# FYS4411/9411 February 13

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$$\psi_T(\vec{r}_1, \vec{r}_2; \alpha, \beta)$$

$$= e^{-\alpha^2(r_1^2 + r_2^2)} \cdot J(r_{12}, \beta)$$

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

$$J(r_{12}, \beta) = e^{\frac{r_{12}}{1+\beta r_{12}}}$$

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

Hydrogen-atom (only radial degrees of freedom)

$\ell = 0$

$$E_\ell(r) = \frac{1}{\psi_r} H \psi_r$$

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \left(-\frac{Z\gamma}{r}\right)$$

$\hbar = 1 = m$

$= \gamma$

$$-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \text{const}$$

limit $r \to 0$

$$\psi_{n\ell} = L_{n\ell}\, e^{-\alpha r} \times Y_{\ell m_\ell}$$

$$\frac{1}{\psi_T}\left(-\frac{1}{2}\frac{d^2}{dr^2}-\frac{1}{r}\frac{d}{dr}-\frac{Z}{r}+\text{const}\right)$$

$$\times\ \psi_T$$

$$\lim_{r\to 0}\frac{d^n}{dr^n}\psi_T=\text{const}$$

$$\lim_{r\to 0} E_L \Rightarrow \frac{1}{\cancel{\psi_T}}\left(-\frac{1}{r}\frac{d\psi_T}{dr}\right.$$

$$\left.-\frac{Z}{r}\cancel{\psi_T}\right)$$

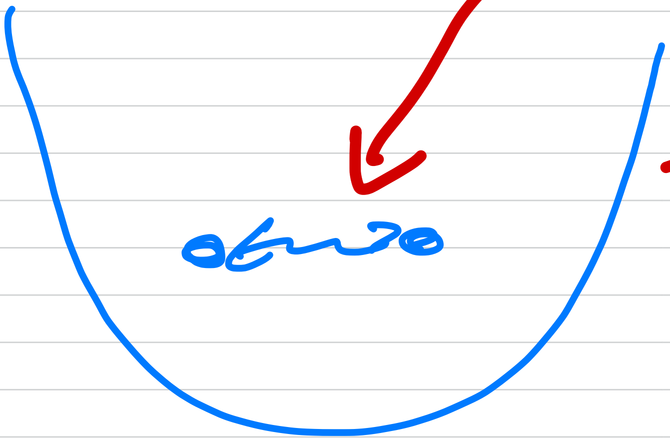
$$-\frac{1}{r}\frac{d\psi_T}{dr}\frac{1}{\psi_T}=Z/r \Rightarrow$$

$$-\frac{d\,\psi_T}{dr} = +Z\,\psi_T$$

$$\psi_T = e^{-Zr}$$

For two particles

$$\frac{\hbar^2}{2m}\left(-\nabla_1^2 - \nabla_2^2 + u(\vec r_1) + u(\vec r_2) + \frac{\gamma}{|\vec r_1 - \vec r_2|}\right)$$



$$\sim u(\vec r_r) = \frac{1}{2} k r_r^2$$

$$\vec R = \frac{\vec r_1 + \vec r_2}{2}$$

$\vec r_1 - \vec r_2$ relative distance

$$A(x \to y) = \min\left(1, q(y,x)\right)$$

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

how do we find this?

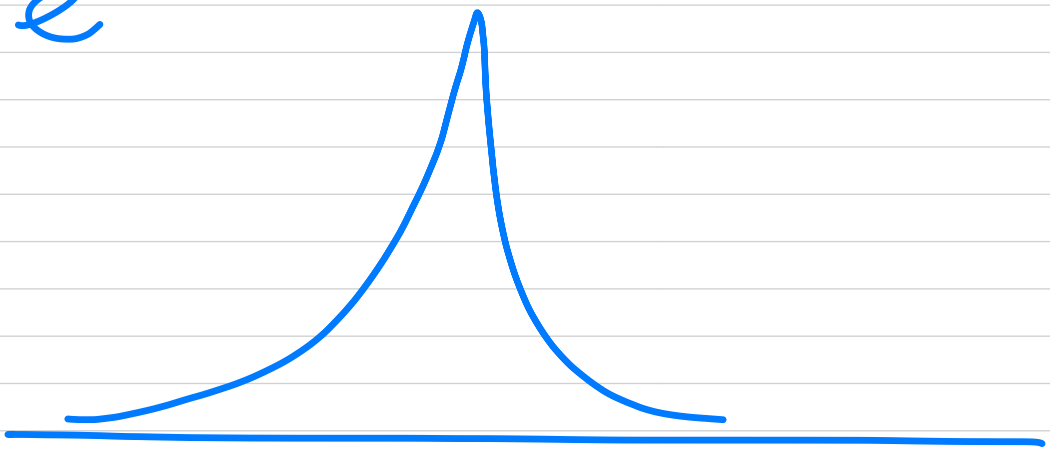
$$\frac{\partial P(\vec{x},t)}{\partial t} = D \nabla_x^2 P$$

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

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

$e^{-r}$

$e^{-|x|}$



$r = |\vec{r}|$

$r = |x|$

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

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

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 $k$

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

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

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

with initial condition

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

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

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

Example: gaussian

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

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

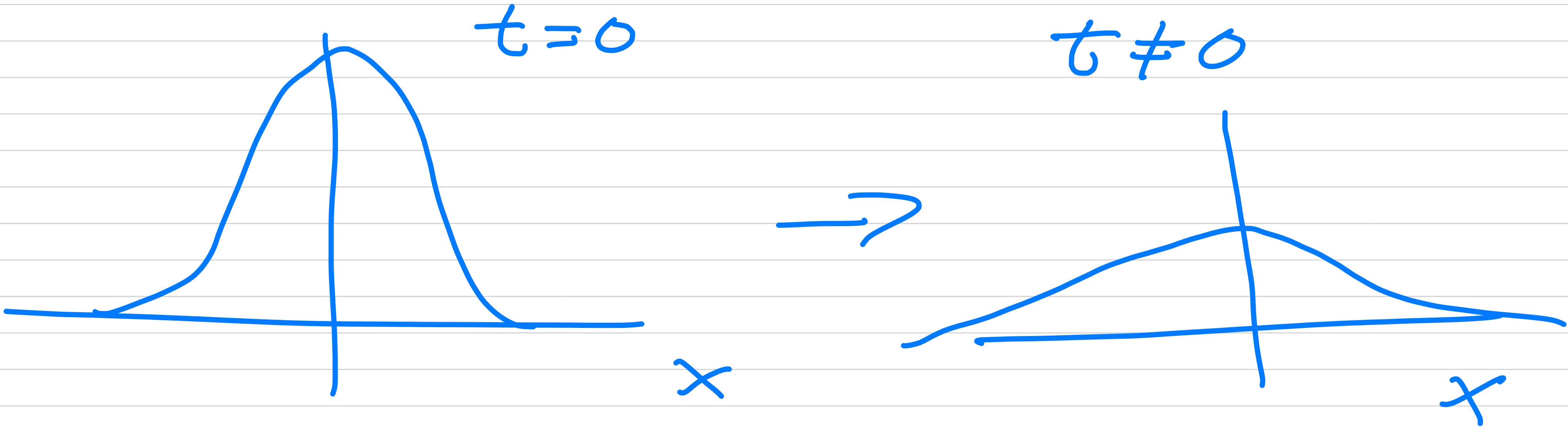
$$\alpha^2 = \frac{1}{4D\,t} \qquad (\text{fixed } t)$$

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

in $n$-dimensions

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

$$\times \exp\left[-|\vec{x}|^2/4Dt\right]$$




known as the fundamental distribution of the diffusion equation

# Convolution theorem

$$y(t) = (x * w)(t)$$

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

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

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

$$= \frac{1}{(4\pi D t)^{n/2}} \int_{\mathbb{R}^n} d\vec{y}^{\,n} \, \underbrace{f(\vec{y})}_{\phi(\vec{y}, t=0)} \exp\left[ -\frac{|x-y|^2}{4Dt} \right]$$

suppose

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

normalized so that

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

$$\phi(\vec{x}, t) = \Phi_0 \left[\frac{\alpha}{4\pi D t}\right]^{n/2}$$

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

Markov-chain

$$\phi(x_i, t) = \sum_j \phi(x_j, t-1)\, W(x_j \to x_i)$$

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

$$= \text{const} \exp\left[ -\frac{(\vec{x} - \vec{y})^2}{4Dt} \right]$$

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

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

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

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

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

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

$G(\vec{x},\vec{y};\Delta t)$ plays the role of a probability of making a transition from $\vec{y}$ to $\vec{x}$ in a time step $\Delta t$,

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

$$= 1$$

Fokker-Planck eq (1-dim)

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

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

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

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

$$\vec{F}(x) = \frac{1}{k_T} \vec{D}\, k_T$$