A variational formulation of electrostatics in a medium with spatially varying dielectric permittivity

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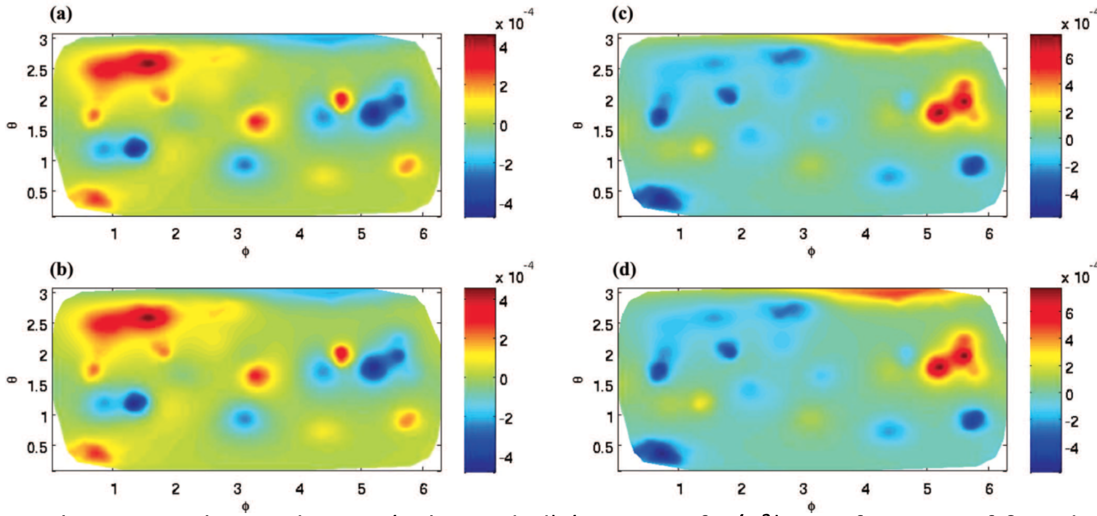
We present a variational formulation of electrostatics specifically designed to treat the problem of dielectric heterogeneities in charged systems. Assuming only the condition of linear response, we construct an energy functional that employs the polarization charge density as its sole variational field. This functional is applicable for any configuration of free charges and arbitrary spatial dependence of the dielectric response.



Polarization charge density (color-coded) (in units of e/σ^2) as a function of ϑ and φ induced on the dielectric sphere from a set of point charges around it. The permittivity inside the sphere is ε_{in} and the permittivity outside the sphere equals ε_{out}. The left column represents the case when $\varepsilon_{in} = 35$ and $\varepsilon_{out} = 80$, while the right column shows the inverse case of $\varepsilon_{in} = 80$ and $\varepsilon_{out} = 35$. (a) and (c) Results from the numerical minimization of the functional $F[\omega_s]$. (b) and (d) Exact results.

For the important case of uniform dielectrics separated by sharp interfaces, we show that, our functional reduces to a functional of only the surface polarization charge density. Such a reduction of the three-dimensional electrostatic problem to a two-dimensional one has many advantages from a computational perspective. The numerical implementation of our minimizing variational principle for a system exhibiting piecewise-uniform dielectric response is illustrated with a system of monovalent ions near a spherical dielectric. We find that the induced density on the spherical interface computed from our methodology is in excellent agreement with exact results.

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