

Problem Set 1

Chemistry 675, Fall 2024

Due Date: September 13, 2024

1. Identify the normalization condition that describes a wavefunction $\Phi(x)$ expanded in terms of a complete orthonormal set of basis functions $\{\phi_i(x)\}$ with coefficients $\{c_i\}$.
2. Consider the wavefunction $\Psi(x) = 0.6i\phi_1(x) + 0.1\phi_2(x) + c_3\phi_3(x) - 0.5\phi_4(x)$, where $\Psi(x)$ is normalized, $\hat{O}\phi_j(x) = j\phi_j(x)$, and $\{\phi_j(x)\}$ form an orthonormal set.
 - (a) Calculate the magnitude of c_3 .
 - (b) Plot the expected distribution of the outcomes of repeated measurements of the operator \hat{O} .
 - (c) Compute $\langle \hat{O} \rangle$.
3. Prove Hermitian operators only have real eigenvalues.
4. Complete Python exercise `problemset1.ipynb`.
 - (a) Download and install Python and Jupyter Notebook.
 - (b) Run the Jupyter notebook `problemset1.ipynb` using “shift-enter” to run each cell.
 - i. Method 1: Run “Anaconda Navigator,” open “JupyterLab,” and import the notebook with “Upload file” (icon with an up arrow).
 - ii. Method 2: Enter the folder of your computer that contains `problemset1.ipynb`, open the command line (terminal), and type `jupyter notebook problemset1.ipynb`.
 - (c) To gain greater understanding of the type of Python code used in class, test how the output of the program varies as you change variables, function names, etc.
 - (d) Complete and submit the answer to the problem marked “Problem Set Exercise” at the end of `problemset1.ipynb` alongside this problem set. Be careful to always label axes.