### HOW do we get D= KbT/....

$$\Delta \mathcal{X} = V_{0,\chi} \Delta t + \frac{f}{2m}(\Delta t)^2 - \mathcal{D}$$

$$\langle \Delta \chi \rangle = \int_0^\infty + \left\langle \frac{f}{2m}(\Delta t)^2 - \mathcal{D} \right\rangle$$

$$= \frac{f}{2m}(\Delta t)^2 - \mathcal{D}$$

$$= \frac{f}{2m}(\Delta t)^2 - \mathcal{D}$$
Even for unbiased random walk
$$= \left\langle (V_{e_{\chi}} \Delta t + \frac{f}{2m} \Delta t - \frac{f}{2m} \Delta t) \right\rangle$$

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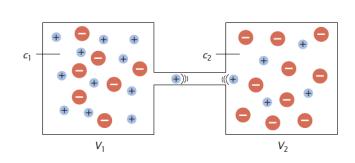
$$= \left\langle (V_{e_{\chi}} \Delta t - \frac{f}{2m} \Delta t) \right\rangle$$

$$= \left\langle ($$

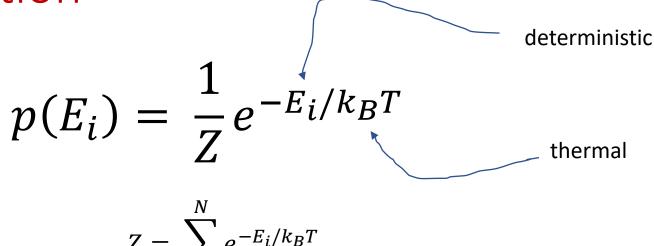
Nelson 4.1.4

# How Thermal energy governs accessibility of microstates of different energy at equilibrium:

**Boltzmann Distribution** 



$$\frac{c_1}{c_2} = \frac{p_1}{p_2} = \frac{e^{-zeV_1/k_BT}}{e^{-zeV_2/k_BT}}.$$

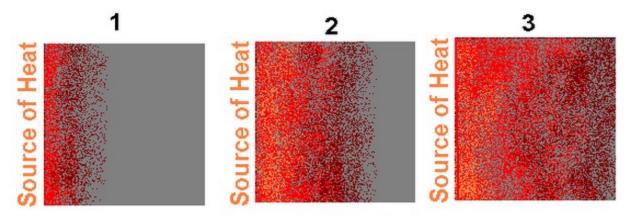


state #2 
$$\sum_{E^{t}} \Delta E_{1-2}$$

# Nano world...incessant motion

- Thermal energy?
- k<sub>B</sub>T
- Ideal gas law?
- How much is  $k_BT$  at room temperature?  $k_B=1.38\times10^{-23}$  J/K. In Joules? In pN-nm?
- Equipartition theorem?

# **HEAT**



Rapidly moving (HOT) molecules
Molecules being bumped and heated up
Cold Molecules

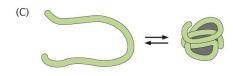
# Heat as a form of energy

- Conservation of energy;
- Energy can be transformed
- Mechanical work on a system produces heat
- Once transformed to heat, transforming to other energies
- Heat = disorganized kinetic energy
- Free energy = Total energy energy related to disorder/randomness in the system
- F=E-TS
- Equilibrium: F minimized
- Non-equilibrium: System evolves in the direction such that F is minimized

# Mechanical, Thermal Chemical Equilibrium

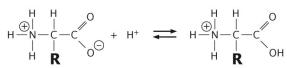
### Nonequilibrium to equilibrium???

#### CHEMICAL EQUILIBRIUM



protein folding and unfolding

(D)



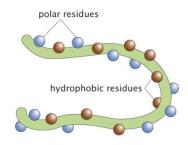
carboxylic acid group becoming protonated and deprotonated

(E)

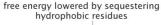
ligand binding and unbinding to receptor

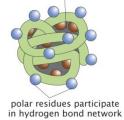
ion channel opening and closing

### Minimization of energy



#### unfolded polypeptide





folded conformation in aqueous environment

Figure 5.8 Physical Biology of the Cell, 2ed. (© Garland Science 2013)

#### Figure 5.7 Physical Biology of the Cell, 2ed. (© Garland Science 2013)

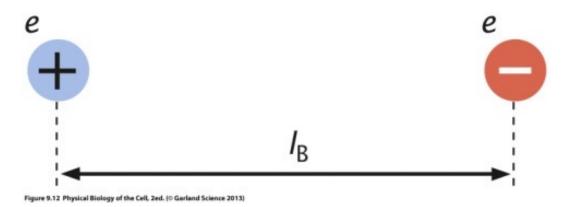
proteins partitioning in a density gradient

MECHANICAL EQUILIBRIUM

microtubule growing against a barrier

(A)

(B)



## Bjerrum Length

- For two unit charges feeling coulomb's attraction/repulsion, what is the effect of  $k_BT$ ? Allowing states otherwise improbable. At what lengthscales does thermal energy start overruling electrostatic energy for a pair of unit charges?
- Monovalent ions in water at room temperature,  $I_B =$ \_\_\_\_(find out)

$$= 9 \times 10^{9}$$

$$l_{B} = \frac{e^{2}}{4\pi \varepsilon k_{B}T}$$

$$e = 1.6 \times 10^{-19}$$

$$k_BT=4 \times 10^{-21}$$

Dielectric constant = 80

Table 1: Length scales that emerge from the interplay of deterministic and thermal energies.

length scale name	energetic term	entropic term	equation	characteristic value	BNID
atmospheric concentration decay length	gravitational	occupation of spatial states	$mgh=k_BT=>h_{th}=\frac{mg}{k_BT}$ $m$ : mass $h$ : height $g$ : acceleration due to gravity	8 km	111406
persistence length	bending	number of states of polymer chain	$E \times I/\xi_P = k_B T \Rightarrow \xi_P = \frac{EI}{k_B T}$ E: Young's modulus I: moment of inertia	DNA: 50 nm actin: 17 μm microtubule: 1.4 mm	103112, 105505, 105534
Bjerrum length	electrostatic interaction	occupation of spatial states	$kq^2/l_B = k_BT \Rightarrow l_B = \frac{kq^2}{k_BT}$ q: charge k: Coulomb's constant	0.7 nm	106405
Debye length	electrostatic interaction	occupation of spatial states	$2c_{\infty}\lambda_D^2q^2/\epsilon_0D=k_BT$ $\Rightarrow \lambda_D=\sqrt{\frac{\epsilon_0Dk_BT}{2c_{\infty}q^2}}$ $c_{\infty}$ : salt conc. D: dielectric constant	1 nm (at 100mM monoionic conc.)	105902

http://book.bionumbers.org/what-is-the-thermal-energy-scale-and-how-is-it-relevant-to-biology/