UNIVERSITY OF CALIFORNIA BERKELEY

Numerical Algorithms Applied to Computational Quantum Chemistry
Grading Rubrics for Homework 3

February 22, 2024

1 GRADING RUBRICS FOR CHEM 279 HW3

1. The problem set is worth 12 points. And the total points are divided into several components, as outlined below:

2. Key Points for Consideration:

   a) **Electron Pair Identification (1 point):** Read the specified format of input for some hydrocarbon molecules and correctly identify the number of electron pairs. An error should be thrown if the number of electron pairs is not an integer.

   b) **Overlap Matrix of Contracted Gaussian Atomic Orbitals (4 points):** Accurately read the basis information and construct a list of basis functions, i.e. contracted Gaussian atomic orbitals (cGTOs). Subsequently, evaluate the overlap matrix of these cGTOs and ensure the overlap matrix is printed. The accuracy of your overlap matrix will be verified using test samples.

   c) **Hamiltonian Matrix (3 points):** Based on the overlap matrix and given empirical parameters, construct the Hamiltonian matrix. Make sure to print the Hamiltonian matrix, as its accuracy will be evaluated using test samples.

   d) **Generalized Eigenvalue Problem and Total Energy Computation (4 points):** Solve the generalized eigenvalue problem and compute the total energy. Make sure to print the total energy, which will be assessed for accuracy using test samples. Pay attention to units and unit conversions.

3. After completing the code, remember to submit the link to your private repository to Gradescope so that your GSI is informed that you have finished your homework. Additionally, don't forget to add your GSI as a collaborator to your repository.