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The Legendre-Transformed Poisson-Boltzmann Electrostatics

The Poisson-Boltzmann (PB) equation for continuum electrostatics is the Euler-Lagrange equation of the PB electrostatic energy functional of electrostatic potentials. The Legendre-transformed PB (LTPB) electrostatic energy functional of all electric displacements is a convex functional dual to the PB functional. It is shown that both formulations are equivalent. A penalty model based on the LTPB electrostatics is constructed and applied to the dielectric variational solvation of charged molecules. The related numerical algorithms, computational results, and convergence analysis are presented.