Variational Monte Carlo

optimize trial wavefunctions

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

computational basis

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

(ex. $|x\rangle \to |\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N\rangle$)

positions of N particles

$\dim(\mathcal{H}) \sim \exp(N)$

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

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

$$E(\vec{\alpha}) = \frac{\sum_x |f(x;\vec{\alpha})|^2 E_L(x)}{\sum_x |f(x;\vec{\alpha})|^2} = \langle E_L \rangle$$

calculate with MC

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

$$\frac{\partial}{\partial \alpha_k} E(\vec{\alpha}) = \langle O_k^{(x)} E_L^* \rangle - \langle O_k \rangle \langle E_L^* \rangle + \langle O_k^* E_L \rangle - \langle O_k^* \rangle \langle E_L \rangle$$

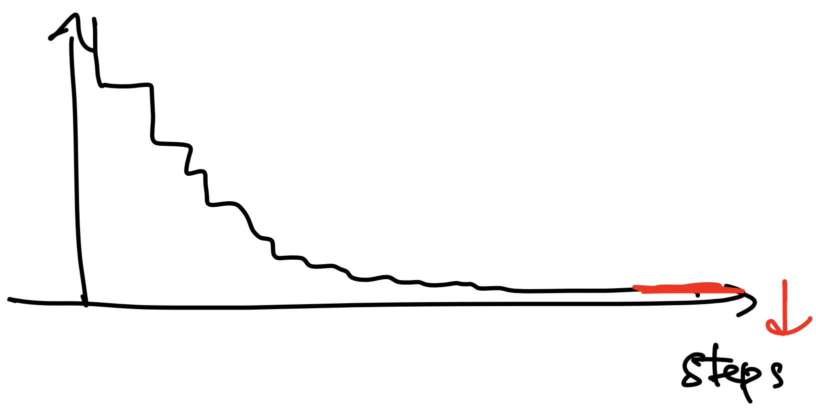
$E(\vec{\alpha})$

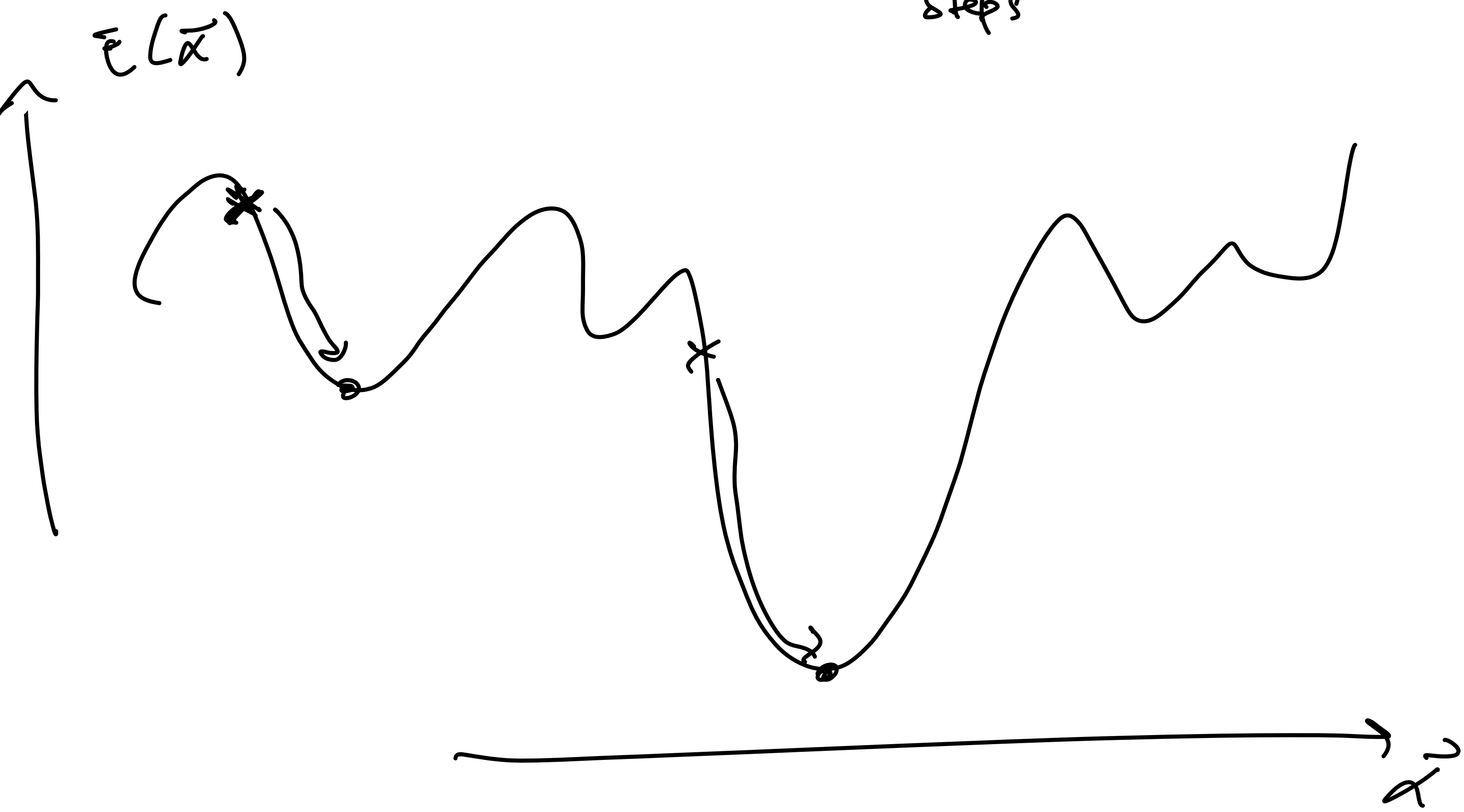
if $f \in \mathbb{R}$ $\quad = 2\left[\langle O_k^{(x)} E_L^{(x)} \rangle - \langle O_k^{(x)} \rangle \langle E_L^{(x)} \rangle\right]$

$$O_k^{(x)} = \frac{\partial}{\partial \alpha_k} \log f(x ; \vec{\alpha})$$

gradient descent $\quad \vec{\alpha} \to \vec{\alpha}' = \vec{\alpha} - \epsilon \vec{\nabla}_{\vec{\alpha}} E$

$\epsilon \ll 1$





Imaginary-time projection as a minimization tool

$$e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}\,|\Psi_T\rangle \rightarrow e^{-\tau\hat{\mathcal{H}}}\,|\Psi_T\rangle$$

$$\frac{it}{\hbar} = \tau \in \mathbb{R}$$

$$t = -i\tau\hbar$$

$|\Psi_T\rangle$ trial wavefunction

$$C_0 = \langle \Psi_T | \Phi_0 \rangle \neq 0$$

$|\Phi_0\rangle$: g.s. of $\hat{\mathcal{H}}$ (is unique)

$$|\Psi_T\rangle = \sum_\gamma c_\gamma |\Phi_\gamma\rangle \qquad \mathcal{H}|\Phi_\gamma\rangle = E_\gamma|\Phi_\gamma\rangle$$

$$= C_0|\Phi_0\rangle + \sum_{\gamma\neq 0} c_\gamma |\Phi_\gamma\rangle \qquad \boxed{E_0 = \min_\gamma E_\gamma}$$

$$e^{-\tau\mathcal{H}}|\Psi_T\rangle = e^{-\tau E_0}\, C_0|\Phi_0\rangle + \sum_{\gamma\neq 0} c_\gamma\, e^{-\tau E_\gamma}|\Phi_\gamma\rangle$$

$$= e^{-\tau E_0}\left[\, c_0|\Phi_0\rangle + \sum_{\gamma\neq 0} e^{-\tau(E_\gamma - E_0)}\, c_\gamma\, |\Phi_\gamma\rangle \right]$$

$$E_\gamma - E_0 > 0$$

$$e^{-\tau(E_\gamma - E_0)} \xrightarrow[\tau\to\infty]{} 0$$

$$\xrightarrow[\tau\to\infty]{} \underbrace{e^{-\tau E_0}\qquad} c_0\, |\Phi_0\rangle$$

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

Imaginary-time projection + variational optimization

$$e^{-\tau H}\,|\Psi(\vec{\alpha})\rangle \simeq \cancel{A}\; |\Psi(\vec{\alpha}+\Delta\vec{\alpha})\rangle$$

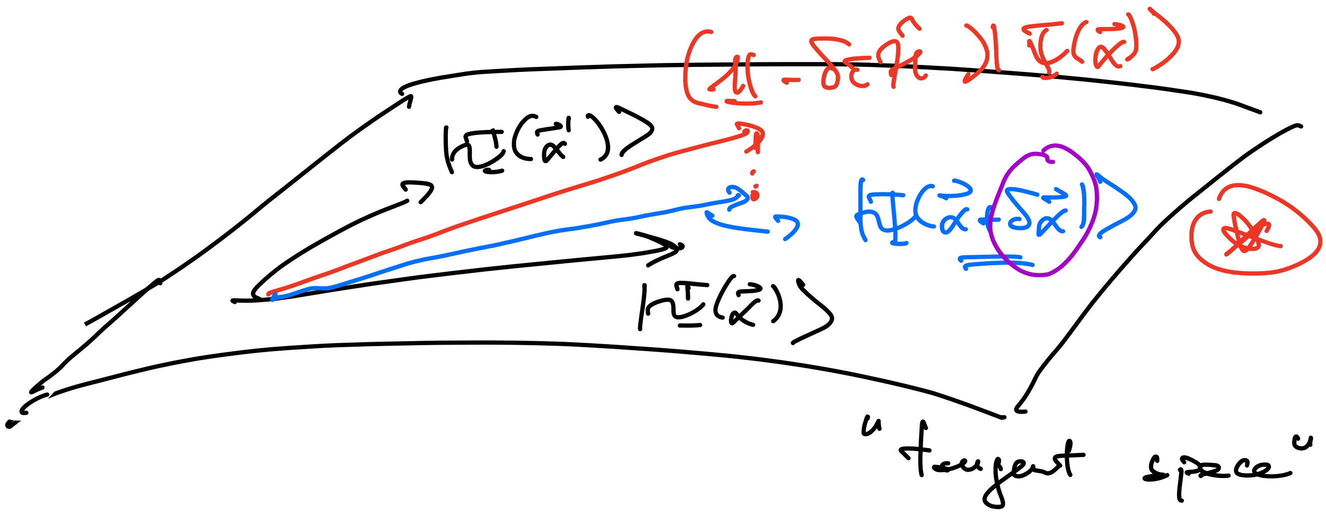
$$\delta\tau$$

$$e^{-\tau\hat{H}} = \lim_{n\to\infty}\left(e^{-\frac{\tau}{n}\hat{H}}\right)^n = \lim_{n\to\infty}\left(\hat{\mathbb{1}} - \delta\tau\,\hat{H}\right)^n$$

infinitesimal imaginary time evolution operator

$$\hat{\mathbb{1}} - \delta\tau \hat{H}$$

$$(\mathbb{1} - \delta\tau \hat{H})\,|\Psi(\vec{\alpha})\rangle \neq \cancel{A}\,|\Psi(\vec{\alpha}')\rangle$$



$$P_{TS}\left[(\mathbb{1} - \delta\tau \hat{H})\,|\Psi(\vec{\alpha})\rangle\right] = |\Psi(\vec{\alpha}+\delta\vec{\alpha})\rangle$$

$|\Psi(\vec{\alpha})\rangle$ is not a normalized vector

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

$$|\Psi(\vec{\alpha}+\delta\vec{\alpha})\rangle = |\Psi(\vec{\alpha})\rangle + \sum_{u=1}^{M} \delta\alpha_u \frac{\partial}{\partial\alpha_u} |\Psi(\vec{\alpha})\rangle + o(\delta\alpha)^2$$

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

$$\dots = \left(\mathbb{1} + \sum_u \delta\alpha_u \hat{O}_u\right)|\Psi(\vec{\alpha})\rangle + o(\delta\alpha)^2$$

$$\hat{O}_u |\Psi(\vec{\alpha})\rangle = \sum_x \left(\frac{\partial}{\partial\alpha_u}\log f\right) f(\vec{x},\vec{\alpha})\,|x\rangle$$

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

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

$$\left[\vec{\alpha} \in \mathbb{R}^M \qquad \alpha_u \in \mathbb{R} \quad \forall u\right]$$

$$f \in \mathbb{C}$$

$$\bar{O}_\mu = \frac{\langle \Psi(\vec{\alpha}) | \hat{O}_\mu | \Psi(\vec{\alpha}) \rangle}{\langle \Psi(\vec{\alpha}) | \Psi(\vec{\alpha}) \rangle} \in \mathbb{C}$$

$$\delta\vartheta = \sum_\mu \mathrm{Im}(\bar{O}_\mu)\,\delta\alpha_\mu$$

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

$$e^{i\delta\vartheta} + o(\delta\alpha)^2$$

$$= \dots = \Big(1 + i \sum_\mu \mathrm{Im}(\bar{O}_\mu)\,\delta\alpha_\mu\Big) |\phi(\vec{\alpha})\rangle$$

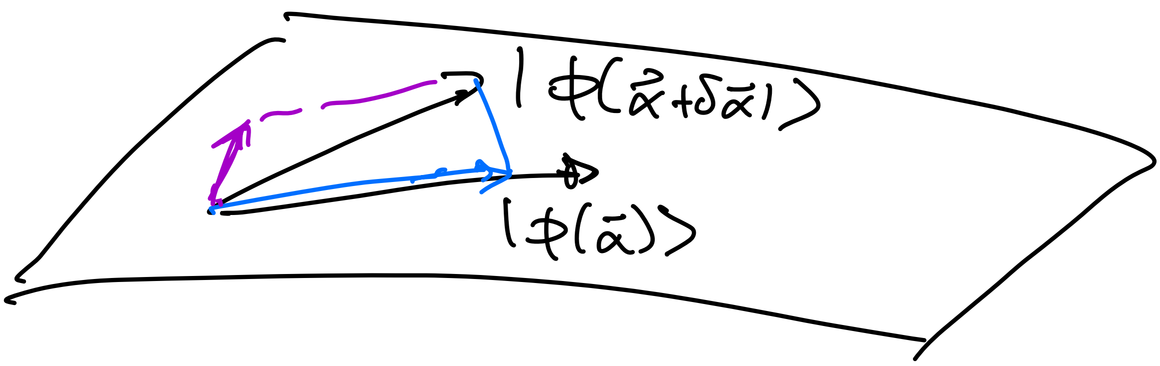
$$+ \sum_{\mu=1}^{n} \delta\alpha_\mu \, |\phi_\mu(\vec{\alpha})\rangle + O(\delta\alpha)^2$$

$$|\phi_\mu(\vec{\alpha})\rangle = (\hat{O}_\mu - \bar{O}_\mu)\,|\phi(\vec{\alpha})\rangle$$

$$\langle \phi(\vec{\alpha}) | \phi_\mu(\vec{\alpha}) \rangle = 0$$

$$e^{i\delta\vartheta}\,\delta\alpha = 1 + o(\delta\alpha)^2$$

$$= \langle \phi(\alpha) | \hat{O}_\mu | \phi(\vec{\alpha}) \rangle - \bar{O}_\mu$$



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

$$e^{i\delta\vartheta}\left[|\phi(\vec{\alpha})\rangle + \sum_k \delta\alpha_k \, |\phi_k(\vec{\alpha})\rangle + o(\delta\alpha)^2\right]$$

$\updownarrow$ (*) equivalent when projected onto tangent space

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

$\downarrow$

$$e^{i\gamma}\langle\phi(\vec{\alpha})|\Psi(\vec{\alpha}+\delta\vec{\alpha})\rangle = \langle\phi(\vec{\alpha})|(\mathbb{1} - \delta\tau\hat{\mathcal{H}})\,|\Psi(\vec{\alpha})\rangle$$

$$e^{i\gamma}\langle\phi_k(\vec{\alpha})|\Psi(\vec{\alpha}+\delta\vec{\alpha})\rangle = \langle\phi_k(\vec{\alpha})|(\mathbb{1} - \delta\tau\hat{\mathcal{H}})\,|\Psi(\vec{\alpha})\rangle$$

$k = 1, \ldots, M$

Conditions on $\delta\vec{\alpha}$

. . . $\gamma = -\delta\vartheta$

$$\underbrace{1 - \delta\tau\langle\phi(\vec{\alpha})|\hat{\mathcal{H}}|\phi(\vec{\alpha})\rangle}_{\in\mathbb{R}} = \underbrace{\cancel{e^{i(\gamma+\delta\vartheta)}}}_{\in\mathbb{R}}^{\,1} \; \overset{1+O(\delta\alpha)}{\frac{\|\Psi(\vec{\alpha}+\delta\vec{\alpha})\|}{\|\Psi(\vec{\alpha})\|}}$$

$$-\delta\tau \langle \phi_u | \hat{\mathcal{H}} | \phi(\vec{\alpha})\rangle = \cancel{e^{i(\gamma+\delta\gamma)}}^{\,1} \left(\cancel{\alpha_i}^{\,1}\right) \quad 1$$

$$\sum_{u'} \langle \phi_u(\vec{\alpha}) | \phi_{u'}(\vec{\alpha})\rangle\, \delta\alpha_{u'}$$

$$+ O(\delta\alpha)^2$$

Condition on $\underline{\delta\vec{\alpha}}$

$$\sum_{u'} \langle \phi_u(\vec{\alpha}) | \phi_{u'}(\vec{\alpha})\rangle\, \delta\alpha_{u'}$$

$$= -\delta\tau\, \underbrace{\langle \phi_u | \hat{\mathcal{H}} | \phi(\vec{\alpha})\rangle}_{\vec{F}/2}$$

$$\langle O_u^* O_{u'} \rangle - \langle O_u^* \rangle \langle O_{u'} \rangle = S_{uu'}$$

$$\boxed{\overleftrightarrow{S}\, \delta\vec{\alpha} = \delta\tau\, \vec{F}/2}$$

$\vec{F}$ = "force"

$$= -2 \left[\langle O_u^* E_L \rangle - \langle O_u^* \rangle \langle E_L \rangle \right]$$

$$\delta\vec{\alpha} = \delta\tau \, \overleftrightarrow{S}^{-1} \, \vec{F}/2$$

imaginary-time evolution algorithm

gradient descent

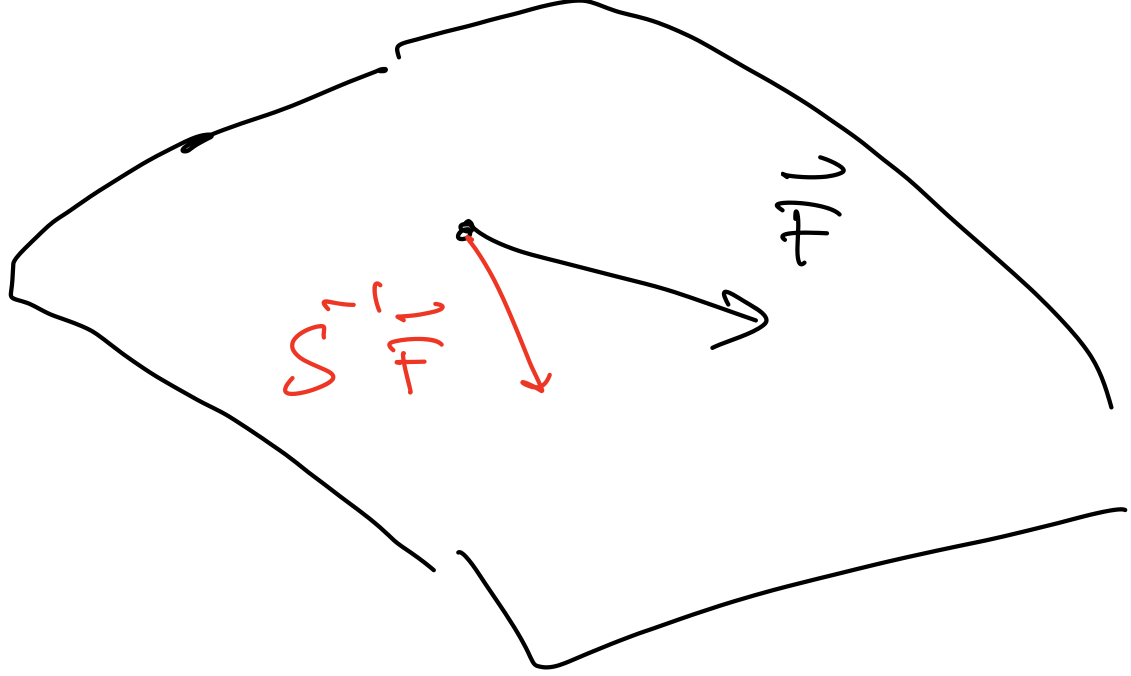
$$\delta\vec{\alpha} = -\overset{(\delta\tau/2)}{\epsilon} \, \nabla_{\vec{\alpha}} \langle \hat{H} \rangle$$

$$= -\overset{(\delta\tau/2)}{\epsilon} \Big[\langle O_k^* E_L \rangle + \langle O_k E_L^* \rangle - \langle O_k^* \rangle \langle E_L \rangle - \langle O_k \rangle \langle E_L \rangle$$

$f \in \mathbb{R}$ $\qquad$ $O_k \in \mathbb{R}$

$$\begin{cases} \delta\vec{\alpha} = \dfrac{\delta\tau}{2} \vec{F} & \text{gradient descent} \\[2ex] \delta\vec{\alpha} = \dfrac{\delta\tau}{2} S^{-1} \vec{F} & \text{imaginary time evolution} \end{cases}$$

S is semi positive definite



gradient descent — Lagrange multiplier

$$\min_{\delta\vec{\alpha}} \left[E(\vec{\alpha}+\delta\vec{\alpha}) + \mu\, |\delta\vec{\alpha}|^2 \right]$$

$\delta\vec{\alpha}^T \cdot \delta\vec{\alpha}$

$$\rightarrow \quad \nabla_{\vec{\alpha}} E = -\mu\, \delta\vec{\alpha}$$

imaginary-time evolution

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

$$\rightarrow \quad \nabla_{\vec{\alpha}} E = -\mu\, S\, \delta\vec{\alpha}$$

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

$$e^{-\tau H} |\Psi(\vec{\alpha})\rangle \simeq |\Psi(\vec{\alpha}+\delta\vec{\alpha})\rangle$$

$$\tau = \frac{it}{\hbar}$$

$$e^{-it/\hbar} |\Psi(\vec{\alpha})\rangle \simeq |\Psi(\vec{\alpha}+\delta\vec{\alpha})\rangle$$

real-time evolution

Improving upon VMC : imaginary-time projection

"Projector" Monte Carlo

$|\Psi_T\rangle$ trial wavefunction

→ it could be an optimized

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

→ any educated guess

$$\lim_{n\to\infty} (\mathbb{1}-\delta\tau\hat{H})^n |\Psi_T\rangle \sim |\Phi_0\rangle$$

$$\sum_{x'} |x'\rangle\langle x'| = \mathbb{1}$$

$$\langle x|(\mathbb{1}-\delta\tau H)^N|\Psi_0\rangle$$

$$|\Psi_0\rangle = |\Psi_T\rangle$$

$$= \sum_{x'} \langle x|(\mathbb{1}-\delta\tau H)|x'\rangle \langle x'|\Psi_0\rangle$$

$$= |\Psi_1\rangle = \sum_x \Psi_1(x)\,|x\rangle$$

$$\Psi_1(x) = \sum_{x'} G_{xx'}\,\Psi_0(x')$$

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

infinitesimal imaginary-time propagator

continue . . .

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

update rule of a quantum state to approach the g.s.

If $G_{xx'} \geq 0$ for $x \neq x'$

$$\underbrace{\langle x | \mathbb{1} - \delta\tau\, \mathcal{H} \,| x' \rangle}_{\hat{=}\; G_{xx'}} = -\delta\tau \underbrace{\langle x | \hat{\mathcal{H}} | x' \rangle}_{\geq 0}$$

≤ 0

$G_{xx} \geq 0$ $\qquad$ $\mathbb{1} - \delta\tau \langle x | \mathcal{H} | x \rangle \geq 0$

condition on $\delta\tau$ ∫

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

Perron-Frobenius theorem

extremal eigenvector → ground state $|\Phi_0\rangle$

$\Phi_0(x) \geq 0$

G.S. wavefunction is semi-positive definite

(Bosons !)

Choose $(\Psi_T) \to \Psi_T(x) \geq 0$

$\Rightarrow$ regard Ψ_T as a probability

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

update rule of a probability distribution