Homework 2 (due September 19, 2019)

(1) Membrane barrier to ion transfer **(15 pts)**

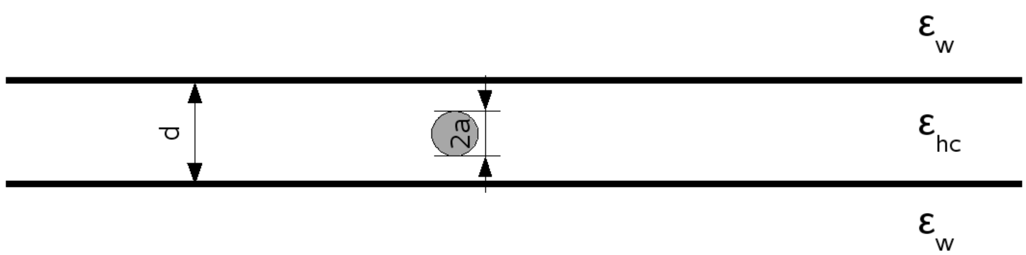
How large is the energetic barrier that prevents an ion to transfer from one side of a lipid bilayer to the other? This is equivalent to asking, "what is the Free Energy to bring that ion from water into the center of the bilayer?" (from where it can easily transfer back to the aqueous environment on either side of the membrane).

a) Let's start with the consideration of the energy required to transfer our ion from a (semi-infinite) reservoir of water ($\varepsilon_w \approx 80$) into a (semi-infinite) reservoir of oil ($\varepsilon_{hc} \approx 2$). Consider a monovalent ion of radius a, such as Na^+ (radius, $a = 1.2$ Å).

(i) What is the difference in Born energies (*i.e.*, the electrostatic self-energies) of Na^+ in oil (read: "hydrocarbons") and in water? Express these energies in k_BT (at $T = 300$ K) and in kJ/mol.

(ii) What is the molecular origin for that difference?

b) Now, this bulk → bulk transfer was only a crude proxy, since a realistic description needs to treat the membrane as a (very) thin slab of hydrocarbons (thickness, $d \approx 3$ nm). The true Free Energy of the ion so close to water/hydrocarbon boundaries on both sides must surely be lower.



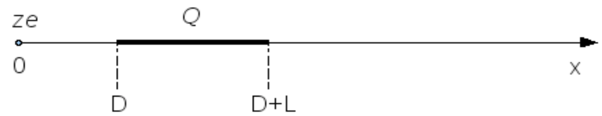
But by how much? In class, we learned that the image charge formalism can be used to "crack" difficult analyses of the Maxwell equations under suitable geometric arrangements that describe the distribution of "oil" and "water" in space by the boundaries between them. Specifically, there were analytical solutions given for an ion within a slab (*i.e.*, a "membrane") and within a sphere (a "protein"). Using the appropriate approximation from class, determine the Born energy of the ion at the center of a membrane as a function of ε_{hc}, d and a.

(i) To verify the correction term (which has not been derived in class), show that the approximation yields reasonable limits for $\varepsilon_{hc} \to \varepsilon_w$, $d \to \infty$, and $a \to 0$.

(ii) How large is the difference in Born energies if you account for the confinement of the ion in a slab (see sketch) of $d = 3$ nm? How big is hence the relative change from the zero-th order result in (a)?

(2) Electrostatic interactions **(15 pts)**

A uniformly charged rod of length L and charge $Q = \lambda L$, where λ is a constant charge per unit length, is oriented along the x axis, starting at a distance D from the origin.



a) Calculate the electric field at the origin generated by the charge as a function of D by integration over all charge elements $dq = \lambda\, dx$.

b) Determine the limiting result for small L, *i.e.*, $L \ll D$. Do you recognize the expression that you obtain in that limit?

c) Determine force that acts on a point charge $+ze$ at the origin.