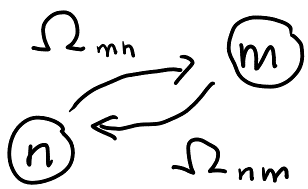
Next step: think about the influence of energy

$\Rightarrow$ biological thermodynamics

system of transitions b/t states



dynamics:

Ω_{nm} — n: end, m: start

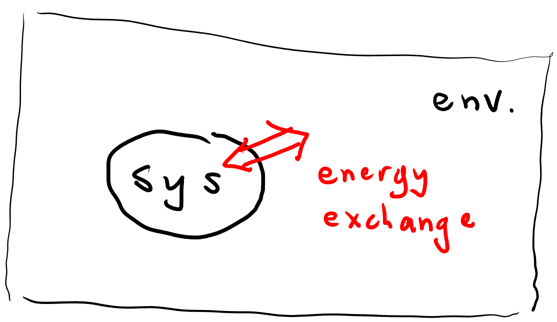
$$\frac{dp_n}{dt} = \sum_m \Omega_{nm} p_m$$

GOAL: connect Ω_{mn} to physical quantities (i.e. energy, chemical potentials, etc.)

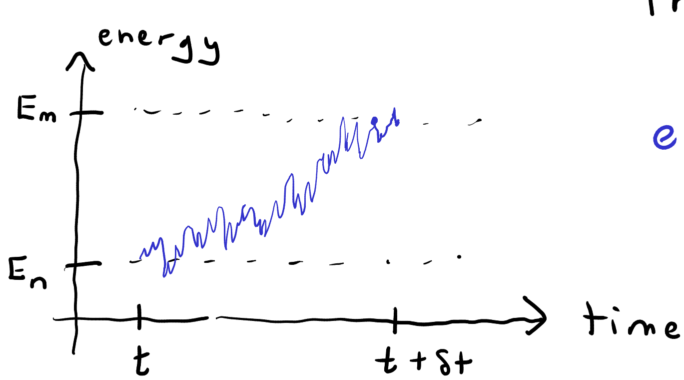
Know: state $n \Rightarrow$ energy E_n

state $m \Rightarrow$ energy E_m } "internal" energy of system

$n \to m$ transition $\Rightarrow$ change in sys. energy $E_m - E_n$



idea: Ω_{mn} should be related to how likely it is to gain/lose $E_m - E_n$ energy from environment

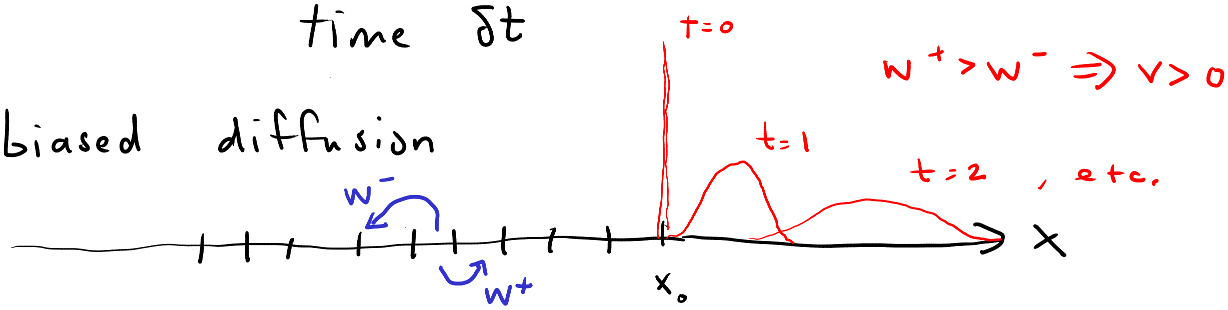


energy exchange: (biased) random walk, w/ env. donating or removing energy in small increments

$\Omega_{mn}\,\delta t$ = prob. for an $n \to m$ trans. in time step δt, given initial state n

$\propto$ prob. system starting w/ energy E_n + ending up with energy E_m after time δt

recall: biased diffusion



continuum approx: $p(x,t) \Rightarrow$ Fokker-Planck equ.

$$\frac{\partial}{\partial t} p(x,t) = -v \frac{\partial}{\partial x} p + D \frac{\partial^2}{\partial x^2} p$$

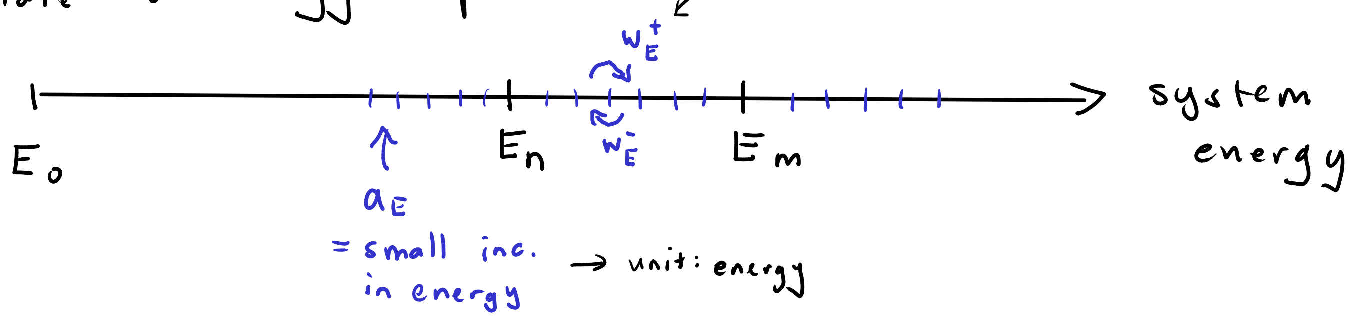
$$D = \frac{(w^+ + w^-)a^2}{2} \qquad v = (w^+ - w^-)a$$

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

↑ initial part. position

translate to energy space:

unit: time^{-1}

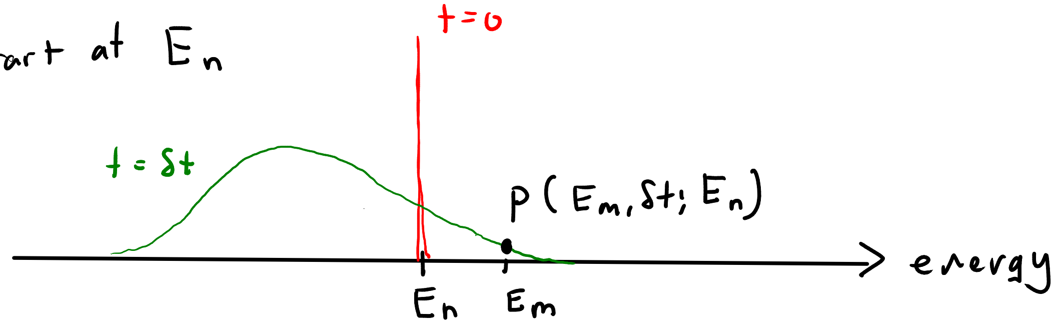


$$V_E = (W_E^+ - W_E^-)\,a_E \qquad \frac{\text{energy}}{\text{time}}$$

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

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

prob. to end up
at E_m after δt
given start at E_n



$$\frac{p(E_m, \delta t; E_n)}{p(E_n, \delta t; E_m)} = \frac{\Omega_{mn}\delta t}{\Omega_{nm}\delta t} = \exp\left[\frac{V_E}{D_E}(E_m - E_n)\right]$$

$$\equiv \exp\left[-\beta(E_m - E_n)\right]$$

$\hookrightarrow$ units: $\frac{1}{\text{energy}}$

$$\underbrace{\beta \equiv -\frac{V_E}{D_E} \equiv \frac{1}{k_B T}}_{\text{definition of temperature}}$$

$T =$ temp. in Kelvin

$k_B = 1.38 \times 10^{-23}\ J/K$

definition of temperature ; $T \equiv -\frac{D_E}{k_B V_E}$

typically : $w_E^- > w_E^+ \Rightarrow V_E < 0 \Rightarrow T > 0$

env. more likely to
take energy than to
give

implications: i) for every $\Omega_{nm} \neq 0$ there
has to be $\Omega_{mn} \neq 0$
(microscopic reversibility)

ii) puts constraints on how energy moves around transition networks