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<title>Impact of Electron-Electron Cusp on Configuration Interaction Energies</title>

<summary> The effect of the electron-electron cusp on the convergence of configuration

interaction (CI) wave functions is examined. By analogy with the

pseudopotential approach for electron-ion interactions, an effective

electron-electron interaction is developed which closely reproduces the

scattering of the Coulomb interaction but is smooth and finite at zero

electron-electron separation. The exact many-electron wave function for this

smooth effective interaction has no cusp at zero electron-electron separation.

We perform CI and quantum Monte Carlo calculations for He and Be atoms, both

with the Coulomb electron-electron interaction and with the smooth effective

electron-electron interaction. We find that convergence of the CI expansion of the wave function for the smooth electron-electron interaction is not significantly improved compared with that for the divergent Coulomb interaction for energy differences on the order of 1 mHartree. This shows that, contrary to popular belief, description of the electron-electron cusp is not a limiting factor, to within chemical accuracy, for CI calculations.

</summary>

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