Current in ion channels described as drift-diffusion of charged hard spheres

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Abstract: The classical description of ionic currents as drift-diffusion in a mean electrical field does not capture particle interactions that arise from the finite diameters of the ions and the discreteness of ionic charge. Such interactions have been included in equilibrium statistical-mechanical descriptions of charged homogeneous fluids, and, via density functional theory (DFT), in those of inhomogeneous fluids. A combination of DFT and drift-diffusion theory is presented here and applied to examples of flux in biological ion channels. Ion channels form molecular pores that distinguish between different ionic species such as Na+, Ca2+, and K+; charged groups lining the pores have been identified as essential for this selectivity. The theory predicts important experimental observations when applied to simple generic models of Ca and Na channels. Ionic selectivity arises from the interaction of the charged groups and mobile ions in a crowded space.