Ground-state methods : → VMC
→ Projector MC

Variational MC

$$\mathcal{H} \xrightarrow{\text{N degrees of freedom}} \quad \mathcal{H}|\Phi_0\rangle = E_0|\Phi_0\rangle \qquad |\vec{x}\rangle \text{ basis of } \mathcal{H}$$

$$|\Psi(\vec{\alpha})\rangle = \sum_{\vec{x}} \underbrace{f(\vec{x}, \vec{\alpha})}_{\in \mathbb{C}} |\vec{x}\rangle \longrightarrow \text{"trial WF"}$$

"Ansatz"

$$\vec{\alpha} = (\alpha_1, \ldots, \alpha_M)$$

$$M \sim \text{poly}(N)$$

$$\min_{\vec{\alpha}} E(\vec{\alpha}) = \min_{\vec{\alpha}} \langle E_L(\vec{x}) \rangle_{|f|^2}$$

$$= \frac{\sum_{\vec{x}} |f(\vec{x}, \vec{\alpha})|^2 \, E_L(\vec{x})}{\sum_{\vec{x}} |f(\vec{x}, \vec{\alpha})|^2}$$

local energy

$$E_L(\vec{x}) = \sum_{\vec{x}'} \frac{f(\vec{x}', \vec{\alpha})}{f(\vec{x}, \vec{\alpha})} \langle \vec{x} | \hat{\mathcal{H}} | \vec{x}' \rangle$$

$$\nabla_{\vec{\alpha}} E(\vec{\alpha}) \rightarrow$$

$$\partial_{\alpha_k} E(\vec{\alpha}) = 2 \,\mathrm{Re}\left[\langle O_k^*(\vec{x}) E_L(\vec{x}) \rangle_{|f|^2} - \langle O_k^* \rangle_{|f|^2} \langle E_L \rangle_{|f|^2} \right]$$

$$O_k(\vec{x}) = \frac{\partial \log f(\vec{x}, \vec{\alpha})}{\partial \alpha_k} \in \mathbb{C}$$

$$\vec{\alpha}^{(0)} \longrightarrow \vec{\alpha}^{(1)} = \vec{\alpha}^{(0)} - \epsilon \, \vec{\nabla}_{\vec{\alpha}} E(\vec{\alpha})$$

gradient descent

Imaginary-time projection

$$e^{-\tau \hat{\mathcal{H}}} = e^{-\frac{it}{\hbar}\hat{\mathcal{H}}} \qquad \tau = \frac{it}{\hbar} \in \mathbb{R}$$

imaginary-time evolution operator

initial wavefunction

$$e^{-\tau \hat{\mathcal{H}}} \, |\Psi_T\rangle \qquad \hat{\mathcal{H}}|\Phi_p\rangle = E_p|\Phi_p\rangle$$

$$|\Psi_T\rangle : \quad \Psi_0^* = \langle \Psi_T | \Phi_0 \rangle \neq 0$$

unique

$$e^{-\tau(\hat{\mathcal{H}} - E_0)} \, |\Psi_T\rangle = e^{-\tau(\hat{\mathcal{H}} - E_0)} \sum_p \Psi_p |\Phi_p\rangle$$

$$\left(\Psi_0 |\Phi_0\rangle + \sum_{p \neq 0} \Psi_p |\Phi_p\rangle \right)$$

$$= \Psi_0 |\Phi_0\rangle + \sum_{p\neq 0} e^{-\tau \overbrace{(E_p - E_0)}^{>0}} \Psi_p |\Phi_p\rangle$$

$$\xrightarrow[\tau \to \infty]{} \Psi_0 |\Phi_0\rangle$$

$$\frac{e^{-\tau(\hat{\mathcal{H}} - E_0)} \, |\Psi_T\rangle}{\| e^{-\tau(\hat{\mathcal{H}} - E_0)} \, |\Psi_T\rangle \|} \xrightarrow[\tau \to \infty]{} |\Phi_0\rangle$$

$$|\Psi_T\rangle \rightarrow |\Psi(\vec{\alpha})\rangle$$

$$e^{-\tau \mathcal{H}} |\Psi(\vec{\alpha})\rangle \rightarrow \text{best approximation to } |\Psi_0\rangle$$

$$\boxed{(\mathbb{1} - \delta\tau \mathcal{H})\, |\Psi(\vec{\alpha})\rangle \neq |\Psi(\vec{\alpha} + \delta\vec{\alpha})\rangle}$$

$$|\Psi(\vec{\alpha})\rangle + \underbrace{\delta\tau \hat{\mathcal{H}} |\Psi(\vec{\alpha})\rangle}_{\delta\tau |\Psi(\vec{\alpha}')\rangle} = |\Psi(\vec{\alpha})\rangle + \delta |\Psi(\vec{\alpha}')\rangle$$

arbitrary

$$\neq |\Psi(\vec{\alpha}'')\rangle$$

Search for $\delta\vec{\alpha}$ such that

$|\Psi(\vec{\alpha} + \delta\vec{\alpha})\rangle$ is the best approximation to $(\mathbb{1} - \delta\tau \mathcal{H})|\Psi(\vec{\alpha})\rangle$

$$\frac{\delta\vec{\alpha}}{\delta\tau} = \ldots \qquad \text{differential equation}$$

$|\Psi(\vec{\alpha} + \delta\vec{\alpha})\rangle$: belonging to a subspace of H

"tangent space" $T_{\vec{\alpha}}$

$$|\Psi(\vec{\alpha} + \delta\vec{\alpha})\rangle = \sum_{\vec{x}} f(\vec{x}; \vec{\alpha} + \delta\vec{\alpha})\, |\vec{x}\rangle$$

$$= |\Psi(\vec{\alpha})\rangle + \sum_{\vec{x}} (\nabla_{\vec{\alpha}} f) \cdot \delta\vec{\alpha}\, |\vec{x}\rangle$$

$$= |\Psi(\vec{\alpha})\rangle + \sum_{\vec{x}} \delta\vec{\alpha} \cdot \underbrace{\left(\frac{\vec{\nabla}_{\vec{\alpha}} f}{f}\right)}_{} f(\vec{x}, \vec{\alpha})\, |\vec{x}\rangle + \mathcal{O}(\delta\alpha)^2$$

$$\sum_n \delta\alpha_n \underbrace{\frac{\partial}{\partial\alpha_n} \log(f(\vec{\alpha};\vec{x}))}_{O_n(\vec{x})}$$

$$= \left(\mathbb{1} + \sum_n \delta\alpha_n \hat{O}_n\right) |\Psi(\vec{\alpha})\rangle + o(\delta\alpha)^2$$

$$\hat{O}_n |\Psi(\vec{\alpha})\rangle = \sum_{\vec{x}} \overbrace{\frac{\partial(\log f)}{\partial\alpha_n}}^{O_n} f\, |\vec{x}\rangle$$

$$\langle \Psi(\vec{\alpha}+\delta\vec{\alpha}) | \Psi(\vec{\alpha}+\delta\vec{\alpha})\rangle = \dots =$$

$$\langle \Psi(\vec{\alpha}) | \Psi(\vec{\alpha})\rangle \left(1 + 2\sum_n \mathrm{Re}(\bar{O}_n)\,\delta\alpha_n\right) + o(\delta\alpha)^2$$

$$\bar{O}_n = \frac{\langle \Psi(\vec{\alpha}) | \hat{O}_n | \Psi(\vec{\alpha})\rangle}{\langle \Psi | \Psi \rangle} = \langle O_n(\vec{x})\rangle_{|f|^2}$$

$$|\phi(\vec{\alpha}+\delta\vec{\alpha})\rangle = \frac{|\Psi(\vec{\alpha}+\delta\vec{\alpha})\rangle}{\| \Psi(\vec{\alpha}+\delta\vec{\alpha}) \|} =$$

$$\frac{|\Psi\rangle}{\|\Psi\|}$$

$$= \dots = e^{i\delta\theta} \left[|\phi(\vec{\alpha})\rangle + \sum_n \delta\alpha_n |\phi_n(\vec{\alpha})\rangle \right] + o(\delta\alpha)^2$$

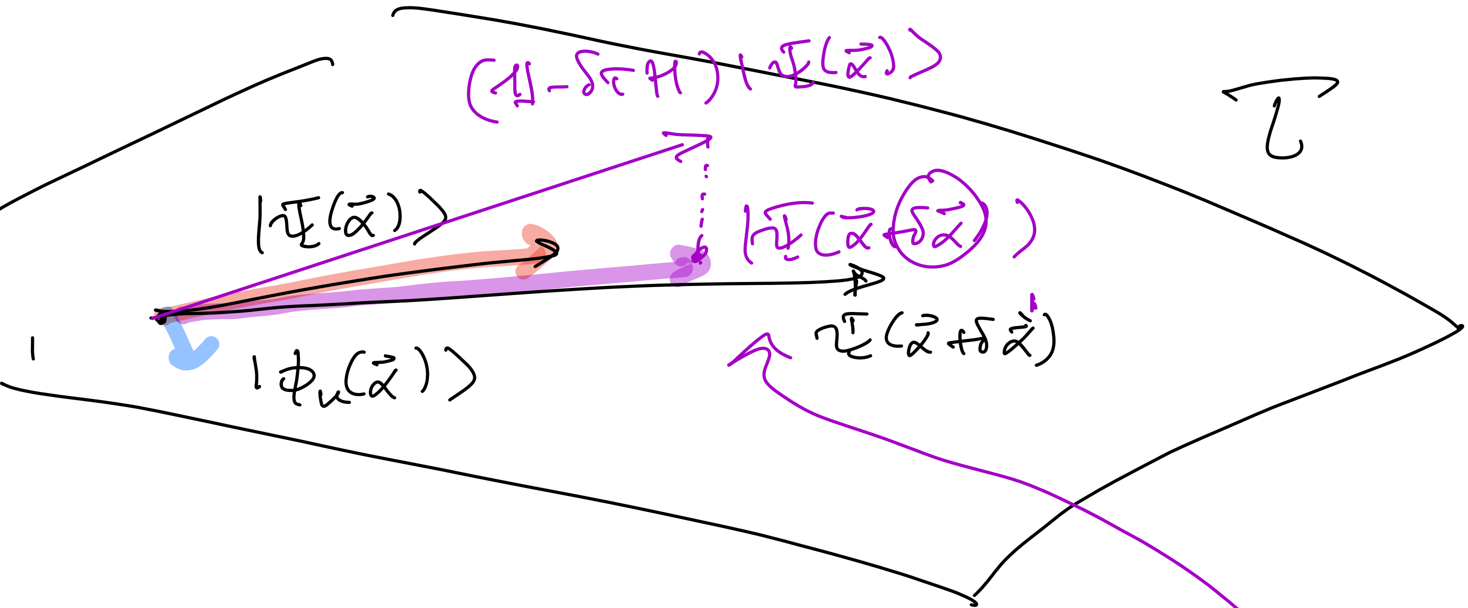
$$|\phi_n(\vec{\alpha})\rangle = (\hat{O}_n - \bar{O}_n) |\phi(\vec{\alpha})\rangle$$

$$e^{i\delta\theta} = 1 + i\sum_n \mathrm{Im}(\bar{O}_n)\,\delta\alpha_n + o(\delta\alpha)^2$$

$$|\phi(\vec\alpha+\delta\vec\alpha)\rangle = \frac{|\Psi(\vec\alpha+\delta\vec\alpha)\rangle}{\| \Psi(\vec\alpha+\delta\vec\alpha) \|} =$$

$$\frac{|\Psi\rangle}{\| \Psi \|}$$

$$= \dots = e^{i\delta\theta}\left[\,|\phi(\vec\alpha)\rangle + \sum_u \delta\alpha_u\, |\phi_u(\vec\alpha)\rangle\right] + o(\delta\alpha)^2$$



$$\mathcal{T} = \text{span}\left\{|\phi(\vec\alpha)\rangle, \{|\phi_u(\vec\alpha)\rangle\}\right\}$$

$$\underbrace{\langle\phi_u(\vec\alpha)|\phi(\vec\alpha)\rangle} = \langle\phi(\vec\alpha)|\left(\hat{O}_u^{\dagger} - \bar{O}_u^{*}\right)|\phi(\vec\alpha)\rangle = 0$$

$$\langle\phi_u(\vec\alpha)|\phi_{u'}(\vec\alpha)\rangle \neq \delta_{uu'}(\dots)$$

fixes γ

$$\boxed{\begin{aligned}\langle\phi(\vec\alpha)|(\mathbb{1}-\delta\tau H)|\Psi(\vec\alpha)\rangle &= e^{i\gamma}\langle\phi(\vec\alpha)|\Psi(\vec\alpha+\delta\vec\alpha)\rangle \\ \langle\phi_u(\vec\alpha)|(\mathbb{1}-\delta\tau H)|\Psi(\vec\alpha)\rangle &= e^{i\gamma}\langle\phi_u(\vec\alpha)|\Psi(\vec\alpha+\delta\vec\alpha)\rangle\end{aligned}}$$

$$-\delta\tau \underbrace{\langle \phi_u^{(\alpha)} | \hat{\mathcal{H}} | \phi(\vec{\alpha})\rangle}_{=} = \sum_{u'} \langle \phi_u(\vec{\alpha}) | \phi_{u'}(\vec{\alpha})\rangle \, \delta\alpha_{u'} + O(\delta\alpha)^2$$

$$S_{uu'} = \langle \phi(\vec{\alpha}) | (\hat{O}_u^{\dagger} - \bar{O}_u^{*}) (\hat{O}_{u'} - \bar{O}_{u'}) | \phi(\vec{\alpha})\rangle$$

$$= \langle O_u^{*} O_{u'} \rangle_{|\phi|^2} - \langle O_u^{*} \rangle_{|\phi|^2} \langle O_{u'} \rangle_{|\phi|^2}$$

Covariance matrix of O_u's

$$\langle \phi(\vec{\alpha}) | (\hat{O}_u^{\dagger} - \bar{O}_u^{*}) \mathcal{H} | \phi(\vec{\alpha})\rangle$$

$$= \underbrace{\langle O_u^{*} E_L \rangle_{|\phi|^2} - \langle O_u^{*} \rangle_{|\phi|^2} \langle E_L \rangle_{|\phi|^2}}_{f_u}$$

$$\sum_{u'} S_{uu'} \, \delta\alpha_{u'} = -\delta\tau \, F_u$$

$$S\left(\frac{\delta\vec{\alpha}}{\delta\tau}\right) = -\vec{F} \qquad \dot{\vec{\alpha}} = S^{-1} \vec{F}$$

$\dot{\vec{\alpha}}$

$$\tau \to it$$

Two algorithms to minimize $E(\vec{\alpha})$

1) $\delta\vec{\alpha} = -\epsilon \nabla_{\vec{\alpha}} E$ $\qquad \dot{\vec{\alpha}} = -\nabla_{\vec{\alpha}} E$

$\delta\tau$ $\qquad$ gradient descent

2) $\delta\vec{\alpha} = -\delta\tau\, S^{-1} \vec{F}$ $\qquad$ imaginary-time evolution

d

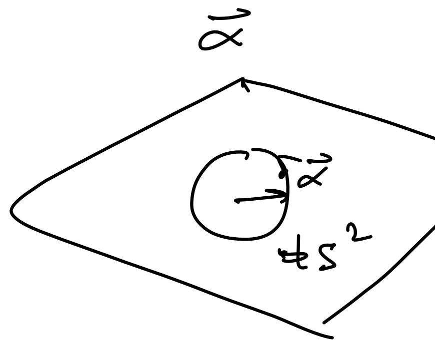
if $f \in \mathbb{R}$ $\qquad \vec{F} = \nabla_{\vec{\alpha}} E$

$\vec{F}$ and $S^{-1}\vec{F}$ go "together"

Geometric picture of gradient descent

view gradient descent as

$$\min_{\delta\vec{\alpha}} \left[E(\vec{\alpha} + \delta\vec{\alpha}) + \mu \underbrace{ds^2(\delta\vec{\alpha})}_{\text{metric}} \right]$$



euclidean metric $\qquad ds^2(\delta\vec{\alpha}) = |\delta\vec{\alpha}|^2$

$$\nabla_{\delta\vec{\alpha}} \left[E(\vec{\alpha} + \delta\vec{\alpha}) + \mu |\delta\vec{\alpha}|^2 \right] = 0$$

$$\delta\vec{\alpha} = -\frac{1}{\mu} \nabla E_{\vec{\alpha}} \qquad \frac{1}{\mu} = \epsilon$$

Geometric picture of imaginary time evolution

metric : $|\delta\vec{\alpha}|^2 \longrightarrow \delta\vec{\alpha}^T S \, \delta\vec{\alpha} = ds^2(\delta\vec{\alpha})$

$$\min_{\delta\vec{\alpha}} \left[E(\vec{\alpha}+\delta\vec{\alpha}) + \mu \boxed{\left(\delta\vec{\alpha}^T S \, \delta\vec{\alpha}\right)} \right]$$

$$\hookrightarrow \quad \delta\vec{\alpha} = -\frac{1}{\mu} S^{-1} \nabla_{\vec{\alpha}} E$$

$$\boxed{\min_{\gamma} \| e^{i\gamma} |\psi(\vec{\alpha}+\delta\vec{\alpha})\rangle - |\psi(\vec{\alpha})\rangle \| = \delta\vec{\alpha}^T S \, \delta\vec{\alpha}}$$

Projector MC $\left\{ \begin{array}{l} \text{Green's function MC} \\ \text{Diffusion MC} \end{array} \right.$

Improvements on VMC

optimized

$|\Psi(\vec{\alpha})\rangle \longrightarrow$ evolve it further in imaginary time without constraining it to be $|\Psi(\vec{\alpha})\rangle$

$$e^{-\tau \mathcal{H}} |\Psi_T\rangle \underset{\tau\to\infty}{\sim} |\Phi_0\rangle$$

$$\downarrow$$

$$\left(e^{-\delta\tau \mathcal{H}}\right)^n |\Psi_T\rangle \underset{n\to\infty}{\sim} |\Phi_0\rangle$$

$\downarrow$ $\delta\tau$ small

$$\underbrace{(\mathbb{1} - \delta\tau \mathcal{H})^{n} |\Psi_T\rangle}_{} \sim |\Phi_0\rangle$$

$\to |\Psi_n\rangle$

$|\vec{x}\rangle$ basis of $\mathcal{H}$

$$|\Psi_{n+1}\rangle = (\mathbb{1} - \delta\tau \mathcal{H})|\Psi_n\rangle + o(\delta\tau)^2$$

$$\langle \vec{x}|\Psi_{n+1}\rangle = \Psi_{n+1}(\vec{x}) = \sum_{\vec{x}'} \langle \vec{x}|(\mathbb{1}-\delta\tau \mathcal{H})|\vec{x}'\rangle \, \Psi_n(\vec{x}')$$

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

$\to$ propagator in imaginary time

$\to$ Green's function

We can sample with MC the expectation values of observables in the imaginary time evolved state of "transition probabilities"

$G_{\vec{x},\vec{x}'} \in \mathbb{R}^+$ $\qquad$ $G_{\vec{x}\vec{x}'} \geq 0$

$$G_{xx'} = \begin{cases} 1 - \delta\tau \langle x | \mathcal{H} | x \rangle & x = x' \\ -\delta\tau \langle x | \mathcal{H} | x' \rangle & x \neq x' \end{cases}$$

$$\begin{cases} \delta\tau < \dfrac{1}{\langle x | \mathcal{H} | x \rangle} \\ \langle x | \mathcal{H} | x' \rangle \leq 0 & x \neq x' \end{cases}$$

What physical systems?

- Bosons without gauge fields
- quantum spin models without frustration

Perron-Frobenius theorem (Feynman's no-node theorem)

ground state $|\Phi_0\rangle \to \Phi_0(x) = \langle x | \Phi_0 \rangle > 0$

Trial wavefunction

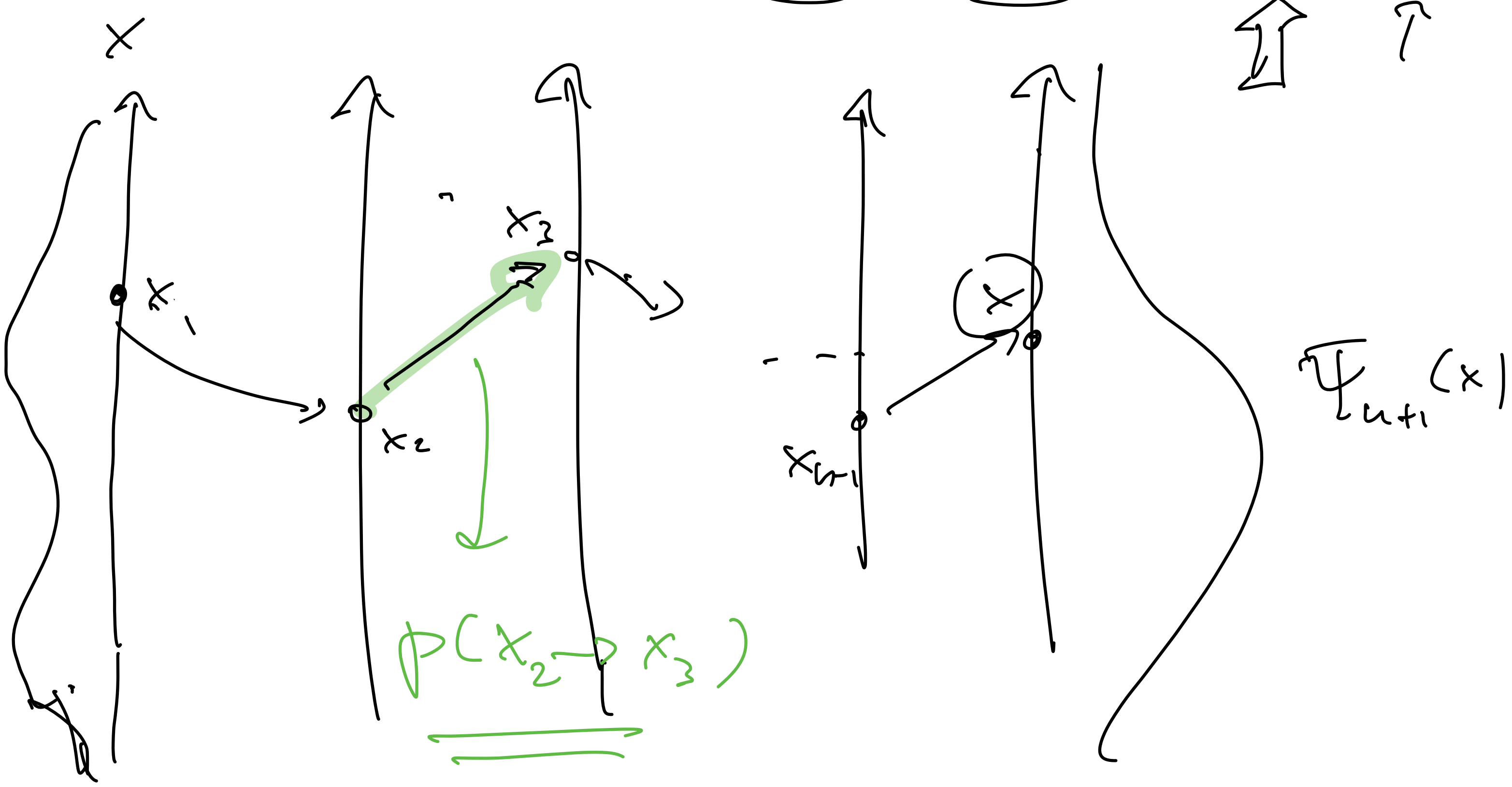
normalized

$|\Psi_T\rangle : \Psi_T(x) = \langle x | \Psi_T \rangle > 0$

$$\boxed{\Psi_{n+1}(x)} = \sum_{x'} G_{xx'} \Psi_n(x)$$

$$= \sum_{x'x''} G_{xx'} G_{xx''} \Psi_{n-1}(x)$$

$$= \dots = \sum_{x_{n-1} x_{n-2} \dots x_1} G_{x x_{n-1}} \, G_{x_{n-1} x_{n-2}} \cdots G_{x_2 x_1} \, \Psi_T(x_1)$$



$\Psi_T(x)$

↪ random walk

$$G_{xx'} = \delta_{xx'} - \delta\tau \, \langle x | \mathcal{H} | x' \rangle \sim p(x' \to x)$$

$$\sum_x p(x' \to x) = 1$$

$$\sum_x G_{xx'} = b_{x'} = \sum_x \left[\delta_{xx'} - \delta\tau \langle x | \mathcal{H} | x' \rangle \right]$$

$$p(x' \to x) = \frac{1}{b_{x'}} G_{xx'}$$

$$\boxed{\Psi_{n+1}(\vec{x})} = \sum_{x_1 x_2 \dots x_n} b_{x_1} b_{x_2} \dots b_{x_n} \, p_{x x_n} \, p_{x_n x_{n-1}} \dots p_{x_2 x_1} \, \Psi_T(x_1)$$

Energy

$$\hat{H} \underbrace{(\mathbb{1} - \delta\tau \hat{H})^n |\Psi_T\rangle}_{} \xrightarrow{n \to \infty} E_0 \, (\mathbb{1} - \delta\tau H)^n |\Psi_T\rangle$$

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

$$E_0 = \lim_{n \to \infty} \frac{\sum_x \left(\sum_{x'} \langle x' | H | x \rangle \right) \overbrace{\langle x | (\mathbb{1} - \delta\tau H)^n | \Psi_T \rangle}^{\Psi_n(x)}}{\sum_x \underbrace{\langle x | (\mathbb{1} - \delta\tau H)^n | \Psi_T \rangle}_{\Psi_n(x)}}$$

$e_L(x)$

$$= \lim_{n \to \infty} \frac{\sum_x e_L(x) \, \Psi_n(x)}{\sum_x \Psi_n(x)}$$

$$= \lim_{n\to\infty} \frac{\langle e_L(x)\, W_n \rangle_{\text{walks}}}{\langle W_n \rangle_{\text{walks}}}$$

$\to x_1 \to x_2 - - \to x_{n-1}$

Importance sampling : guiding wavefunction

$$\Psi_{n+1}(x) = \sum_{x'} G_{xx'}\, \Psi_n(x')$$

(≥ 0)

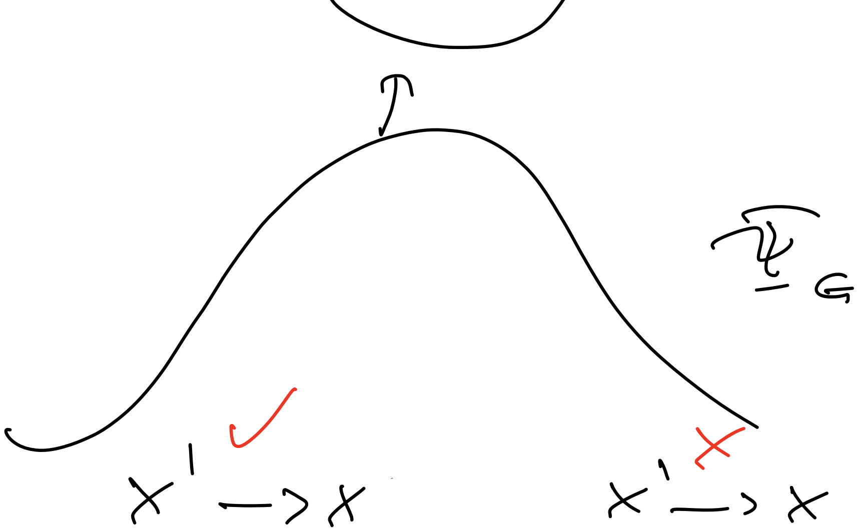
Guess of the ground state $\Psi_G(x)$

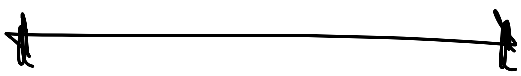
$(= \Psi_T(x))$

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

$$\tilde{\Psi}_{n+1}(x) = \sum_{x'} \tilde{G}_{xx'}\, \tilde{\Psi}_n(x')$$

$$\tilde{G}_{xx'} = \frac{\Psi_G(x)}{\Psi_G(x')}\, G_{xx'} = \tilde{b}_{x'}\, \tilde{p}(x' \to x)$$





Application : continuous space

Diffusion MC

N particles in continuous space

$$|X\rangle \to |\vec{R}\rangle = \underbrace{|\vec{r}_1, \vec{r}_2 \ldots \vec{r}_N\rangle}$$

$|\Psi_T\rangle$: symm.

antisymm.

$$|\Psi_n\rangle = \overbrace{(\mathbb{1} - \delta\tau H)^n}\, |\Psi_T\rangle$$

has the same symmetry under permutation

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

$$H = \sum_i \frac{p_i^2}{2m} + U(\vec{R})$$

potential energy

primitive approximation

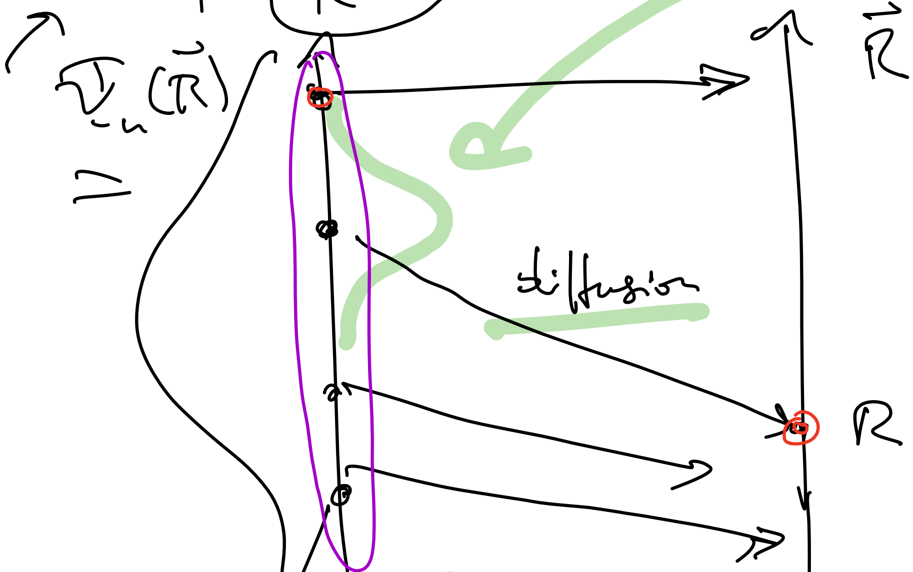
$$G(\vec{R}, \vec{R}'; \tau) \underset{\tau \to 0}{\simeq} \left(\frac{m}{2\pi\hbar^2 \tau} \right)^{\frac{dN}{2}}$$

$$e^{-\frac{\tau}{2}\left[U(\vec{R}) + U(\vec{R}') - 2E_T\right]} \; e^{-\frac{m}{2\tau\hbar^2}(\vec{R} - \vec{R}')^2} + O(\tau^3)$$

$$\boxed{\Psi_{n+1}(\vec{R})} = \int d\vec{R}' \left(\quad \right)^{\frac{dN}{2}}$$

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

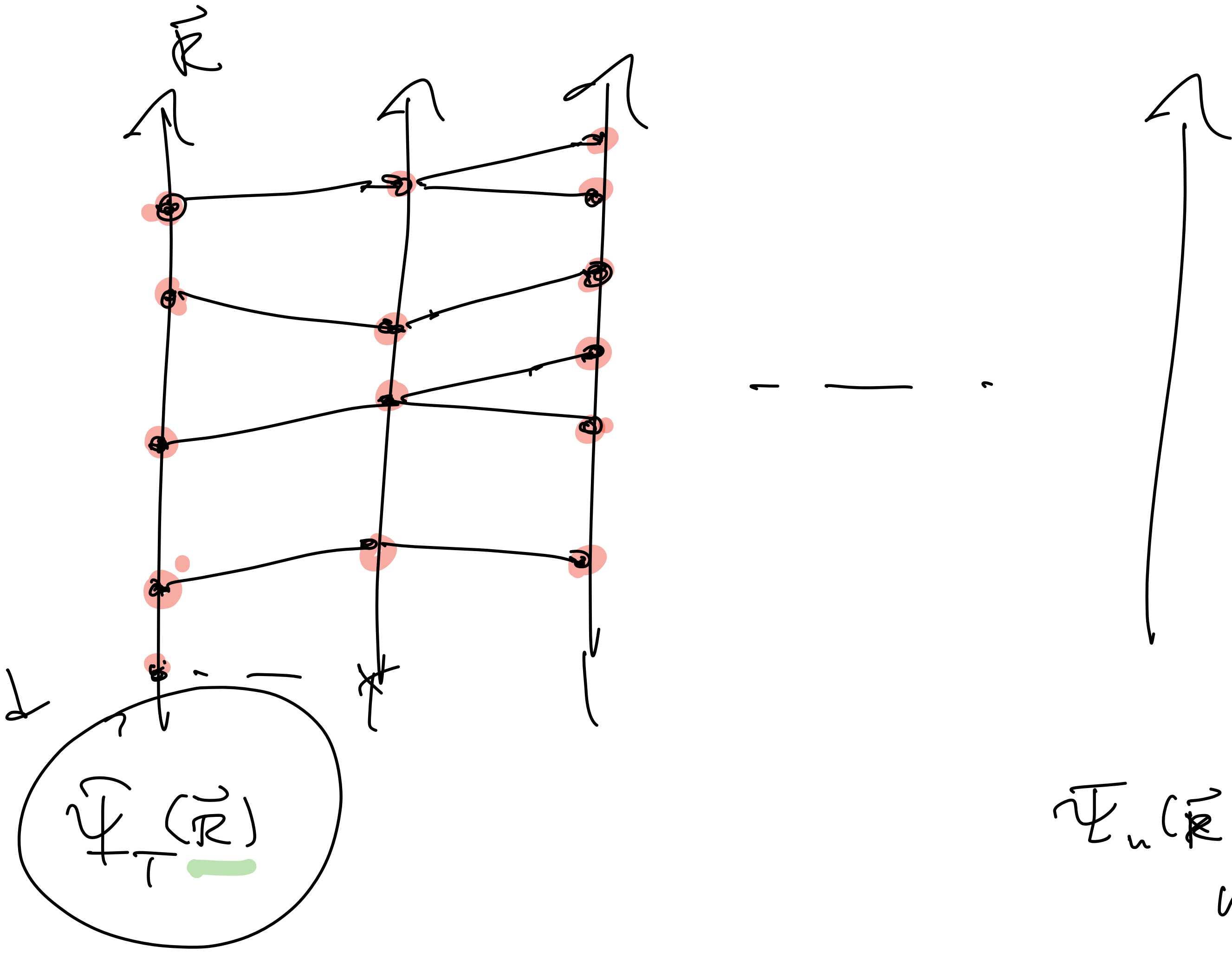
P



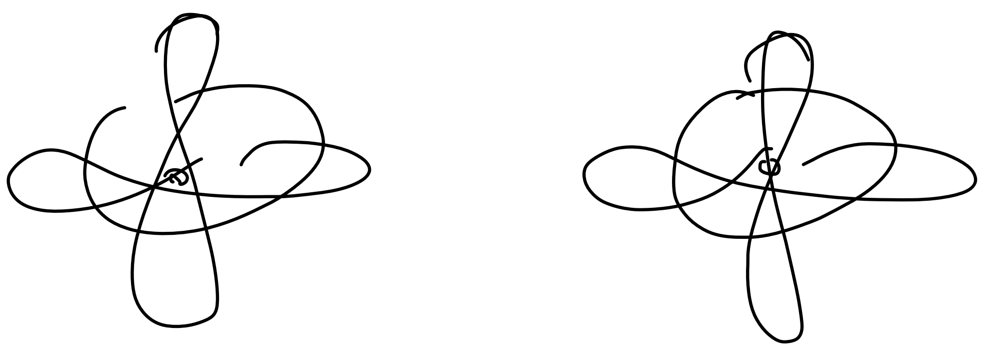
P < 1 : walker survives with probability P "walkers"

P > 1 : walker survives and it replicates with prob. P − 1

"Many-walker" formulation of DMC



$$\Psi_n(\vec{R}) \underset{n\to\infty}{\sim} \Phi_0(\vec{R})$$



H_2

$$\Psi_T(\vec{R},\vec{\sigma}) = \sum_\gamma c_\gamma D_\gamma(\vec{R},\vec{\sigma})$$

T

$$G(\vec{R},\vec{R}';\tau) \rightarrow \tilde{G} = \underbrace{\frac{\Psi_T(\vec{R})}{\Psi_T(\vec{R}')} G(\vec{R};\vec{R}';\tau)}$$

Fixed-node approximation