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Continuous Markov chain

$$w(\vec{y}, t+\Delta t) = \int_{x \in D} W(\vec{y}, t+\Delta t | \vec{x}\vec{y}) \times w(\vec{x}, t)\, d\vec{x}$$

How does this link with QM?

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

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

$$\hat{H}^{-1}\hat{H}|\phi_0\rangle = E_0 H^{-1}|\phi_0\rangle$$

$\hat{H}$ is a differential operator

1-particle

$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2m} + v(\vec{r})$$

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

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

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

$$\langle \vec{y} | \phi_0 \rangle = \Phi_0(\vec{y})$$

$$= E_0 \int_{-\infty}^{\infty} \langle \vec{y} | \hat{H}^{-1} | \vec{x} \rangle \underbrace{\langle \vec{x} | \phi_0 \rangle}_{\Phi_0(\vec{x})} d\vec{x}$$

Green's function / propagator

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

probability of making a transition from $\vec{x} \to \vec{y}$

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

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

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

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

parallel to

$$\frac{\partial W(\vec{y}, t+\Delta t \,|\, \vec{x} t)}{\partial t} =$$

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

$$W(\vec{y}, t+\Delta t | \vec{x} t) =$$

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

Trial wf in code example

$\hbar = m = e = \varepsilon_0 = 1$

$$H = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} + \frac{1}{2} r_1^2 + \frac{1}{2} r_2^2 + \frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

$$\Psi_T = e^{-\alpha^2 (r_1^2 + r_2^2)/2} f(r_{12}, \beta)$$

$$r_{12} = |\vec{r}_1 - \vec{r}_2| = \sqrt{(x_1-x_2)^2 + (y_1-y_2)^2 + (z_1-z_2)^2}$$

$$f(r_{12}, \beta) = \exp\left\{\frac{r_{12}}{1+\beta r_{12}}\right\}$$

$$\vec{\alpha} = \{\alpha, \beta\}$$

(i) Metropolis ratio

$$R = \frac{|\psi(\vec{R}_{new})|^2}{|\psi(\vec{R}_{old})|^2}$$

(ii) Quantum Force

$$\vec{F}_i = 2\frac{1}{\psi}\vec{\nabla}_i\psi$$

(iii) Kinetic energy

$$\frac{1}{\psi}\left(-\frac{\nabla_i^2}{2}\psi\right)$$

(i) can move all particles

$$\vec{R}_{old} = \{\vec{r}_{1old}, \vec{r}_{2old}, \dots, \vec{r}_{Nold}\}$$

$$\vec{R}_{new} = \{\vec{r}_{1new}, \vec{r}_{2new}, \dots \vec{r}_{Nnew}\}$$

Then perform Metropolis test, $\vec{F}$, + Kinetic energy.

(ii) Move one particle at the time, and then

test (R) and compute
$\bar{F}$ and K ,

Trial wf in p1 .

$\psi_T(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N) \propto$

$\varphi_{\alpha_1}(\vec{r}_1)\, \varphi_{\alpha_2}(\vec{r}_2) \ldots \varphi_{\alpha_N}(\vec{r}_N)$

$$R = \frac{\varphi_{\alpha_1}(\vec{r}_{1\,new})\, \cancel{\varphi_{\alpha_2}(\vec{r}_{2\,old}) \ldots \varphi \ldots}}{\varphi_{\alpha_1}(\vec{r}_{1\,old})\, \cancel{\varphi_{\alpha_2}(\vec{r}_{2\,old}) \ldots}}$$

$$= \frac{\varphi_{\alpha_1}(\vec{r}_{1\,new})}{\varphi_{\alpha_1}(\vec{r}_{1\,old})}$$

$$= e^{-\frac{1}{2}\alpha^2(\vec{r}_{1\,new}^{\,2} - \vec{r}_{1\,old}^{\,2})}$$

Basic elements of VMC code

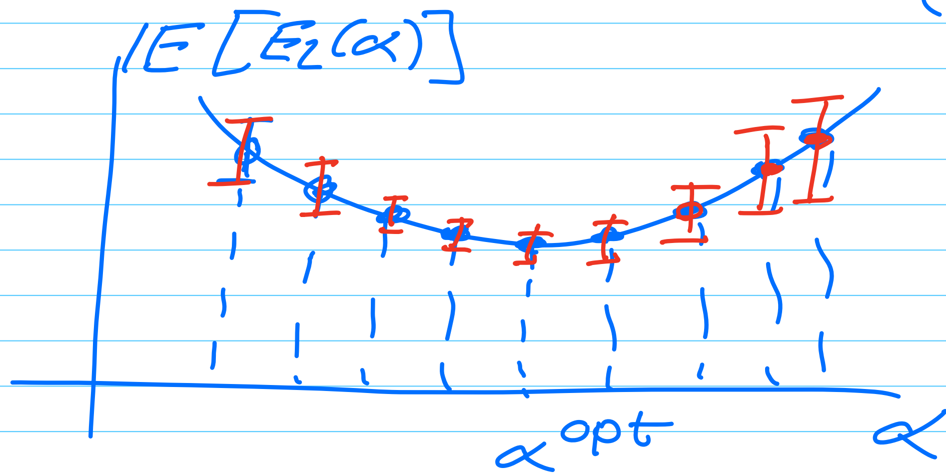
- Metropolis + Markov chains
- Expression for $E_L(\vec{R};\vec{\alpha})$
  $\psi_T(\vec{R};\vec{\alpha})$, $P_T \sim |\psi_T|^2$

- importance sampling
  (Metropolis–Hastings)

$$\vec{F} = 2 \frac{1}{\psi_T} \vec{\nabla} \psi_T$$

- optimization part

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



each point is obtained with the same amount of Monte carlo cycles

$$\alpha^{opt} = \hat{\alpha} = \underset{\alpha \in \mathbb{R}^m}{\arg\min}\, \mathbb{E}[E_L(\alpha)]$$

Can we optimize the search for $\hat{\alpha} = \alpha^{opt}$ with less

Monte Carlo?

yes → gradient methods:

- gradient descent
- stochastic gradients
- stochastic reconfig.
- steepest descent
- conjugate descent