

PC5215, Numerical Recipes with Applications, Lab 2 (Due Friday, 2 Oct 2020)

1. Using the polynomial interpolation Python code `polint.py` of “Numerical Recipes in C”, compute and then plot a curve for x in the interval $[-1, 4]$, passing through exactly the points $(x,y) = (-1, 1.25), (1, 2), (2,3), (4,0)$ with a cubic polynomial. For plotting, you can use `gnuplot`, or `Origin`, or the plotting function in `MATLAB`, or even Python itself (need `import matplotlib`). Label the axis, mark the points with circles and the interpolated curve with solid line.

2. Implement the Romberg integration method in Python [following the “Numerical Recipes” code `qromb()`, `trapzd.py` and `polint.py`], and compute the integral:

$$\int_0^2 x^4 \ln(x + \sqrt{x^2 + 1}) dx.$$

The \ln means natural logarithm (base e). Use different parameters (such as number of iterations `JMAX`, and convergence criteria `EPS`), compare the results. What is your most accurate estimation of the integral? Give an error estimate of the answers. Compare with the exact answer. Also try with the symbolic integration system, such as *Mathematica* to get exact, or highly accurate (say 16 digits) results.

3. (This is a more challenging problem) The Hamiltonian of a hydrogen molecule with two fixed protons and two electrons is given by

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 - \frac{e^2}{4\pi\epsilon_0 r_{A1}} - \frac{e^2}{4\pi\epsilon_0 r_{B1}} - \frac{e^2}{4\pi\epsilon_0 r_{A2}} - \frac{e^2}{4\pi\epsilon_0 r_{B2}} + \frac{e^2}{4\pi\epsilon_0 r_{12}} + \frac{e^2}{4\pi\epsilon_0 r_{AB}},$$

where m is the mass of the electron, ϵ_0 is the dielectric constant of vacuum, e is the magnitude of the electron charge, \hbar is the reduced Planck constant. We assume that the two protons are located at (3D) fixed vector positions \mathbf{r}_A and \mathbf{r}_B , and the two electrons are at \mathbf{r}_1 and \mathbf{r}_2 . The distance is defined by $r_{\alpha\beta} = |\mathbf{r}_\alpha - \mathbf{r}_\beta|$, where α or β can be A, B, 1 or 2. In a simplest possible approximation for the electron wave function, we use atomic orbital of the ground state hydrogen atom in the symmetrized form,

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \varphi(r_{A1})\varphi(r_{B2}) + \varphi(r_{A2})\varphi(r_{B1}), \quad \varphi(r) = e^{-r/a_0}$$

where a_0 is Bohr radius. Note that the wave function is not normalized.

Estimate numerically lower bounds to the hydrogen molecule bonding energy by evaluating the integrals through a Monte Carlo method with the Metropolis algorithm,

$$E(r_{AB}) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$

For internal computer calculation, it is best to use atomic units ($\hbar=1, e=1, m=1, 4\pi\epsilon_0=1$). Outline your method, and report the results in units of ångström (for distance r_{AB} between two protons) and eV (for energy). Make a plot of energy (with error bars) vs. r_{AB} .

[For background, read any quantum mechanics textbooks, or Chapter 2 of “Molecular Modelling, principles and applications”, by Andrew R. Leach.]