Lecture FYS4411, February 9, 2024

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

Diffusion eq

$$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial x^2} \qquad (1\text{-Dim})$$

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

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

Fourier transforms to momentum

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

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

with initial condition

$$\tilde{\phi}(k,0) = \tilde{f}(k)$$

unique solution

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

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

$$\left[\quad \tilde{g}(k,t) = \int_{\mathbb{R}^n} dx\, e^{-ikx} g(x,t) \right]$$

$$f(x) = F^{-1}[\tilde{f}]$$

Example

For a Gaussian distribution

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

$$F[e^{-a^2x^2}] = \frac{\sqrt{\pi}}{a} e^{-\frac{k^2}{4a^2}}$$

$a^2 = \frac{1}{4D\cdot t}$ and treating -t- as a fixed parameter

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

in $-n-$ dimensions

$$\mathcal{F}^{-1}\left[e^{-D|\vec{k}|^2 t}\right]$$

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

also known as the fundamental distribution of the diffusion equation,

$$\mathcal{F}^{-1}\left[e^{-D|\vec{k}|^2 t}\right] = S_n(\vec{x}, t)$$

convolution theorem

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

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

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

normalized so that

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

$$\phi(x,t) = \phi_0 \left[\frac{a}{4\pi^2 D t}\right]^{n/2}$$

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

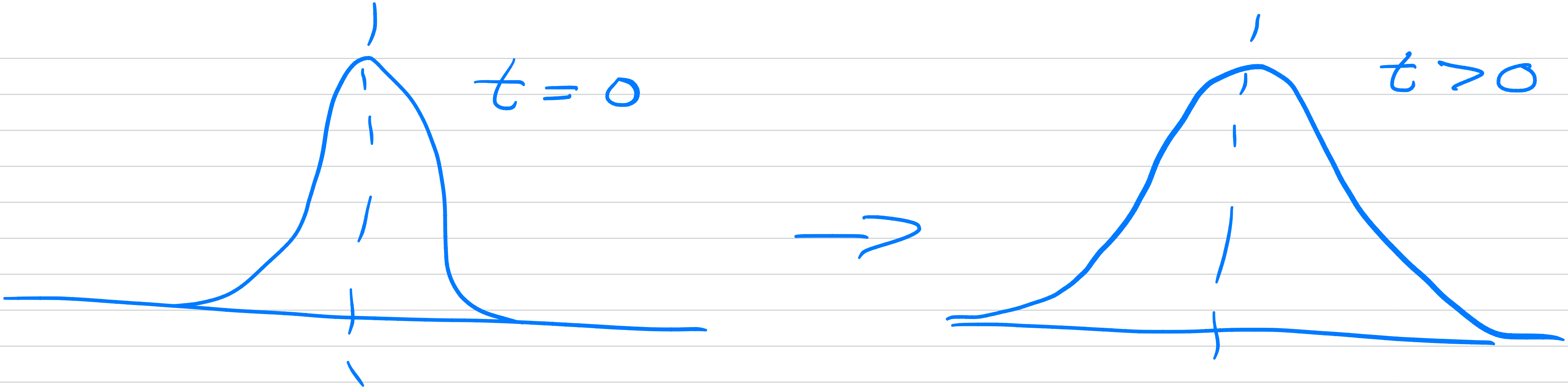
Markov chain (continuous distribution)

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

$$S_n(\vec{x},t)$$

$$\phi(x,t) = \phi_0 \left[\frac{a/\pi}{1+4aDt} \right]^{n/2} \times \exp\left[- \frac{a|\vec{x}|^2}{1+4aDt} \right]$$

an initial gaussian remains a Gaussian with a spreading linear with t. the peak at $x=0$, diminishes as function of $t^{-1/2}$



$$f(\vec{x}) = \phi_0 \, \delta^{(n)}(\vec{x})$$

$$\phi(x,t) = \frac{\phi_0}{(4\pi D t)^{n/2}} \int_{\mathbb{R}^n} \delta^{(n)}(\vec{y}) \times \exp\left[-\frac{|x-y|^2}{4Dt} \right] d^n y$$

$$= \phi_0 \, S_n(\vec{x}, t)$$

$$\frac{\partial \phi}{\partial t} - D D^2 \phi = F(x,t)$$

$$S_u(x,t) \Longrightarrow G(\vec{x}\,t;\vec{y}\,t')$$

(Green's function)

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

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

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

$$T(j \to i) \to G(\vec{x}\, t ; \vec{y}\, t')$$

$$= G(\vec{x}\, t \,|\, \vec{y}\, t')$$

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

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

$$G(\vec{x}, \vec{y} ; \Delta t) = \frac{1}{(4\pi D \Delta t)^{n/2}}$$

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

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

$$= \min\left(1, \frac{|\psi_T(\vec{x})|^2}{|\psi_T(\vec{y})|^2}\right)$$

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

Fokker-Planck equation

3dim

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

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

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

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

Computational considerations

need $\vec{\nabla}\Psi_T(\vec{x})$ in quantum force and local energy

$\nabla^2\Psi_T(\vec{x})$ in local energy

$$\Psi_T(\vec{x}) \propto \varphi_{OB}(\vec{x}_1, \vec{x}_2 \ldots \vec{x}_N)\,\varphi_C(|\vec{x}_i - \vec{x}_j|)$$

$$\vec{x} = \{\vec{x}_1, \vec{x}_2, \ldots \vec{x}_N\}$$

$$\frac{1}{\Psi_T} \nabla \Psi_T = \nabla$$