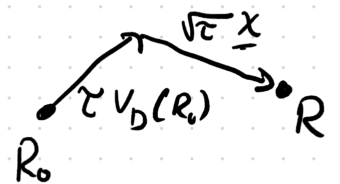
Diffusion Monte Carlo

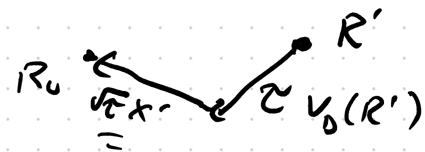
Biased Metropolis

$$v_D(R) = \frac{\nabla \psi(R)}{\psi(R)}$$

$$T(R_0 \to R')$$



$$T(R' \to R_0)$$



$$\frac{P(R_0 \to R')}{P(R' \to R_0)} = \frac{\psi_T^2(R')}{\psi_T^2(R_0)}$$

$$T(R_0 \to R') = e^{-\chi^2/2\tau} = e^{-(R' - \tau v_D(R_0) - R_0)^2/2\tau}$$

$$T(R' \to R_0) = e^{-(R_0 - \tau v_D(R') - R')^2/2\tau}$$

Proposal 1:

9-10: DMC

10:30-12:30: Hands on

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Proposal 2

9-10: Hands-on

10:30-11:30: Lecture

11:50-12:30: Hands-on

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Basic idea:

$|\psi_T\rangle$ from VMC

Energy Eigenstates

$$e^{-H\tau}|\psi_T\rangle = \sum c_i e^{-E_i\tau}|\Phi_i\rangle$$

$$\frac{\langle\psi_T|H e^{-H\tau}|\psi_T\rangle}{\langle\psi_T|e^{-H\tau}|\psi_T\rangle} = \frac{\sum E_i \boxed{c_i^2 e^{-E_i\tau}}}{\sum \boxed{c_i^2 e^{-E_i\tau}}} \xrightarrow[\tau\to\infty]{} E_0$$

Monte Carlo implementation

$$\frac{\langle \psi_T | H e^{-\tau H} | \psi_T \rangle}{\langle \psi_T | e^{-\tau H} | \psi_T \rangle} = \frac{\int \langle \psi_T | H | R_0 \rangle \langle R_0 | e^{-\tau H} | R_1 \rangle \langle R_1 | \psi_T \rangle dR_0 dR_1}{\int \underbrace{\langle \psi_T | R_0 \rangle \langle R_0 | e^{-\tau H} | R_1 \rangle \langle R_1 | \psi_T \rangle}_{\tilde{\rho}(R_0, R_1)} dR_0 dR_1}$$

$$= \int \underbrace{\frac{\langle \psi_T | H | R_0 \rangle}{\langle \psi_T | R_0 \rangle}}_{\text{Average this}} \underbrace{\frac{\tilde{\rho}(R_0, R_1)}{\int \tilde{\rho}(R_0, R_1) dR_0 dR_1}}_{\text{Sample this}} dR_0 R_1$$

Diffusion Monte Carlo:

- Stochastic process to sample

$$\rho \propto \psi_T^*(\underbrace{R_0) \langle R_0 | e^{-\tau H} | R_1 \rangle \psi_T(R_1}_{\text{path}})$$

- For energy

$$\langle E \rangle = \langle E_{Loc}(R_0) \rangle_{R_0, R_1 \sim \rho}$$

Sampling the path

- Two approaches
  - generate R_0, R_1 with probability $\rho(R_0, R_1)$
  - Sample another distribution $p(R_0, R_1)$ and weight so that $pw = \rho$

$$\langle E \rangle = \frac{\sum w_i E_L(R_i)}{\sum w_i}$$

$$\frac{\int E_L \rho}{\int \rho} = \frac{\int E_L w p}{\int w p} = \frac{\langle E_L w \rangle}{\langle w \rangle}$$

DMC Strategy

$$R_0 \sim \psi_T^2$$

$$R_1 \sim \frac{\langle R_1 | e^{-\tau H} | R_0 \rangle \, \psi_T(R_1)}{\psi_T(R_0)}$$

$$\psi_T(R_1) \langle R_1 | e^{-\tau H} | R_0 \rangle \, \psi_T(R_0)$$

Approximating $\langle R_1 | e^{-\tau H} | R_0 \rangle$

Differential eqn	Green function
$-\frac{\partial \psi}{\partial \tau} = -\frac{1}{2} \nabla^2 \psi$	$e^{-(R_1 - R_0)^2/2\tau}$ — Diffusion
$-\frac{\partial \psi}{\partial \tau} = V \psi$	$e^{-\tau V(R_0)} \delta(R_0 - R_1)$ — Population
$-\frac{\partial \psi}{\partial \tau} = -\frac{1}{2} \nabla^2 \psi + V \psi = \hat{H} \psi$	$\langle R_1 \| e^{-\tau H} \| R_0 \rangle = e^{-\tau V(R_1)/2} e^{-(R_1 - R_0)^2/2\tau} e^{-\tau V(R_0)/2} + \mathcal{O}(\tau^2)$

Diffusion Monte Carlo without importance sampling

$$R_0 \sim \psi_T^2$$

$$R_1 = e^{-(R_1 - R_0)^2/2\tau}$$

$$R_2 = e^{-(R_2 - R_1)^2/2\tau}$$

We sampled:

$$p = \psi_T^2(R_0)\, e^{-(R_1 - R_0)^2/2\tau}\, e^{-(R_2 - R_1)^2/2\tau}$$

Wanted

$$\rho = \underline{\psi_T(R_0)}\, \underline{e^{-kR_0^2/2}}\, \underline{e^{-(R_1 - R_0)^2/2\tau}}\, \underline{e^{-kR_1^2}}\, \underline{e^{-(R_2 - R_1)^2}}\, \underline{e^{-kR_2^2/2}}\, \psi_T(R_2)$$

Weight:

$$w = \frac{\rho}{p} = e^{-kR_0^2/2}\, e^{-kR_1^2}\, e^{-kR_2^2/2}\, \frac{\psi_T(R_2)}{\psi_T(R_0)}$$

Issues

Variance in weight $\rightarrow$ inefficiency

$$w = e^{-kR_0^2/2} e^{-kR_1^2} e^{-kR_2^2/2} \frac{\psi_T(R_2)}{\psi_T(R_0)}$$

- $\dfrac{\psi_T(R_N)}{\psi_T(R_0)}$ varies a lot.
- $e^{-\tau V}$ varies a lot
- $\dfrac{\psi_T(R_N)}{\psi_T(R_0)}$ averages to zero $\rightsquigarrow$ Sign problem!

Importance sampling

Differential eqn	Green function
$\psi_T\left(-\frac{\partial \psi}{\partial \tau}\right) = \psi_T \hat{H} \psi$	$\approx \underbrace{e^{-\tau E_L(R_0)/2}}_{\text{weights}} \underbrace{e^{-(R_0 - R_1 - v(R_1)\tau)/2\tau}}_{\text{sample}} \underbrace{e^{-\tau E_L(R_1)/2}}$
	$= \langle R_0 \mid e^{-\tau H} \mid R_1 \rangle \frac{\psi(R_1)}{\psi(R_0)}$

See Reynolds, Ceperley, Lester or Foulkes Rev. Mod. Phys.

Example:

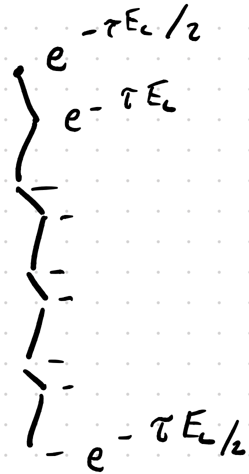
$\bullet\ \Psi_T^2$

$$\downarrow \quad e^{-(R_1 - R_0 - v_D(R_0))^2/2\tau}$$

$\bullet\ R_1$

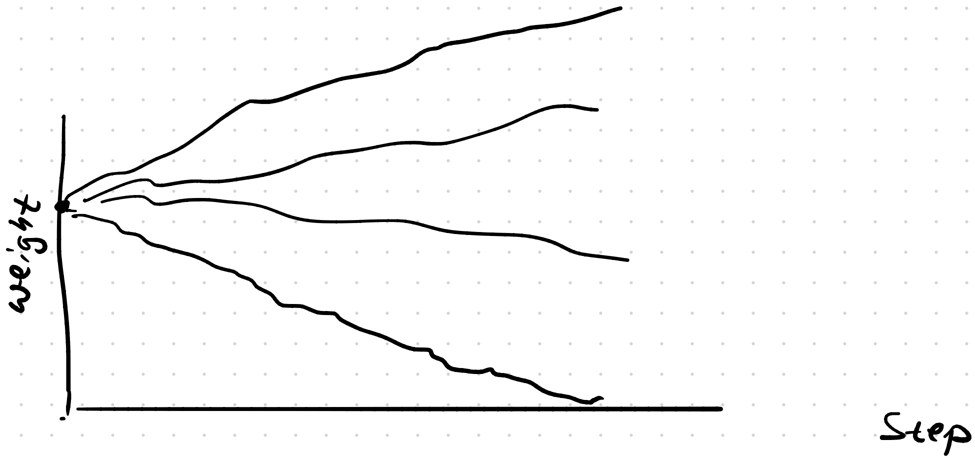
weight: $e^{-(E_L(R_0) + E_L(R_1))\tau/2}$

Long paths



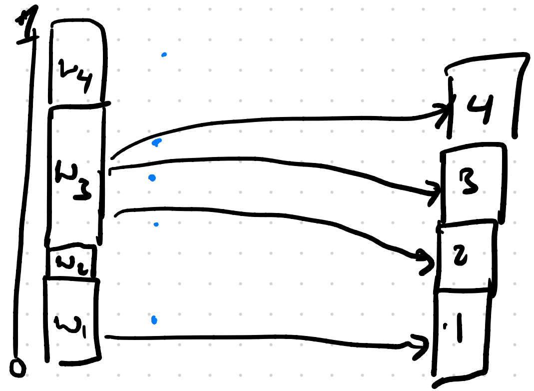
Shift using E_T so $e^{-\tau(E_L - E_T)} \sim 1$

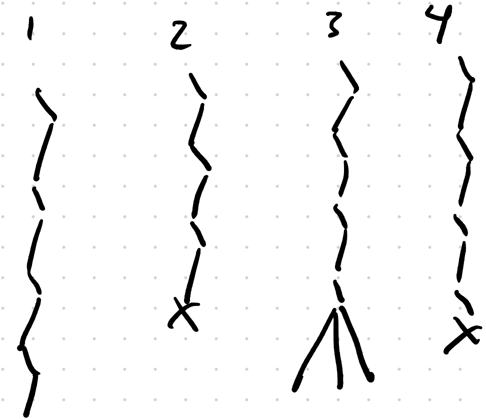
Efficiency problem



Eventually variance of weights gets too big.

Branching





Summary: DMC

① Sample $R_0 \sim \psi_T^2$

② Iterate:

ⓐ $R_{n+1} = R_n + \sqrt{\tau}\,\chi + \tau v_D(R_n)$

ⓑ $w_{n+1} = w_n + e^{-\left(E_L(R_n) + E_L(R_{n+1}) - 2E_T\right)\tau/2}$

ⓒ update E_T

ⓓ Branching