Homework 6

179, Spring 2025

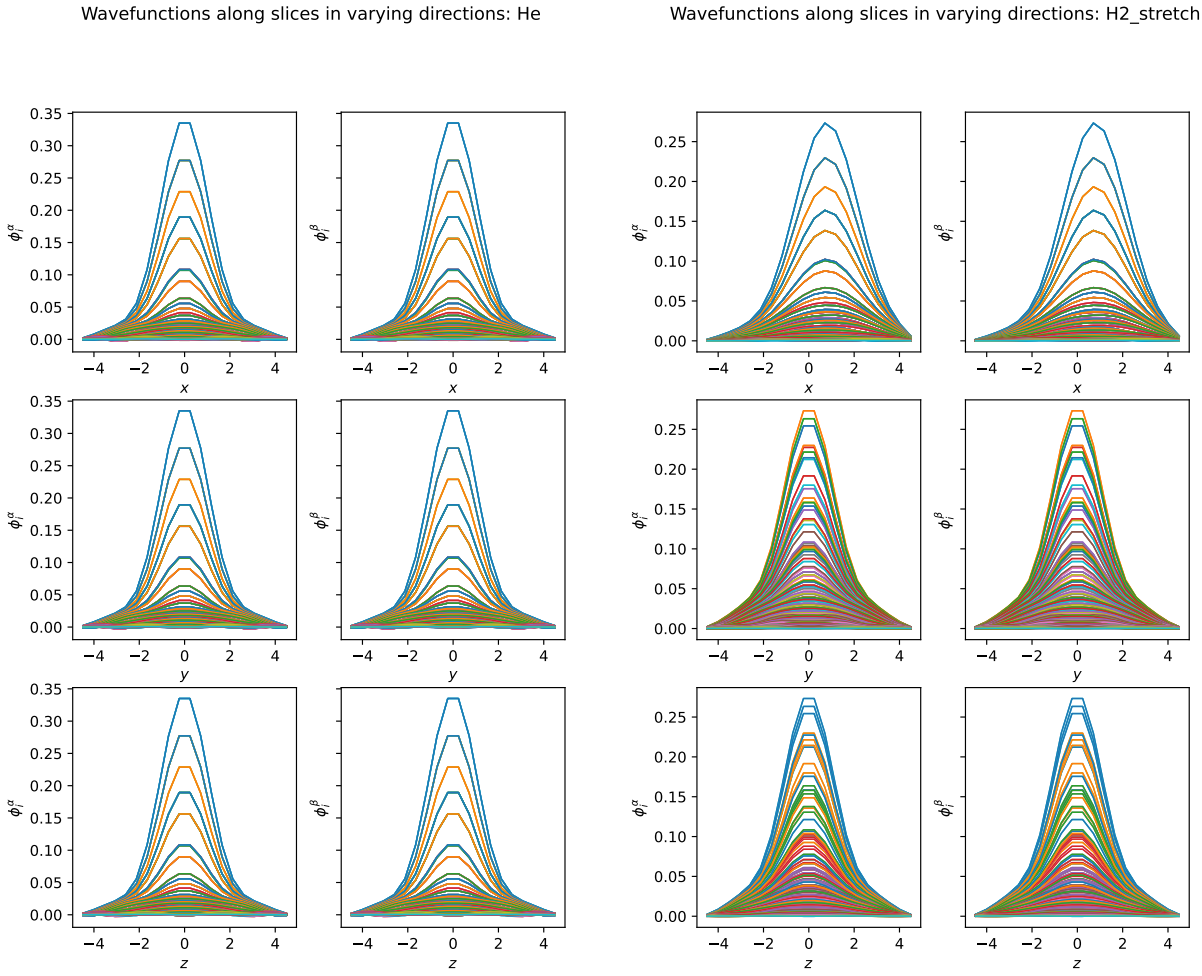
Johan Vonk*

May 11, 2025

My code is at: `https://github.com/Berkeley-Chem-179-279/hw6-jvonk`

HW6.1: I implemented my DFT code using both the density fitting and a Poisson solver. The density fitting gave slightly different results compared to the reference solution, but the Poisson solver matched within $0.000\,001\,E_\mathrm{h}$ for H and H_2 using all the terms, which was also the convergence tolerance.

HW6.2: I debugged the code for Hydrogen with only the external potential. With a Poisson solver, it exactly matches the reference solution.



HW6.3:

*vonk@berkeley.edu