Stochastic density functional theory for ions in a polar solvent

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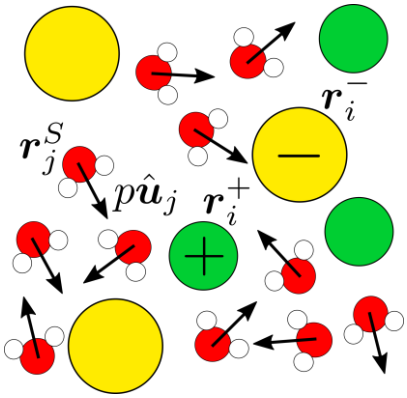
In recent years, the theoretical description of electrical noise and fluctuation-induced effects in electrolytes has gained a renewed interest, enabled by stochastic field theories like stochastic density functional theory (SDFT). Such models, however, treat solvents implicitly, ignoring their generally polar nature. In the present study, starting from microscopic principles, we derive a fully explicit SDFT theory that applies to ions in a polar solvent. These equations are solved to compute observables like dynamic charge structure factors and dielectric susceptibilities. We unveil the relative importance of the different contributions (solvent, ions, cross terms) to the dynamics of electrolytes, which are key to understand the couplings between ions and the fluctuations of their microscopic environment.



Reference

[1] P. Illien, A. Carof, B. Rotenberg, Stochastic density functional theory for ions in a polar solvent, arXiv:2407.17232.