

Homework 6

179, Spring 2025

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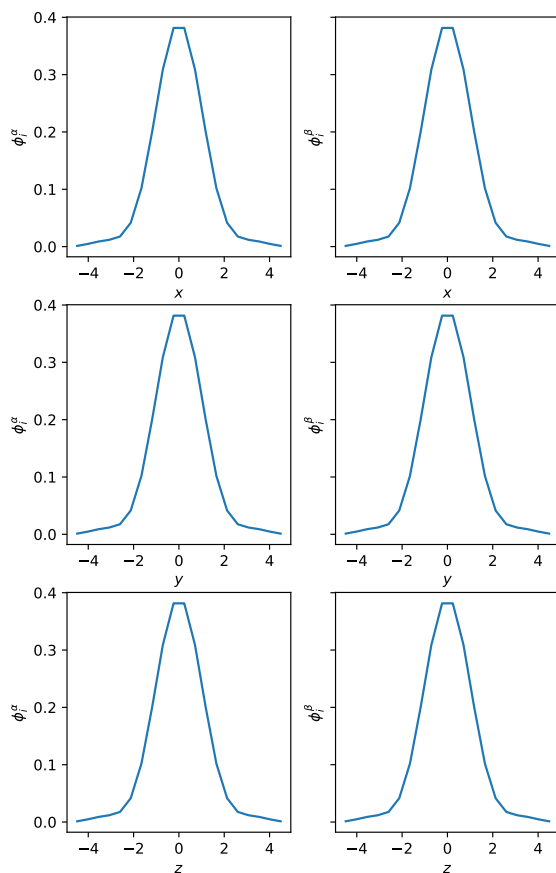
May 3, 2025

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

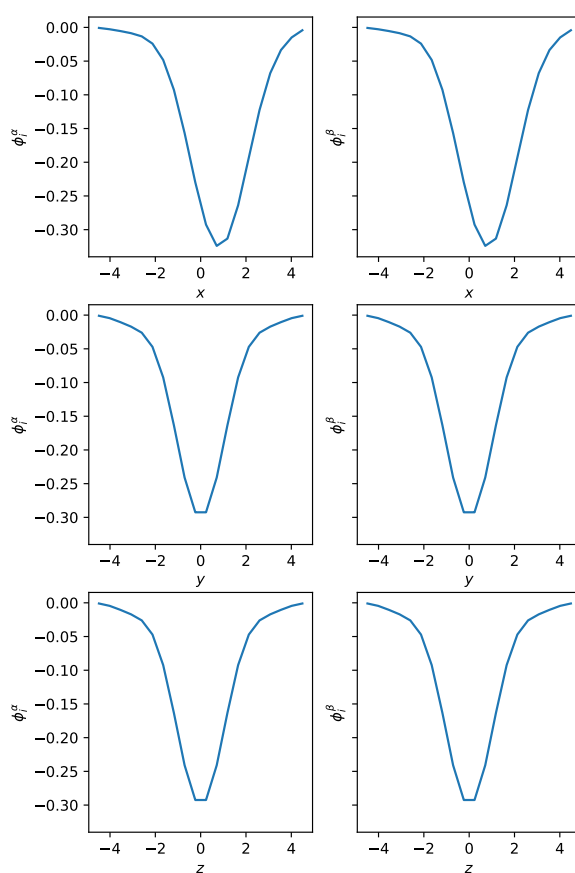
HW6.1: I implemented my DFT code using both the density fitting and a Poisson solver. Both the density fitting and the Poisson solver gave slightly different results compared to the reference solution. Since the differences were small, it is likely that my Poisson solver uses different convergence criteria than the reference solution.

HW6.2: I debugged the code for Hydrogen with only the external potential. Without density fitting, it almost exactly matches the reference solution.

Wavefunctions: He



Wavefunctions: H2_stretch



HW6.3:

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