FYS4411/9411 FEB 17, 2022

$$W_i(t+\Delta t) \to W(\vec{y}, t+\Delta t)$$

$$= \int_{x\in D} \underbrace{W(\vec{y}, t+\Delta t \mid \vec{x}\, t)}_{\text{unknown}} w(\vec{x}, t)\, d\vec{x}$$

continuous Markov chain

How do these expression relate to quantum mech?

$$\hat{H}|\phi_0\rangle = E_0|\phi_0\rangle$$

$$\hat{H}\hat{H}^{-1} = \hat{H}^{-1}H = \mathbb{1}$$

$$\hat{H}^{-1}\hat{H}|\Phi_0\rangle = E_0\hat{H}^{-1}|\Phi_0\rangle$$

$\hat{H}$ is a differential operator

$$\hat{H} = -\frac{\nabla^2\hbar^2}{2m} - V(\vec{r}) \quad \text{(1 single particle)}$$

$\hat{H}^{-1}$ is an integral operator

insert $\int_{-\infty}^{\infty} |\vec{x}\rangle\langle\vec{x}|\, dx$

and multiply from the left with $\langle\vec{y}|$

$$\langle\vec{y}|\Phi_0\rangle = \Phi(\vec{y}) =$$

$$E_0 \int_{-\infty}^{\infty} \langle\vec{y}|H^{-1}|\vec{x}\rangle\langle\vec{x}|\Phi_0\rangle\, d\vec{x}$$

$$= E_0 \int_{-\infty}^{\infty} \underline{\langle\vec{y}|H^{-1}|\vec{x}\rangle}\, \Phi_0(\vec{x})\, d\vec{x}$$

Green's function / propagator

$$G(\vec{y},\vec{x}) = \langle\vec{y}|H^{-1}|\vec{x}\rangle$$

$$\Phi_0(\vec{y}) = \hat{H}(\vec{y})\,\hat{H}^{-1}\Phi_0(\vec{y})$$

$$= \int_{-\infty}^{\infty} \hat{H}(\vec{y})\, G(\vec{y},\vec{x})\,\Phi_0(\vec{x})\, d\vec{x}$$

$$\hat{H}(\vec{y})\, G(\vec{y},\vec{x}) = \delta(\vec{y}-\vec{x})$$

$$\hat{H}(\vec{x})\, G(\vec{x},\vec{y}) = \delta(\vec{x}-\vec{y})$$

Connection with Diffusion equation (1-Dim)

$$\frac{\partial w(x,t)}{\partial t} = D \frac{\partial^2 w(x,t)}{\partial x^2}$$

$$w(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left\{-\frac{x^2}{4Dt}\right\}$$

$$w(y,t+\Delta t) = \int_{-\infty}^{\infty} W(y\; t+\Delta t \,|\, x\; t)\, w(x,t)\, dx$$

$$\frac{\partial W(y\; t+\Delta t \,|\, x\; t)}{\partial t} = D \frac{\partial^2}{\partial x^2} W(y, t+\Delta t \,|\, x\; t)$$

$$W(y\; t+\Delta t \,|\, x\; t) =$$

$$\frac{1}{\sqrt{4\pi D \Delta t}} \exp\left\{-\frac{(y-x)^2}{4D\Delta t}\right\}$$

Factor q in Metropolis Hastings;

$$q = \frac{W(y\, t+\Delta t \mid x\, t)\, w(y\, t+\Delta t)}{W(x\, t \mid y\, t+\Delta t)\, w(x\, t)}$$

without quantum force

$$q = \frac{w(y\, t+\Delta t)}{w(x\, t)}$$

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Basic elements in a VMC code

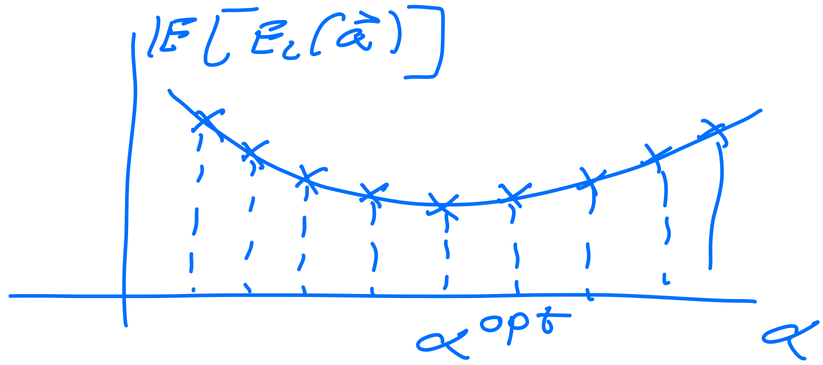
- Metropolis sampling ✓
- Analytical expression for $E_L(\vec{R}; \vec{\alpha})$ ✓

- importance sampling

$$\vec{F} = \frac{2}{\psi_T} \vec{\nabla} \psi_T$$

- optimization of

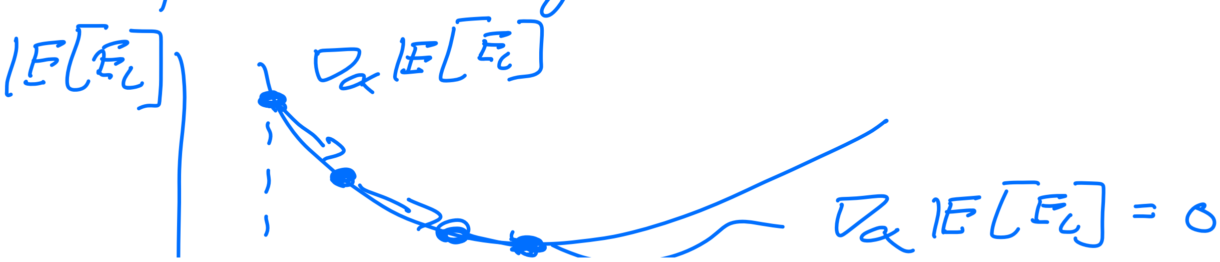
$$\mathbb{E}[E_L(\vec{\alpha})]$$

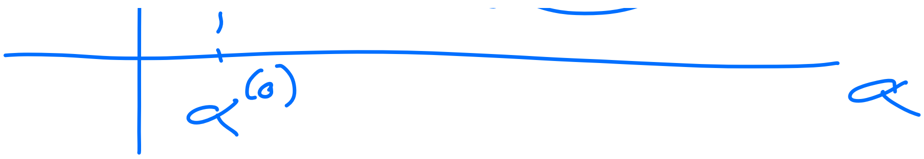


$$\alpha^{opt} = \arg\min_{\alpha \in \mathbb{R}^M} \mathbb{E}[E_L(\vec{\alpha})]$$

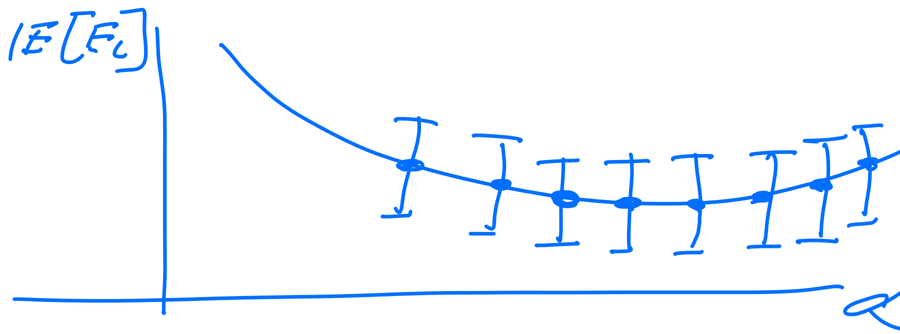
Can we optimize the search for α^{opt} with less Monte Carlo cycles?

Yes $\rightarrow$ gradient methods





- Gradient optimization
- After this: stochastic resampling method: we want proper estimation of errors



error (standard deviation) estimate.

Post analysis with resampling methods: Blocking, Bootstrap, Jackknife

- parallelization

- Gradient optimization

$\langle E \rangle = \int d\vec{R}\, P(\vec{R};\vec{\alpha}) E(\vec{R};\vec{\alpha})$

$$\mathbb{E}[E_L(\vec{\alpha})] = \int d\vec{R}\, P(\vec{R};\vec{\alpha}) E_L(\vec{R};\vec{\alpha})$$

$$\simeq \frac{1}{M} \sum_{i=1}^{M} E_L(\vec{R}_i;\vec{\alpha})$$

$$P_T(\vec{R};\alpha) = \frac{|\psi_T(\vec{R};\vec{\alpha})|^2}{\int d\vec{R}\, |\psi_T|^2}$$

$$E_L(\vec{R};\vec{\alpha}) = \frac{1}{\psi_T} \hat{H} \psi_T(\vec{R};\vec{\alpha})$$

$$\psi_T(\vec{R};\vec{\alpha}) \rightarrow \psi_T(\vec{\alpha})$$

$$P_T(\vec{R};\vec{\alpha}) \rightarrow P_T(\vec{\alpha})$$

$$E_L(\vec{R};\vec{\alpha}) \rightarrow E_L(\vec{\alpha})$$

$$\frac{\partial\, \mathbb{E}[E_L(\vec{\alpha})]}{\partial \vec{\alpha}} = 0 \quad ?$$

$$= \int d\vec{R} \left[\frac{d P_T(\vec{\alpha})}{d\vec{\alpha}} E_L(\vec{\alpha}) + P_T(\vec{\alpha}) \frac{d E_L(\vec{\alpha})}{d\vec{\alpha}} \right]$$

Example : HO in 1 Dim

$$\psi(\vec{\alpha}) = \psi(\alpha) = e^{-\frac{1}{2}\alpha^2 x^2}$$

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$$\frac{d P(\alpha)}{d\alpha} \quad \wedge \quad \frac{d E_L(\alpha)}{d\alpha}$$

$$\frac{d p(\alpha)}{d\alpha} = \frac{d}{d\alpha}\left[\frac{e^{-\frac{1}{2}\alpha^2 x^2 \cdot 2}}{\int dx\, e^{-\alpha^2 x^2}}\right]$$

$$\frac{d\, \mathbb{E}[E_L(\alpha)]}{d\alpha} =$$

$$2\left[\mathbb{E}\left[\frac{d \ln \psi(\alpha)}{d\alpha} E_L(\alpha)\right] - \mathbb{E}\left[\frac{d \ln \psi(\alpha)}{d\alpha}\right]\mathbb{E}\left[E_L(\alpha)\right]\right]$$

$$= 0$$

new integral

$$\int dx \frac{d \ln \psi(x,\alpha)}{d\alpha} E_L(x;\alpha)$$

new integral

$$\int dx \frac{d \ln \psi(x,\alpha)}{d\alpha}$$

$$\frac{\left(\frac{d\,\psi(\alpha)}{d\alpha}\right)}{\psi(\alpha)}$$

- set up 3 integrals, two new ones and $\int dx\, p(x;\alpha)\, E_L(x;\alpha)$
- use automatic differentiation