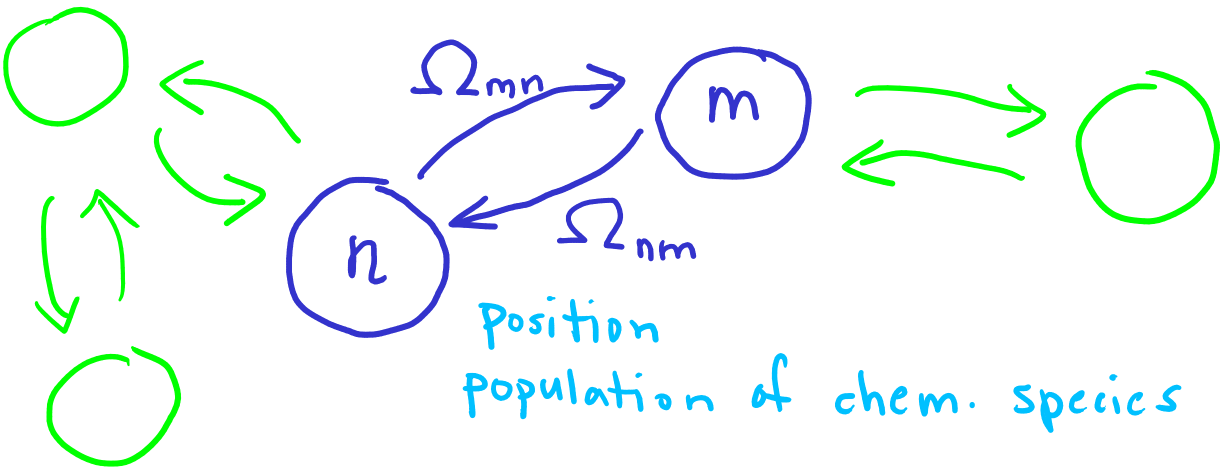
PHYS 320/420 Lecture 16

summary of course so far:

description of biophys. systems in terms of states

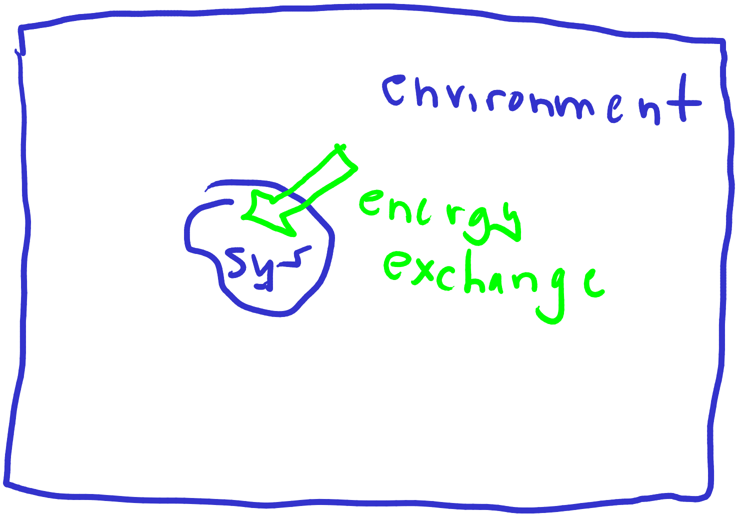


dynamics: $$\frac{dp_n}{dt} = \sum_m \Omega_{nm} p_m$$

Focus on trans. b/t two states n & m in our network.

Know: each state n has a certain associated E_n.

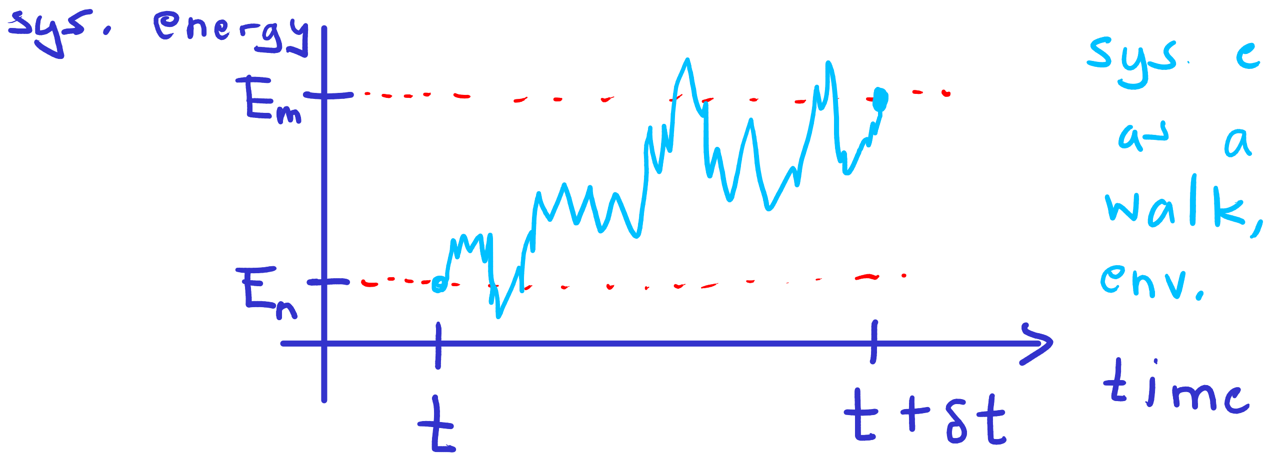
trans. from $n \to m$ involves an energy change in system: $E_m - E_n$



any system change in energy must come from outside: environment

Idea: rate Ω_{mn} of $n \to m$ transition should be related to prob. of environ. being able to supply $E_m - E_n$ energy needed for the transition

Make this more concrete:

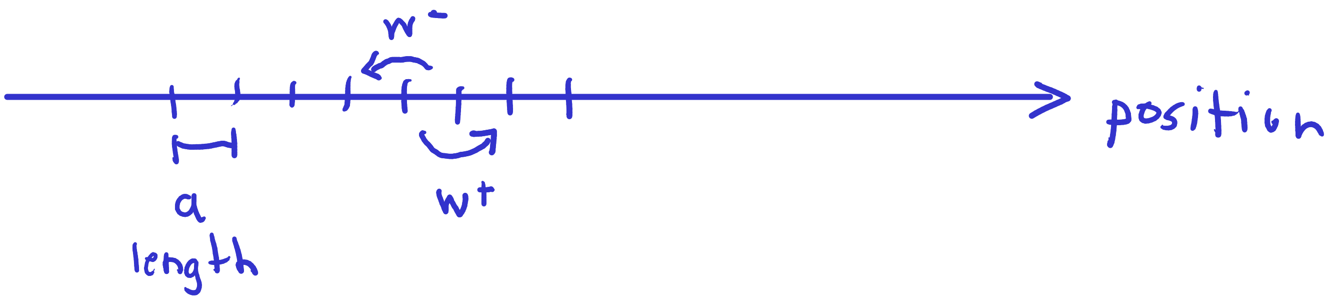


sys energy as a random walk, with env. donating + taking back small increments of energy

$$\Omega_{mn} \delta t = \text{prob. that } n \to m \text{ trans. occurs in time step } \delta t, \text{ starting at } n$$

$\propto$ prob. that sys. starts with energy E_n and ends up with energy E_m after time δt

recall position diffusion in 1D:



if there is net bias (air flow) then $w^- \neq w^+$

$\rightsquigarrow$ master equ $\rightsquigarrow$ Continuum approx.

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

cont. pos. x

$$\frac{\partial P}{\partial t} = -v \frac{\partial P}{\partial x} + D \frac{\partial^2 P}{\partial x^2}$$

$$v = a(w^+ - w^-)$$ mean speed of biasing flow

$$D = \frac{(w^+ + w^-)a^2}{2}$$

init. pos.

solution: $$P(x,t;x_0) = \frac{1}{\sqrt{4\pi D t}} \exp\left[-\frac{(x-x_0-vt)^2}{4Dt}\right]$$

when x starts at x_0

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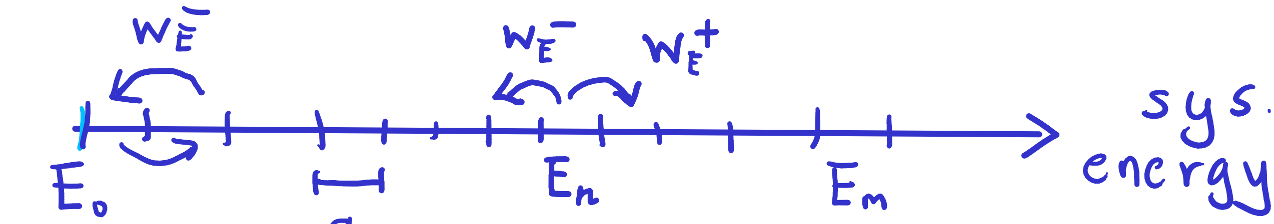
translate this to energy:



$$V_E = (W_E^+ - W_E^-)\,a_E \quad \frac{\text{energy}}{\text{time}}$$

$$D_E = \frac{1}{2}(W_E^+ + W_E^-)\,a_E^2 \quad \frac{\text{energy}^2}{\text{time}}$$

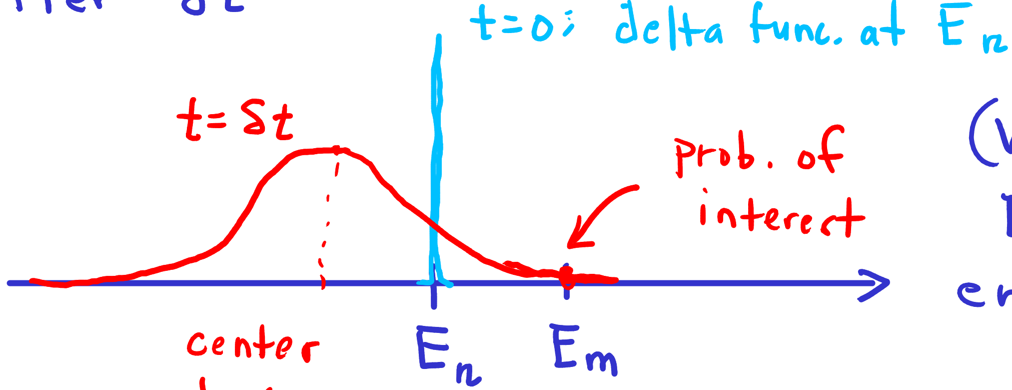
$\Rightarrow$ same as previous picture

prob. that we end up in E_m starting at E_n after δt

$$P(E_m, \delta t; E_n)$$

initial energy

$$= \frac{1}{\sqrt{4\pi D_E \delta t}} \exp\left[-\frac{(E_m - E_n - V_E \delta t)^2}{4 D_E \delta t}\right]$$

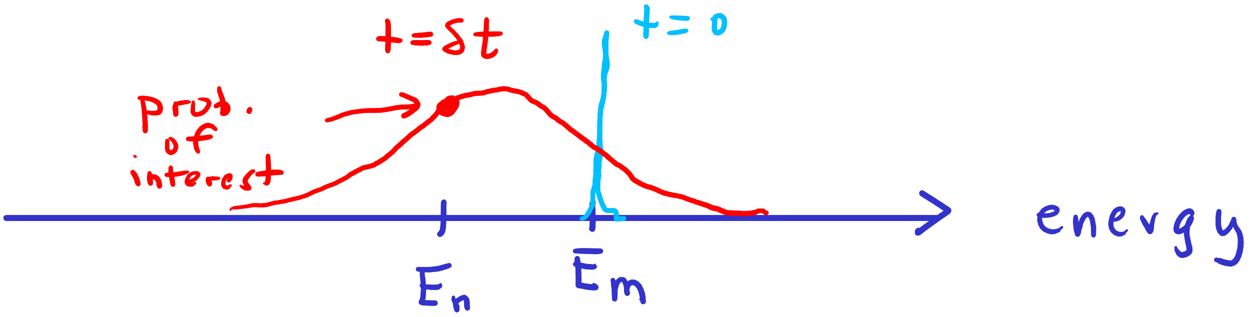


$(V_E < 0)$

$E_m > E_n$

energy

What about reverse trans. $m \to n$?



$$\frac{\Omega_{mn}\,\delta t}{\Omega_{nm}\,\delta t} = \frac{P(E_m, \delta t; E_n)}{P(E_n, \delta t; E_m)} \quad \leftarrow \text{plug in}$$

$$= \exp\left[\frac{V_E}{D_E}(E_m - E_n)\right]$$

(detailed balance relation)

$$\Rightarrow \boxed{\frac{\Omega_{mn}}{\Omega_{nm}} = \exp\left[-\beta(E_m - E_n)\right]}$$

definition of temp.

$$\beta \equiv -\frac{V_E}{D_E} \equiv \frac{1}{k_B T} \sim \frac{1}{\text{energy}}$$

T = temp. in K

k_B = Boltzmann's const. $= 1.38 \times 10^{-23} \frac{J}{K}$

$$\frac{1}{k_B T} = \beta = -\frac{(w_E^+ - w_E^-)\, a_E}{\frac{1}{2}(w_E^+ + w_E^-)\, a_E^2} = \frac{2(w_E^- - w_E^+)}{(w_E^+ + w_E^-)\, a_E}$$

w_E^+, w_E^-, a_E prop of the environment

$\Rightarrow$ temp. encodes certain ratio of these properties