FYS4411 Lecture Feb 4

importance sampling:

$$W(j \to i) = \underset{\text{acceptance probability}}{A(j \to i)}\, \underset{\text{Transition}}{T(j \to i)}$$

PDF : $P_i^{(t)}$ $\left[P(\vec{R}_i; \vec{\alpha}) = \dfrac{|\psi_T(\vec{R}_i; \alpha)|^2}{\int |\psi_T|^2 d\vec{R}} \right.$

Metropolis algo
($t \to \infty$)

$$A(j \to i) = \min\left(1, \frac{P_i\, T(i \to j)}{P_j\, T(j \to i)}\right)$$

$$T(i \to j) = T(j \to i)$$

Make a model for $T(j \to i)$

standard Diff eq

$$P_j^{(t)} \to P(\vec{x}_j; t)$$

$$\boxed{\frac{\partial P}{\partial t} = D \sum \frac{\partial^2}{\partial x^2} P}$$

$\partial t \qquad \sum_i \qquad \partial x_i^2$

Fokker-Planck, introduce drift velocity due to some external force F_i

$$\boxed{\frac{\partial P}{\partial t} = \sum_i D \frac{\partial}{\partial x_i}\left(\frac{\partial}{\partial x_i} - F_i(\vec{x})\right)P}$$

we want P to converge in limit $t \to \infty$

$$P(\vec{x}) = \frac{|\psi^2(\vec{x})|}{\int |\psi(\vec{x})|^2 d\vec{x}}$$

at equilibrium $\frac{\partial P}{\partial t} = 0$

$$\sum_i D\left[\frac{\partial^2 P}{\partial x_i^2} - \frac{\partial}{\partial x_i}(F_i P)\right] = 0$$

$$\underline{\frac{\partial^2 P}{\partial x_i^2}} = P\frac{\partial F_i}{\partial x_i} + F_i\frac{\partial P}{\partial x_i}$$

F_i takes the form

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$$\boxed{F = g(p)\frac{\partial p}{\partial x}}$$

in order to have a 2nd derivative on the rhs

$$\underline{\frac{\partial^2 p}{\partial x_i^2}} = p\frac{\partial g}{\partial p}\left(\frac{\partial p}{\partial x_i}\right)^2 + \underbrace{\underline{p \cdot g}\frac{\partial^2 p}{\partial x_i^2}} + g\left(\frac{\partial p}{\partial x_i}\right)^2$$

$g = 1/p$

then all terms cancel.

$$p = \frac{|\psi|^2}{\int|\psi|^2 dx} \Rightarrow$$

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

= "quantum Force".

Desired p in limit $t \to \infty$

in statistical mechanics,

the trajectories in the Fokker-Planck eq (FP) are generated by the Langevin eq.

$$\frac{\partial x}{\partial t} = D\, F(x(t)) + \underset{\text{random fluctuations}}{\eta}$$

integrating (δt)

$$\vec{y} = \vec{x} + D\, \underline{F(\vec{x})}\, \underline{\delta t} + \underset{\text{Gaussian RN}}{X}$$

$\mu = 0$

$\sigma^2 = 2 D \delta t$

Brute Force MC, we have a step size δ

Here we need to tune δt

$\delta t = \{10^{-1}, 10^{-2}, 10^{-3}\}$, then extrapolate to $\delta t = 0$

Metropolis Sampling

$$T(i \to j) \to G(\vec{y}, \vec{x}; \delta t)$$

$$A(j \to i) \to A(\vec{y}, \vec{x})$$

$$= \min\left(1, \frac{\psi^2(\vec{y})\, G(\vec{y}, \vec{x}; \delta t)}{\psi^2(\vec{x})\, G(\vec{x}, \vec{y}; \delta t)}\right)$$

$$\frac{\partial P}{\partial t} = \mathcal{L} P$$

$$\mathcal{L} = D \vec{\nabla}(\vec{\nabla} - \vec{F})$$

$$G(\vec{y}, \vec{x}; \delta t) \propto \exp\left[D \delta t (\nabla^2 - \vec{\nabla} F - \vec{F} \vec{\nabla})\right]$$

F varies little when we move from $\vec{x} \to \vec{y}$

$$G(\vec{y}, \vec{x}; \delta t) =$$

$$\frac{1}{(4\pi D\delta t)^{3N/2}} \exp\left\{ \left[-(\vec{y}-\vec{x}-D\delta t \vec{F}(\vec{x})) \right]^2 / 4D^2\delta t^2 \right.$$

variance $2D\delta t$

$$\boxed{\begin{aligned} &- \quad \vec{F}(\vec{x}) = \frac{2}{\psi(\vec{x})} \underline{\vec{\nabla}\psi(\vec{x})} \\ &- \quad \vec{y} = \vec{x} + D\underline{\vec{F}(\vec{x})}\delta t + \chi \\ &- \quad G(y, x; \delta t) \end{aligned}}$$

Python code (2-dim electron)

$$\psi_T(\vec{r}_1, \vec{r}_2) = e^{-\alpha(r_1^2+r_2^2)} J(|\vec{r}_1-\vec{r}_2|)$$

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

$$J(|\vec{r}_1-\vec{r}_2|) = J(r_{12})$$

$$= e^{\frac{r_{12}}{1+\beta r_{12}}}$$

— computational issues —

- Metropolis Test

$$P = \quad \psi_{\text{new}} \quad \psi^{\text{new}}$$

$$R = \frac{\cdots}{\psi_{0B}^{old}\,\psi_C^{old}}$$

$$\psi_{0B}^{new} = \varphi(r_1^{new})\,\varphi(r_2^{old}) \cdots \varphi(r_N^{old})$$

move one particle at the time

$$\frac{\nabla\psi}{\psi} = \frac{(\vec{\nabla}\psi_{0B})\psi_C + \psi_{0B}\nabla\psi_C}{\psi_{0B}\psi_C}$$

Quantum force = local energ

$$= \frac{\nabla\psi_{0B}}{\psi_{0B}} + \frac{\nabla\psi_C}{\psi_C}$$

$$\frac{1}{\psi}\nabla^2\psi = \frac{1}{\psi_{0B}\psi_C}\left(\nabla^2(\psi_{0B}\psi_C)\right)$$

local energy

$$= \frac{1}{\psi_{0B}\cancel{\psi_C}}(\nabla^2\psi_{0B})\cancel{\psi_C}$$

$$+ \frac{1}{\psi_C}\nabla^2\psi_C$$

$$+ 2\frac{1}{\psi_{0B}\psi_C}\vec{\nabla}\psi_{0B}\,\vec{\nabla}\psi_C$$