One Dimensional Mimicking of Electronic Structure: The Case for Exponentials

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In order to model the electron-electron repulsion in one dimension, some other interaction from that of the Coulomb interaction must be chosen. The reason for this is that the chemistry of the one dimensional Coulomb interaction does not allow electrons to bind or molecules to form. Since we want to investigate the properties of three dimensional systems, but with less costly computation, we use an alternative interaction in one dimension. The most common interaction is a soft-Coulomb, but we show that an exponential is extremely close to the results from the soft-Coulomb. This interaction also makes our computations faster and solvable on a smaller system than the long ranged soft-Coulomb [1].

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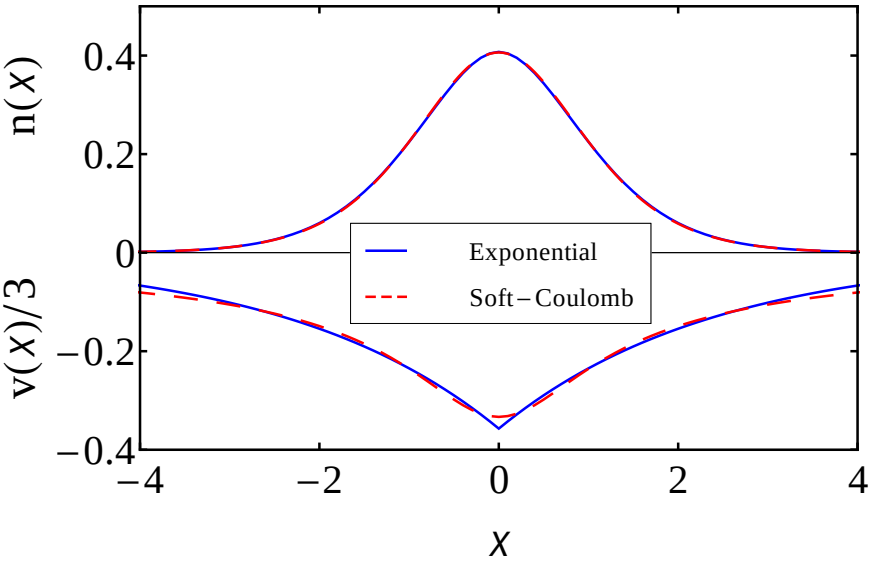

An exponential can match the chemistry of a soft-Coulomb interaction.

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[1] Thomas E. Baker, E. Miles Stoudenmire, Lucas O. Wagner, Kieron Burke, and Steven R. White, "One dimensional mimicking of electronic structure: The case for exponentials," ArXiv:1504.05620 (2015).