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A Leiden duet, Einstein and Ehrenfest

"Einstein should be allowed his mistakes"

Dear Sir or Madam,

Einstein should be allowed his mistakes, like the rest of us, and Weinberg ("Einstein's Mistakes", PHYSICS TODAY, November, 2005, p. 31) understandably points out only the most newsworthy. I write to point out another misunderstanding—mistake, if you will—in Einstein's work only because the mistake is continued in a substantial number of publications today.

Einstein described diffusion as motion of particles without charge on atomic (Brownian) length and time scales. He used a stochastic differential equation—a Langevin equation—in the high friction limit to describe diffusive trajectories. Einstein did not discuss how his treatment could accommodate macroscopic boundary conditions or produce macroscopic flow, which is, after all, what Fick thought diffusion is all about.

Langevin equations, in the spirit of Einstein's work, are widely used to describe the motion and fluctuations of density of charged particles in (for example) aqueous solutions. The electric force in these equations is usually described by a steady function. Fluctuations in number density of charged particles are allowed but fluctuations in net charge and electric potential are not. Such Langevin equations seem inconsistent with the idea that charge creates electric force and so are unlikely to be helpful, at least in my view. It is hard to imagine systems in which the number density of ions can fluctuate while the number density of charge does not.

I believe Einstein's description of Brownian motion must be coupled self-consistently to equations describing the electric field when the diffusing particle has significant charge. The ink particles studied by Brown were surely charged. In these cases, the electric field can be computed self-consistently from the density of ink particles, ions, and solvent molecules using Poisson's or Maxwell's equations and boundary conditions that force (for example) macroscopic flow. The self-consistent treatment of diffusion and the electric field forms the basis of computational electronics used to design the transistors and integrated circuits of our electronic technology.[1-3] Diffusion and the electric field are not treated self-consistently in most of computational chemistry and biology, for example, in simulations of molecular dynamics of ions or proteins, although self-consistent treatments are found in analyses of ionic motion through protein channels.[4-9]

Ever yours
Bob Eisenberg

1. Selberherr, S. Analysis and Simulation of Semiconductor Devices (Springer-Verlag, New York, 1984).
2. Damocles. in http://www.research.ibm.com/DAMOCLES/home.html (2005).
3. Jacoboni, C. & Lugli, P. The Monte Carlo Method for Semiconductor Device Simulation (Springer Verlag, New York, 1989).
4. Kurnikova, M. G., Coalson, R. D., Graf, P. & Nitzan, A. A Lattice Relaxation Algorithm for 3D Poisson-Nernst-Planck Theory with Application to Ion Transport Through the Gramicidin A Channel. Biophysical Journal 76, 642-656 (1999).
5. Im, W. & Roux, B. Brownian Dynamics simulations of ions channels: a general treatment of electrostatic reaction fields for molecular pores of arbitrary geometry. Biophysical Journal 115, 4850-4861 (2001).
6. Aboud, S., Marreiro, D., Saraniti, M. & Eisenberg, R. A Poisson P3M Force Field Scheme for Particle-Based Simulations of Ionic Liquids. J. Computational Electronics, in the press, (2004).
7. Saraniti, M., Aboud, S. & Eisenberg, R. The Simulation of Ionic Charge Transport in Biological Ion Channels: an Introduction to Numerical Methods. Reviews in Computational Chemistry (in the press). (2004).

8. van der Straaten, T. A., Kathawala, G., Eisenberg, R. S. & Ravaioli, U. BioMOCA - a Boltzmann transport Monte Carlo model for ion channel simulation. . Molecular Simulation 31, 151–171 (2004).
9. Corry, B. & Chung, S.-H. Influence of protein flexibility on the electrostatic energy landscape in gramicidin A. European Biophysics Journal 34, 208-216 (2005).