# Models of Membrane Electrostatics

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***Short Abstract* — I derive formulas for the electrostatic potential of a charge in or near a membrane modeled as one or more dielectric slabs lying between two semi-infinite dielectrics. One can use these formulas in Monte Carlo codes to compute the distribution of ions near cell membranes more accurately than by using Poisson-Boltzmann theory or its linearized version. Here I use them to discuss the electric field of a uniformly charged membrane, the image charges of an ion, the distribution of salt ions near a charged membrane, the energy of a zwitterion near a lipid slab, and the effect of including the phosphate head groups as thin layers of high electric permittivity.**

## CELL MEMBRANES

THE plasma membrane of an animal cell and the membranes of the endoplasmic reticulum, the Golgi apparatus, the endosomes, and other membrane-enclosed organelles are lipid bilayers about 5-nm thick studded with proteins. The lipid constituents are mainly phospholipids, sterols, and glycolipids.

Of the four main phospholipids in membranes, three---phosphatidylethanolamine (PE), phosphatidylcholine (PC), and sphingomyelin (SM)---are neutral, and one, phosphatidylserine (PS), is negatively charged. In a living cell, PE and PS are mostly in the cytosolic layer of the plasma membrane; PC and SM are mostly in the outer layer~\cite{Zwaal1999, *MBoC4587}; and the electrostatic potential of the cytosol is 20 to 120 mV lower than that of the extracellular environment.

After pioneering work by Gouy, Chapman, and Wagner, and by Onsager and Samaras, many scientists have studied the electrical properties of cell membranes. This paper presents the exact electrostatic potential due to a charge in or near a membrane in the continuum limit in which the membrane is taken to be one or more dielectric slabs lying between two different infinite dielectric media. Because of the superposition principle, this monopole potential also gives the multipole potential due to any array of charges in or near a membrane.

One can use these formulas to simulate the interactions of ions with other ions and with fixed charges near membranes while modeling water and other neutral molecules as bulk media. For instance, one can use them in Monte Carlo simulations to compute the behavior of salt ions and protons in water near neutral or charged membranes even in the presence of fixed charges of arbitrary geometry. This method is more accurate than the Poisson-Boltzman mean-field approximation and much more accurate than its linearized version. These formulas also provide a context for and a check on all-atom computer simulations.

As early as 1924, Wagner noted that an ion in water near a lipid slab induces image charges that repel the ion. No mean-field theory can describe this simple effect, but work-arounds are available for the Poisson-Boltzmann theory.

## OUTLINE

Formulas for the electrostatic potential of a charge in or near a cell membrane modeled as a single slab are derived in section II. As pedagogical illustrations of their utility, I use them to compute the electric field of a charged membrane in section III and the response of bound charge to an ion in section IV. In section V, I use them to simulate the distribution of salt ions near a charged membrane. I discuss the Debye layer in section VI and the energy of a zwitterion near a lipid slab in section VII. In section VIII, I calculate the potential of a charge near a membrane modeled as several dielectric layers of different permittivities between two different semi-infinite dielectrics. I use this analysis in section IX to model a phospholipid bilayer as a lipid layer bounded by two layers of head groups of high electric permittivity. The phosphate head groups cause the membrane to attract rather than to repel ions. I summarize the paper in section X.

## REFERENCES

**[1]** Cahill, K (2012) Models of Membrane Electrostatics *Phys. Rev. E* **85**,051921.

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