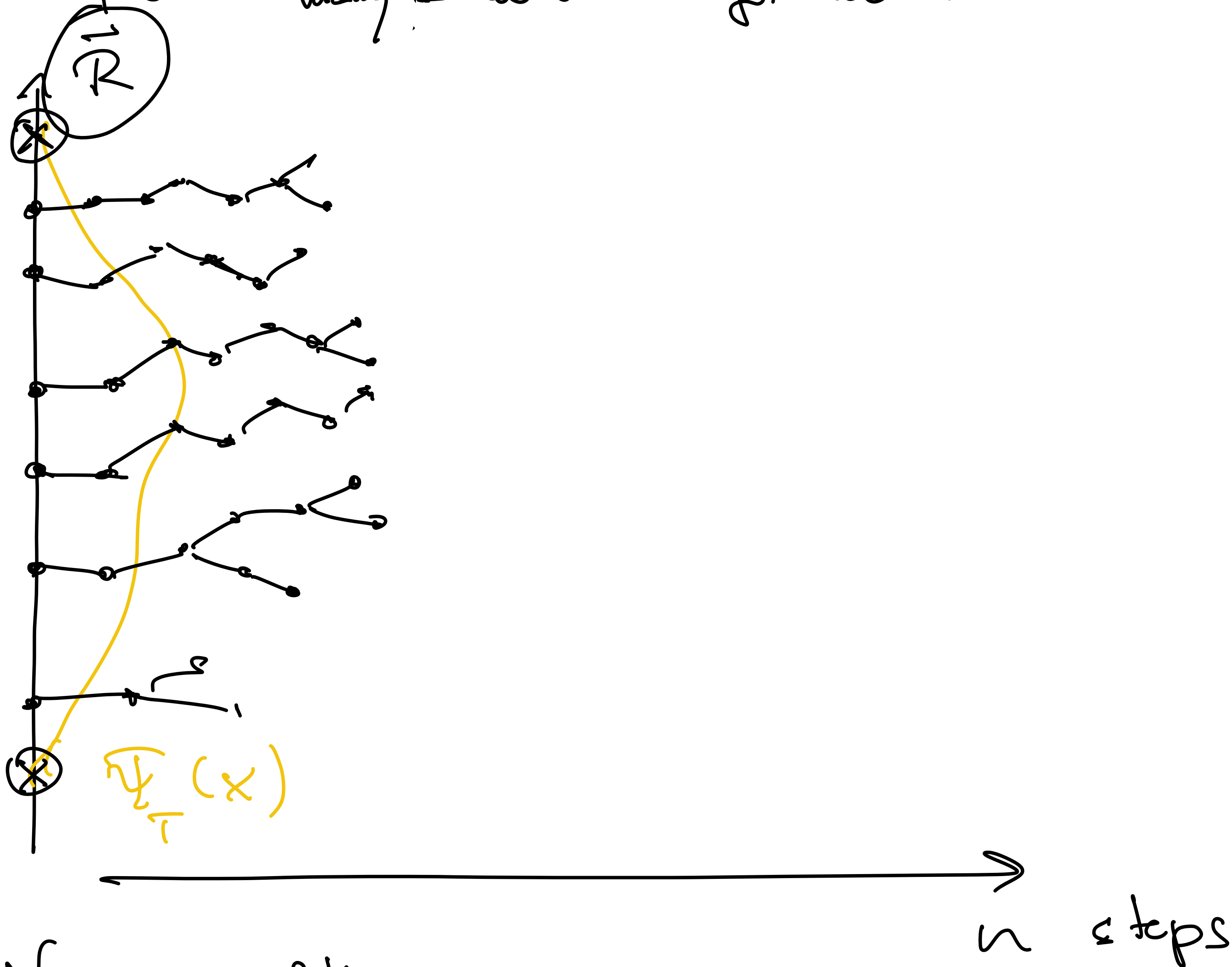
suppression / branching process

many-walkers approach



P : $\begin{cases} P \leq 1 & \text{walker survives with prob. } P \text{ or "dies" with prob. } 1-P \\ P > 1 & \text{walker continues and it may replicate with prob. } P-1 \end{cases}$

Complete many-walker formulation



N_w walkers

E_T is adjusted along the propagation

so as to keep $N_w \simeq$ const

→ correlates the walkers.

$E_T \simeq E_0$

Guiding wavefunctions (importance sampling)

reweight imaginary-time propagation

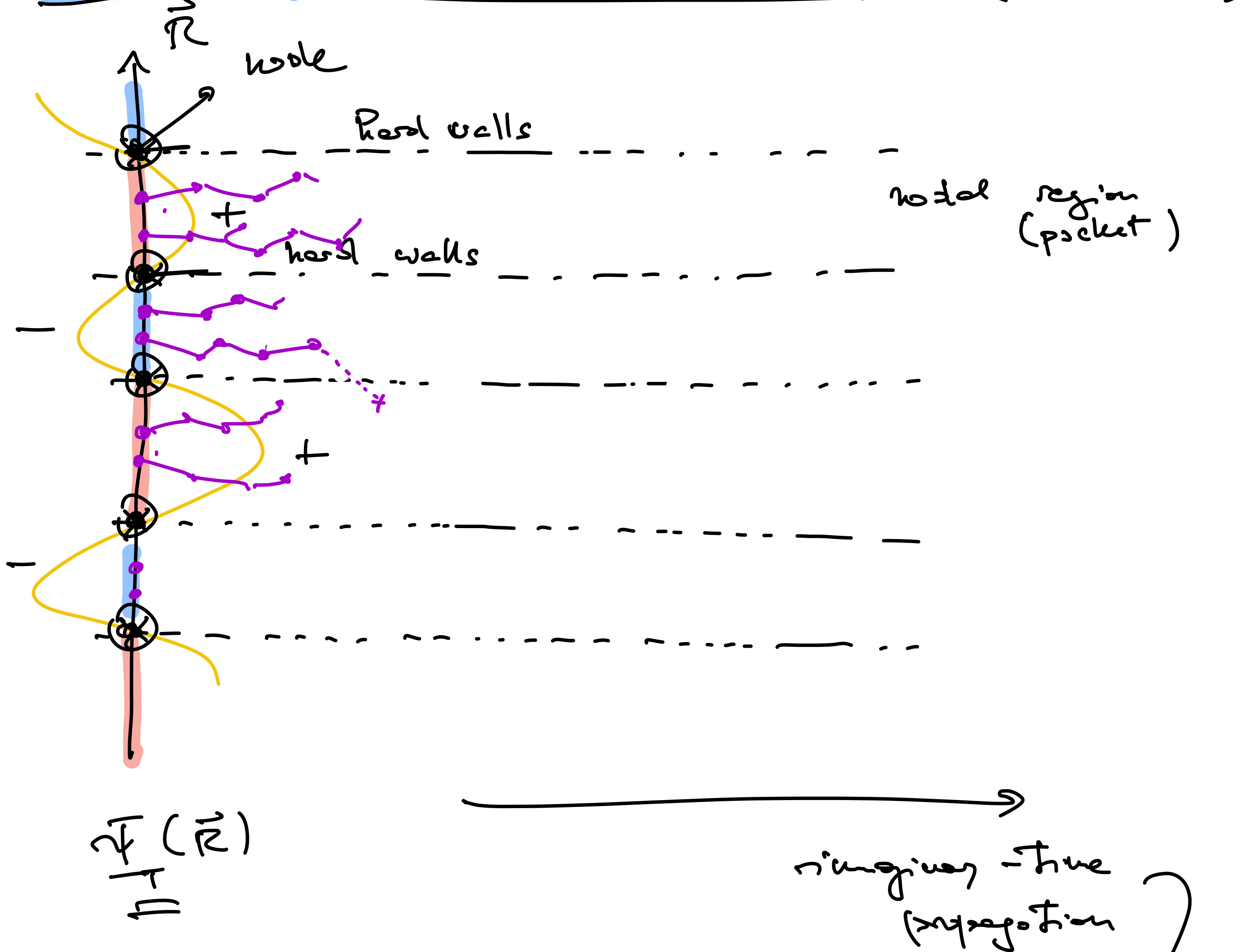
$$\underbrace{\Psi_T(\vec{R})\,\Psi_n(\vec{R})}_{\tilde{\Psi}_n} = \int d\vec{R}'\, \underbrace{\frac{\Psi_T(\vec{R})}{\Psi_T(\vec{R}')}\, G(\vec{R},\vec{R}';\tau)}_{\tilde{G}}\, \underbrace{\Psi_T(\vec{R}')\,\Psi_{n-1}(\vec{R}')}_{\tilde{\Psi}_{n-1}}$$

$\Psi_T \geq 0$ bosons

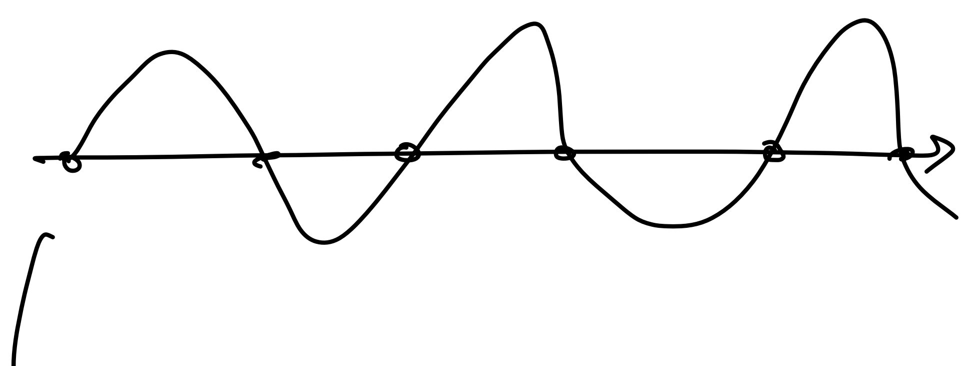
What if $\Psi_T < 0$?

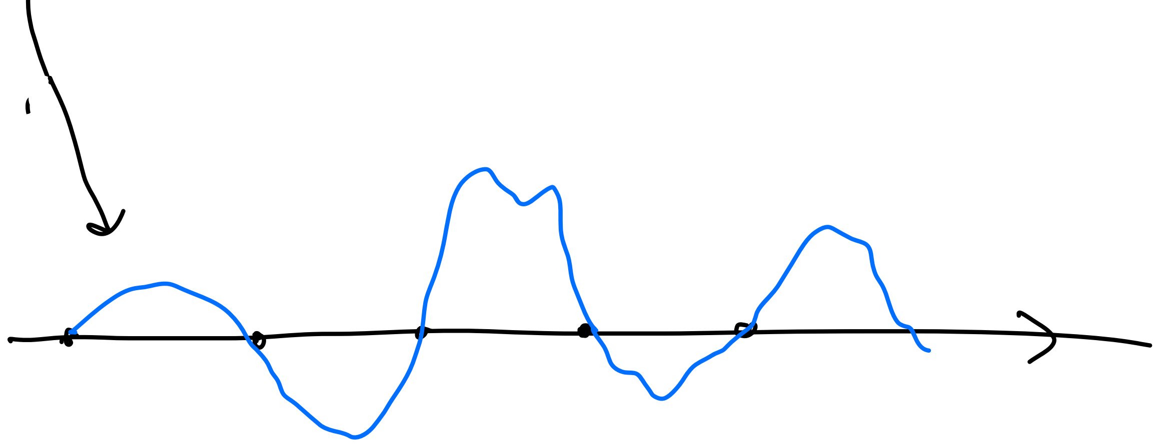
<u>Fermions</u>

Fixed-node Diffusion Monte Carlo (FN-DMC)



Best wavefunction with a fixed nodal structure imposed by the trial wavefunction





<u>Bics</u> : fixed nodal structure