Convexity and fluctuations in dual Poisson-Boltzmann free energies

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The sign of free energy functionals based on the electrostatic potential has long interested and puzzled the community of molecular simulators: A recent paper states "The fact that the functional cannot be identified with the electrostatic energy away from the minimum a priori precludes its use in a dynamical 'on the fly' optimization…"

In this talk we discuss dual variational formulations of the Poisson-Boltzmann equation which allow one to produce a true minimizing principle for electrostatic free energies.

Though constructed from mean field theory the dual free free energy gives also the correct one-loop contribution calculated from field theory. It presumably contains information on self energies and image charge effects which are known to be important near surfaces.