Lecture FYS4411, february 2, 2024

Metropolis algorithm

– Markov chain

$$w_i(t) = \sum_j W(j \to i)\, w_j(t')$$

$$\lim_{t \to \infty} w_i(t) = w_i$$

$$w = W w$$

$$W(j \to i) = T(j \to i)\, A(j \to i)$$

From detailed balance

$$\frac{A(j \to i)}{A(i \to j)} = \frac{w_i \, T(i \to j)}{w_j \, T(j \to i)}$$

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

$$w_i = \frac{|\Psi_T(\vec{R}_i)|^2}{\int d\vec{R} \, |\Psi_T(\vec{R})|^2}$$

Model for $T(i \to j)$

importance sampling.

Bird's eye view

$$I = \int_0^1 f(x)\,dx$$

uniform distribution

$$p(x)\,dx = \begin{cases} dx & 0 \le x \le 1 \\ 0 & \text{else} \end{cases}$$

$$I = \mathbb{E}[f(x)] = \int_0^1 p(x) f(x)\,dx$$

(i) change of variables
(ii) importance sampling

$$\int_{-\infty}^{\infty} p(x)\,dx = \underline{1}$$

$$p(x)\,dx = p(y)\,dy$$

integrate

$$x(y) = \int_0^y p(y')\,dy'$$

$$p(y)\,dy = e^{-y}\,dy \qquad y \in [0,\infty)$$

$$x(y) = \int_0^y e^{-y'}\,dy' = 1 - e^{-y}$$

$$\Rightarrow \quad y(x) = -\ln(1-x) \Bigg| \begin{matrix} x=0 \\ y=0 \\ x=1 \\ y \Rightarrow \infty \end{matrix}$$

$$x \in [0,1]$$

$$p(x) = \frac{1}{3}(4-2x) \qquad x \in [0,1]$$

$$\int_0^1 p(x)\,dx = \underline{1}$$

$$p(y)\,dy = dy \qquad y \in [0,1]$$

$y \sim$ uniform distribution

$$y(x) = \frac{1}{3}x(4-x)$$

$$x = 2-(4-3y)^{1/2}$$

y

$y=0 \;\wedge\; x=0$

$y=1 \;\wedge\; x=\underline{1}$

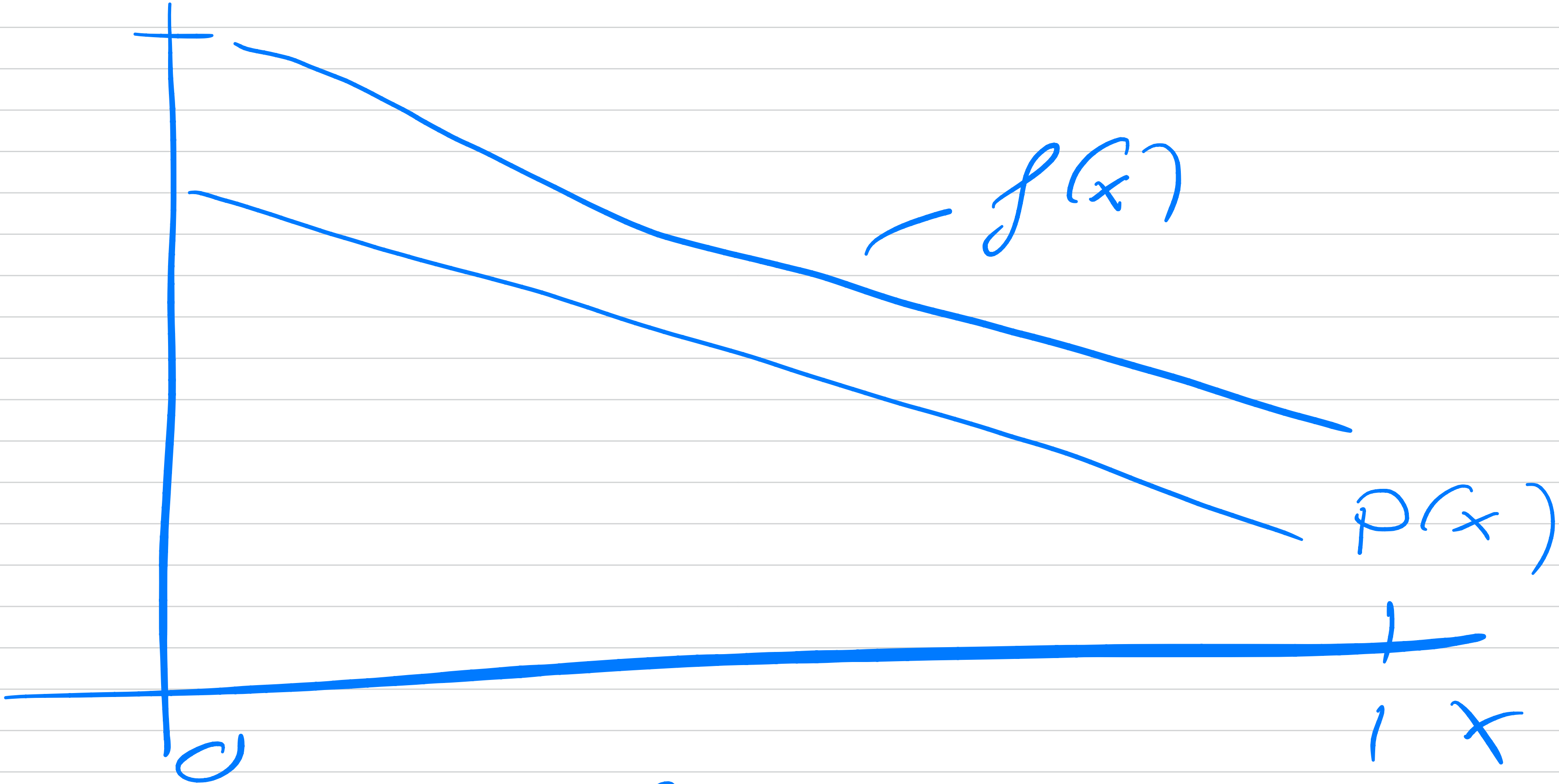
$$I = \int_0^1 \frac{1}{1+x^2}\,dx = \frac{\pi}{4} = \int_0^1 f(x)\,dx$$

Importance sampling

$$I = \int_0^1 p(x)\,\frac{f(x)}{p(x)}\,dx$$

$p(x)$ is a PDF

$$\frac{f(0)}{p(0)} = \frac{f(1)}{p(1)} = 3/4$$



$$\frac{f(x)}{p(x)} \approx \text{constant}$$

$$I = \int p(y) f(y)\, dy = \mathbb{E}[f]$$

$$\mathrm{Var}[f] = \int p(y) f^2(y)\, dy$$

$$- \left[\int p(y) f(y)\, dy \right]^2$$

$$\mathrm{STD}[f] = \sqrt{\mathrm{var}[f]} \Rightarrow$$

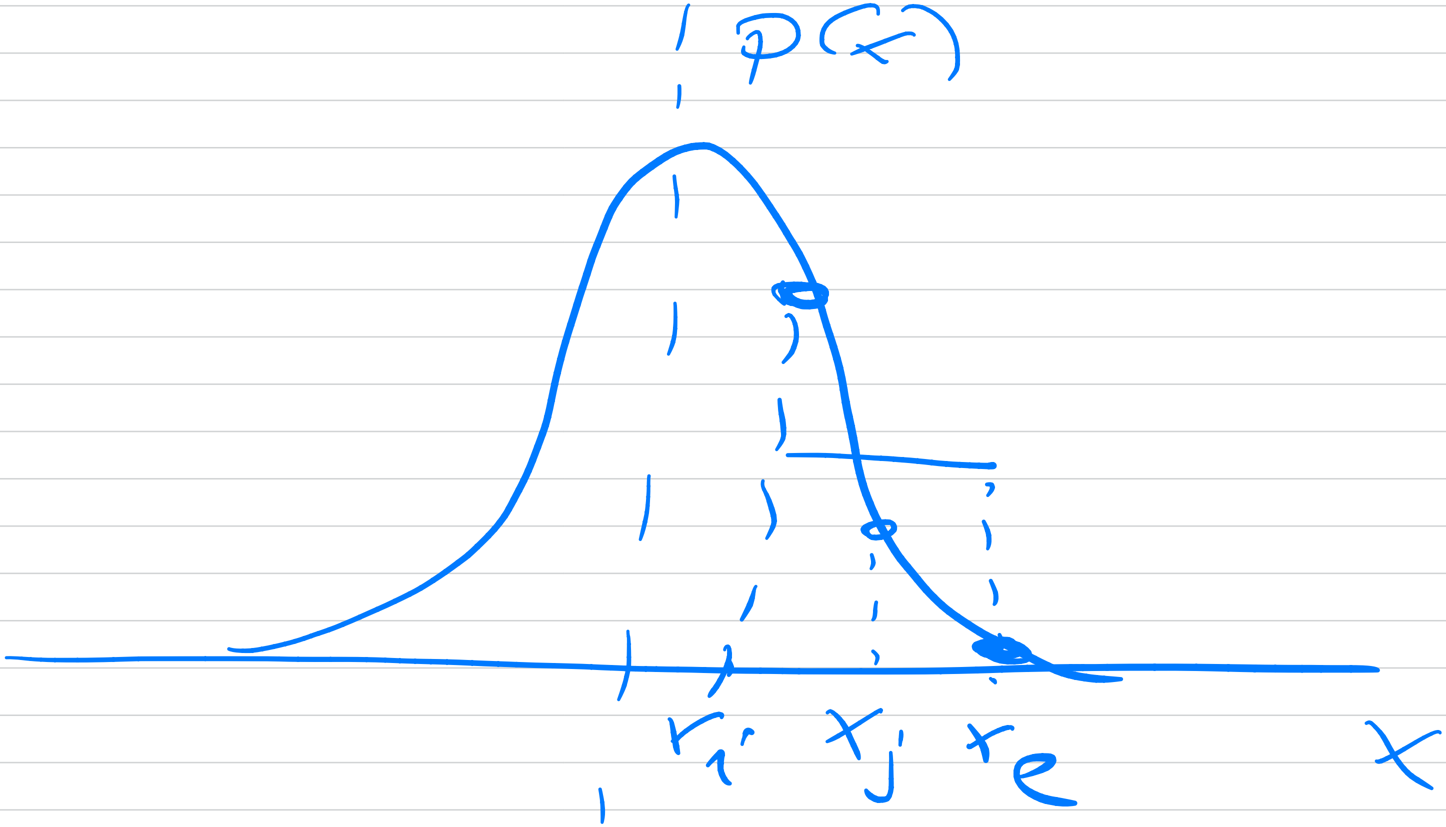
$$I = \mathbb{E}[f] \pm \mathrm{STD}[f]$$

$$I = \int_0^1 p(x) \frac{f(x)}{p(x)} dx$$

$$p(y)dy = dy = p(x)dx$$

$$p(x) = \frac{dy}{dx} \Rightarrow$$

$$I = \int_0^1 \frac{f(x(y))}{p(x(y))} dy$$



$x_j \to x_i'$

$r \sim [0,1]$

$$x_i' = x_j' + \delta(r - 0.5)$$

step size

Ansatz for ψ_T

$$E_L(\vec{R}) = \frac{1}{\psi_T(\vec{R})} H \psi_T(\vec{R})$$

electron in hydrogen

$$\frac{1}{\psi_T(\vec{R})} \left(-\frac{1}{2} \nabla^2 - \frac{Z}{R} \right) \psi_T(\vec{R})$$

Radial equation

$$E_L(R) = \frac{1}{R_T(R)} \left(-\frac{1}{2} \frac{d^2}{dR^2} - \frac{1}{2} \frac{d}{dR} - \frac{Z}{R} \right) R_T$$

+ Finite term

$$\lim_{R\to 0} \frac{d^n R_T}{dR^n} = M < \infty$$

$$\frac{d^2 R_T}{dR^2} \wedge \frac{dR_T}{dR} \text{ are finite } \quad R \to 0$$

$$\lim_{R\to 0} \left(\frac{1}{R_T(R)} \left[-\frac{1}{R}\frac{d}{dR} - \frac{Z}{R} \right] R_T \right)$$

$$\frac{1}{R_T}\frac{dR_T}{dR} = -Z \Rightarrow$$

$$R_T(R) = e^{-ZR}$$

Two particles which interact through $\dfrac{1}{r_{12}}$

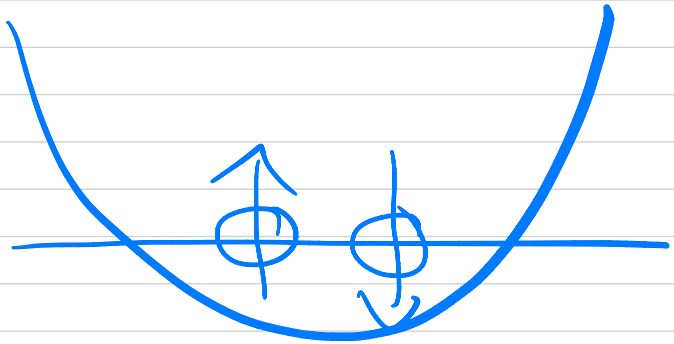
$$r_{12} = |\vec{r}_1 - \vec{r}_2|$$

$$R_T(r_{12}) \propto e^{\beta r_{12}}$$

Ansatz for ground state of atomic Helium

$$\Psi_T(\vec{r}_1, \vec{r}_2) = e^{-\alpha r_1} e^{-\alpha r_2} \cdot e^{\beta r_{12}}$$

Examples:



$n_{x_1}, n_{x_2} = 0$

$$\Psi_T(\vec{r}_1, \vec{r}_2) = \underbrace{e^{-\alpha(r_1^2+r_2^2)}}_{\substack{\Psi_{OB}(\vec{r}_1,\vec{r}_2) \\ \text{onebody}}} \underbrace{e^{f(r_{12})}}_{\substack{\text{correlation} \\ \Psi_C(r_{12})}}$$

Jastrow factor

In Examples

$$\psi_T(\vec{r}_1, \vec{r}_2) = e^{-\alpha(r_1^2 + r_2^2)} \, e^{\frac{a r_{12}}{1+\beta r_{12}}}$$

more general form

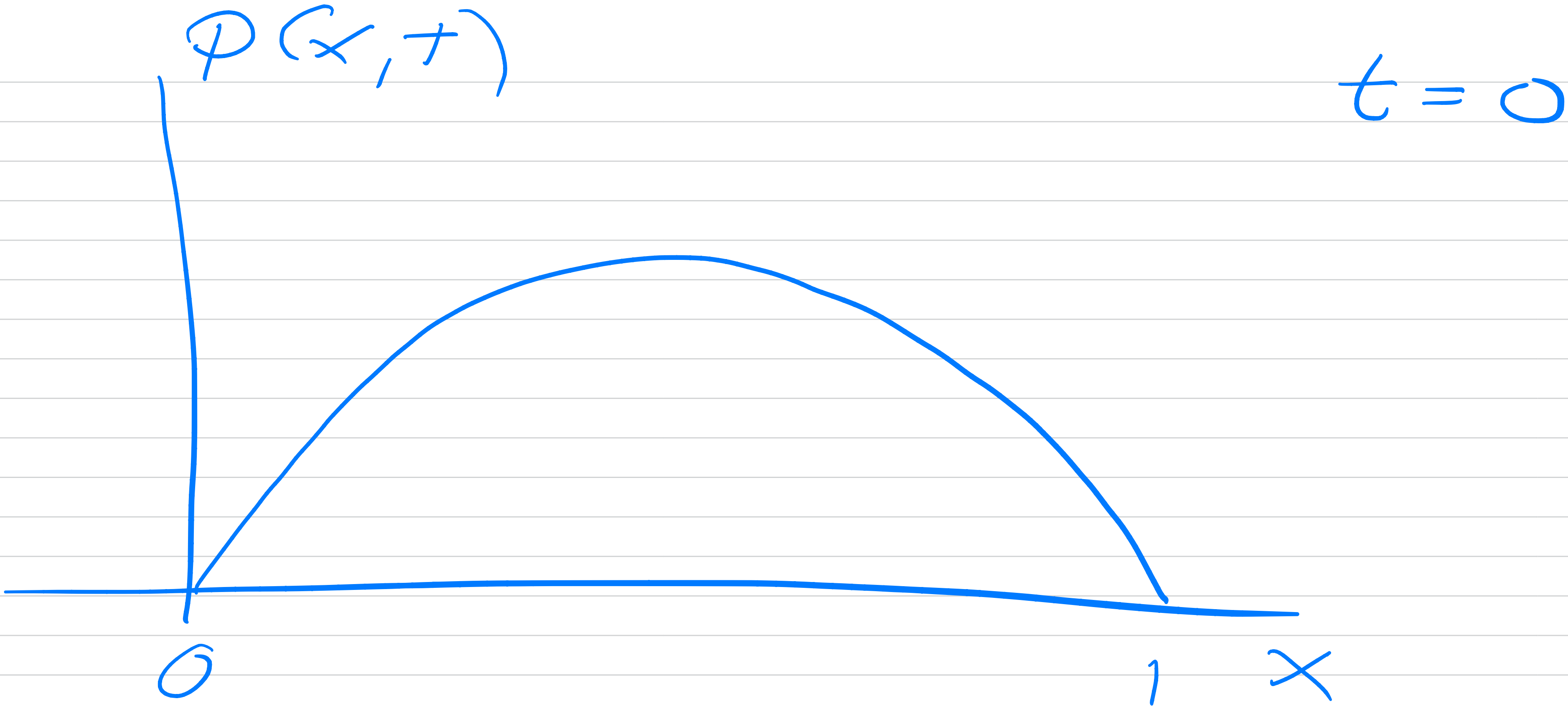
$$\exp\left[\frac{\sum_k r_{ij}^k \beta_k}{1+\sum_l \alpha_l r_{ij}^l}\right]$$

α_l and β_k are variational parameters.

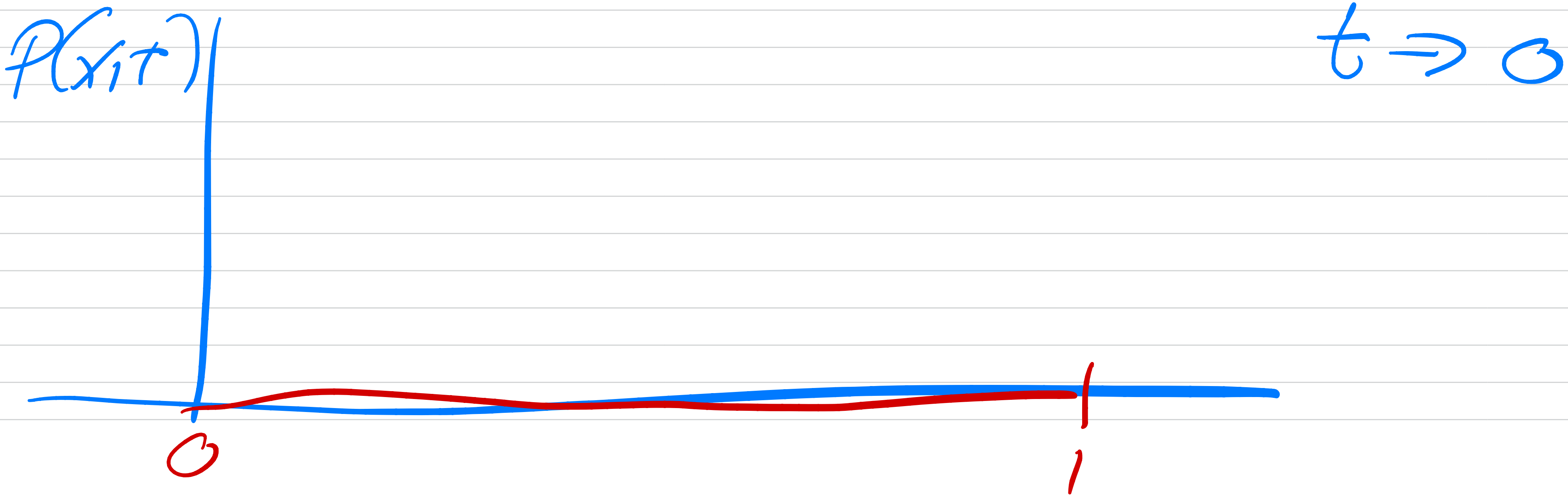
Small technicality in Metropolis test with ψ_{OB} only

$$\frac{e^{-\alpha(r_1'^2+r_2^2)}}{e^{-\alpha(r_1^2+r_2^2)}} = \frac{e^{-\alpha r_1'^2}}{e^{-\alpha r_1^2}}$$

$$= e^{-\alpha(r_1'^2 - r_1^2)}$$



P(x,t)
t = 0
0
1
x



P(x,t)
t -> 0
0
1