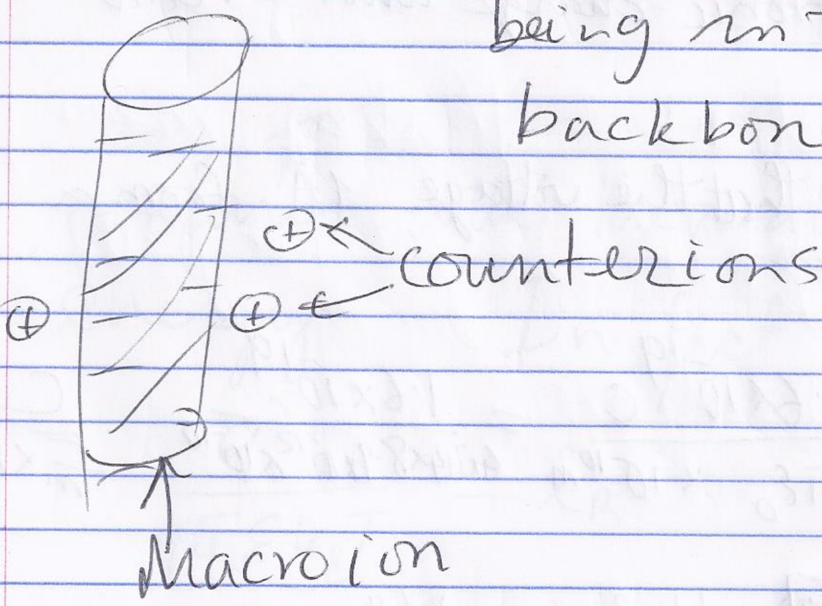
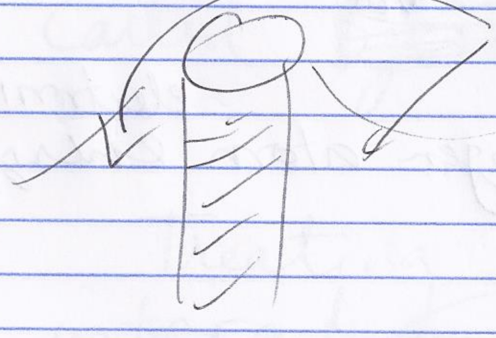
Electrostatic interaction

Many ~~mol~~ macromolecules in biology are charged. DNA is usually negatively charged (it's an acid), usually charge being in the phosphate backbone





cloud of counterions 'diffusing' around.

Diffuse chargelayer

~~D~~ Electric double layer.

Gauss Law, units etc.

$$\vec{\nabla}\cdot\vec{E} = \frac{\rho}{\varepsilon}$$ Permittivity

$$\varepsilon_0 = 8.9\times10^{-12}\ F/m = 8.9\times10^{-12}\ \frac{m^2}{NC^2}$$

$\varepsilon \simeq 80\,\varepsilon_0$ for water.

Electronic charge unit $= 1.6\times10^{-19}$ C

Note that the voltage $1\,\text{Å}$ from a proton is

$$\frac{1.6\times10^{-19}\ C}{4\pi\varepsilon_0 \times 10^{-10}\,m} = \frac{1.6\times10^{-19}}{4\times3.14\times8.9\times10^{-12}\times10^{-10}} \quad \frac{C}{\frac{F}{m}\times m}$$

$$= 14.3 \quad \text{Volts}$$

Remember hydrogen atom electronic energies $\sim -10\,eV$

In water $\varepsilon = 80\,\varepsilon_0$

For a charge $q \sim Ze$

$$\frac{q^2}{4\pi\varepsilon l} = \frac{Z^2 e^2}{4\pi\varepsilon l} = \frac{14.3 \times 1.6 \times 10^{-19}}{80} \frac{Z^2}{(l/1\text{Å})} \text{ J}$$

$$= 2.9 \times 10^{-20} \frac{(Z^2)}{(l/1\text{Å})} \text{ J} = 2.9 \times 10^{-21} \frac{(Z^2)}{(l/1\text{nm})} \text{ J}$$

Remember $k_B T = 4.1 \times 10^{-21}$ J

So, for $l \sim 1$ nm Coulomb energy compares with thermal fluctuation energy. In fact

$$\frac{q^2}{4\pi\varepsilon k_B T} = l_B \quad \text{is a length scale}$$

Called ~~Bjerrum~~ Bjerrum length.

Treating multiple counterions interacting with macroion.

$$\boxed{-\nabla^2 \Phi = \frac{\rho}{\varepsilon} = \frac{1}{\varepsilon}\sum_i q_i c_i e^{-q_i \Phi / k_B T}}$$

$-\nabla \Phi = \vec{E}$

i species of charges.

Poisson-Boltzmann equation. Makes meanfield assumption regarding charge distribution.