FYS4411/9411 lecture, February 14, 2025

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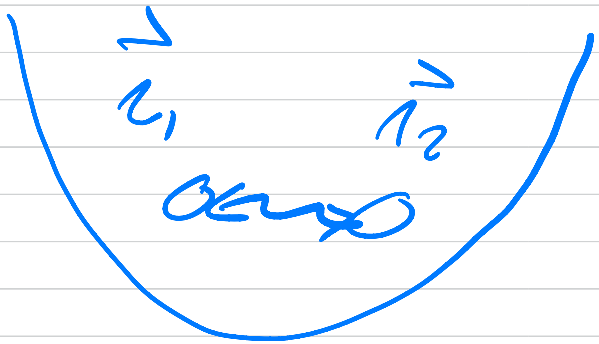
$$\Psi_T(\vec{r}_1, \vec{r}_2; \alpha, \beta) = \underbrace{e^{-\alpha^2(r_1^2+r_2^2)}}_{OB} \underbrace{\times\, e^{\frac{r_{12}}{1+\beta r_{12}}}}_{C}$$

$$r_i^2 = x_i^2 + y_i^2$$

$$r_{12} = \sqrt{(x_1-x_2)^2+(y_1-y_2)^2}$$



$$\vec{F}_i = \frac{1}{\Psi_T}\vec{\nabla}_i \Psi_T$$

kinetic energy

$$\nabla_i^2 \Psi_T$$

$$\Psi_T(\vec{R};\vec{\alpha}) = \varphi_{OB}(\vec{R};\vec{\alpha}) \times \varphi_C(\vec{R};\vec{\alpha})$$

$$\nabla_i^2 \psi_T = \nabla_i^2 \left(\varphi_{0B}(\vec{R};\vec{r}) \, \varphi_c(\vec{R};\vec{r}) \right)$$

$$\frac{1}{\psi_T} \nabla_i^2 \psi_T = \frac{1}{\varphi_{0B}} \nabla_i^2 \varphi_{0B}$$

$$+ \frac{1}{\psi_T} \vec{\nabla}_i \varphi_{0B} \, \vec{\nabla}_i \varphi_c$$

$$+ \frac{1}{\varphi_c} \nabla_i^2 \varphi_c$$

$$q(y,x) = \frac{T(x \to y)}{T(y \to x)} \frac{|\psi_T(y)|^2}{|\psi_T(x)|^2}$$

$$\frac{\partial P}{\partial t} = D \nabla^2 P$$

$$P \to T \propto e^{-(y-x)^2/4Dt}$$

$$\frac{T(x \to y)}{T(y \to x)} = \frac{e^{-(y-x)^2/4D\tau}}{e^{-(x-y)^2/4D\tau}}$$

$$= 1$$

$P(x,t) \rightarrow \phi(x,t)$

$$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial x^2}$$

initial conditions

$$\phi(x, t=0) = f(x)$$

Boundary conditions

$$\lim_{x \to \pm\infty} \phi(x,t) = 0 \quad \forall t$$

Fourier transform to $-k-$

$$\phi(x,t) \longrightarrow \tilde{\phi}(k,t)$$

$$\tilde{\phi}(k,t) = \int_{x\in D} dx\, e^{ikx} \phi(x,t)$$

$$\frac{\partial \tilde{\phi}(k,t)}{\partial t} = -Dk^2 \tilde{\phi}(k,t)$$

with initial condition

$$\tilde{\phi}(k,0) = \tilde{f}(k) = \int dx\, e^{ikx} f(x)$$

unique solution

$$\tilde{\phi}(k,t) = \tilde{f}(k)\, e^{-Dk^2 t}$$

$\phi(x,t)$ is given by inverse Fourier transform

$$\phi(x,t) = \int_{k \in D} dk\, e^{-ikx}\, \tilde{\phi}(k,t)$$

Example: gaussian

$$f(x) = e^{-\alpha^2 x^2}$$

$$F\left[e^{-\alpha^2 x^2}\right] = \frac{\sqrt{\pi}}{\alpha} e^{-k^2/4\alpha^2}$$

$$\alpha^2 = \frac{1}{4D \cdot t} \quad (\text{fixed } t)$$

$$F^{-1}\left[e^{-Dtk^2}\right] = \frac{e^{-x^2/4Dt}}{\sqrt{4\pi D t}}$$

in n-dimensions

$$F^{-1}\left[e^{-D|\vec{k}|^2 t}\right] = \frac{1}{(4\pi D t)^{n/2}} \exp\left[-\frac{|x|^2}{4Dt}\right]$$

also known as the fundamental distribution of the diffusion equation,

$$F^{-1}\left[e^{-D|\vec{k}| t}\right] = S_n(\vec{x}, t)$$

convolution theorem

$$y(t) = (x * w)(t) = \int_{s \in D} ds\, x(s)\, w(t-s)$$

$$\phi(\vec{x}, t) = (f * S_n)(\vec{x}, t)$$

$$= \frac{1}{(4\pi D t)^{n/2}} \int_{\mathbb{R}^n} d^n y\, f(\vec{y}) \times \exp\left[-\frac{|\vec{x}-\vec{y}|^2}{4Dt}\right]$$

$$\left[w_i(t) = \sum_j W(j \to i)\, w_j(t') \right]$$

suppose

$$f(x) = \left(\frac{\alpha}{\pi}\right)^{n/2} \phi_0 \, e^{-\alpha|\vec{x}|^2}$$

normalized so that

$$\int_{\mathbb{R}^n} d^n x \, f(\vec{x}) = \phi_0$$

$$\phi(\vec{x},t) = \bar{\Phi}_0 \left[\frac{\alpha}{4\pi^2 D t}\right]^{n/2}$$

$$\times \int_{\mathbb{R}^n} d^n y \, \exp\left[-\alpha|\vec{y}|^2 - \frac{|\vec{x}-\vec{y}|^2}{4Dt}\right]$$

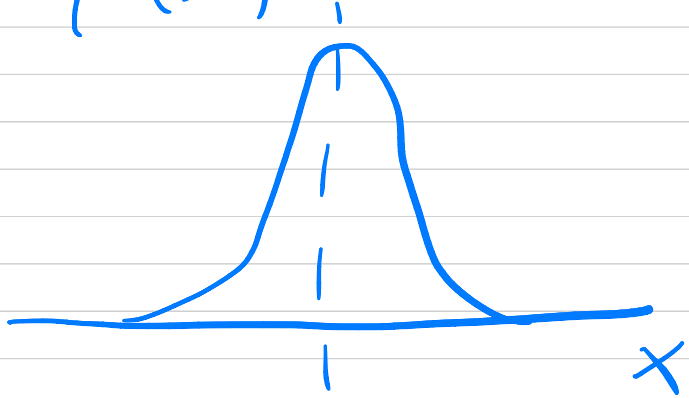
Markov-chain continuous dist.

$$\phi(\vec{x},t) = \int_{\mathbb{R}^n} d^n y \; \phi(\vec{y})\, W(\vec{x},\vec{y},t)$$

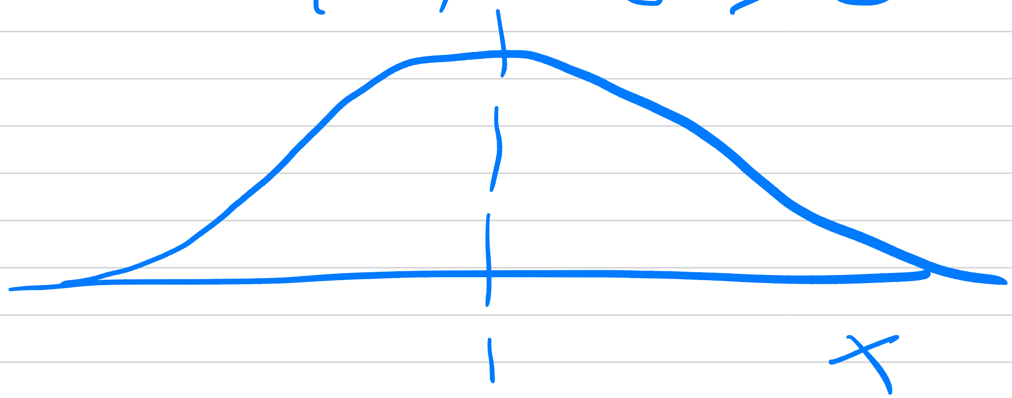
$$= \phi_0 \left[\frac{\alpha/\pi}{1+4\alpha D t} \right]^{n/2}$$

$$\times \exp\left[- \frac{\alpha |\vec{x}|^2}{1+4\alpha D t} \right]$$

$\phi(x)$; $t=0$



$\phi(x)$; $t>0$



$$S_n(\vec{x}, t) \rightarrow G(\vec{x}\, t; \vec{y}\, t')$$

$$\frac{\partial\, G(\vec{x}\, t; \vec{y}\, t')}{\partial t} - D \nabla^2 G(\vec{x}\, t; \vec{y}\, t')$$

$$= \delta(t - t')\, \delta^{(n)}(\vec{x} - \vec{y})$$

$$t - t' = \Delta t$$

$$G(\vec{x}, \vec{y}; \Delta t) = \frac{1}{\sqrt{4\pi D \Delta t}^{\,n}}$$

$$\times \exp\left[- \frac{|\vec{x} - \vec{y}|^2}{4 D \Delta t} \right]$$

$G(\vec{x}, \vec{y}; \Delta t)$ plays same role as $W(j \rightarrow i)$

$$\phi(\vec{x},t) = \int_0^t dt' \int_{\mathbb{R}^n} d^n y\; G(xt;yt')$$

$$\times\, F(\vec{y},t')$$

Metropolis - Hastings

j = position y

i = — " — x

$$A(j\to i) = \min\left(1,\; \frac{|\psi_T(\vec{x})|^2\, G(\vec{x},\vec{y};\Delta t)}{|\psi_T(\vec{y})|^2\, \underbrace{G(\vec{y},\vec{x};\Delta t)}_{\curvearrowright\, G(\vec{x},\vec{y};\Delta t)}}\right)$$

$= 1$

is just the Diffusion eq. solution. Need something different ?

Fokker-Planck eq

$$\frac{\partial \phi(x,t)}{\partial t} = D \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} - F\right] \times \phi(x,t)$$

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

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

3-Dim

$$\frac{G(\vec{y},\vec{x};\Delta t)}{G(\vec{x},\vec{y};\Delta t)} \neq 1$$

$$\vec{F}(x) = \frac{1}{\Psi_T}\vec{\nabla}\Psi_T$$

$\vec{\nabla}\Psi_T$ is also needed when evaluating $\nabla^2\Psi_T$