Computational Physics Lab

(PH49012)

Spring-2021, IIT KGP

Assignment 08

Q1. Consider the following expression:

$$\int_a^b f(x)\mathrm{d}x = h\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{N-1} f(a+kh)\right] + \frac{1}{12}h^2\left[f'(a) - f'(b)\right] + O(h^4)$$

This result gives a value for the integral on the left which has an error of order h^4—a factor of h^2 better than the error on the trapezoidal rule and as good as Simpson's rule. We can use this formula as a new rule for evaluating integrals. We might call it the "Euler-Maclaurin rule".
Write a program to calculate the value of the integral $\int_0^2 (x^4 - 2x + 1)\mathrm{d}x$. The order-$h^2$ term in the formula involves the derivatives $f'(a)$ and $f'(b)$, which you should evaluate using central differences centered on a and b respectively. Note that the size of the interval you use for calculating the central differences does not have to equal the value of h used in the trapezoidal rule. An interval of about 10^{-5} gives good values for the central differences.
Use your program to evaluate the integral with $N = 10$ slices and compare the accuracy of the result with that obtained from the trapezoidal rule alone with the same number of slices. (10 points)

Q2. Find the first three bound state energies of finite square well potential by solving the equation:

$$\tan(za) = 2\frac{\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}}{\left[2 - \left(\frac{z_0}{z}\right)^2\right]} \tag{1}$$

For $a = 1.0$, $z_0 = \sqrt{\frac{2m}{V_0\hbar}} = 10.0$ and $z^2 = z_0^2 + 2mE/\hbar^2$
First plot separately the LHS and RHS of equation (1) on the same graph to obtain initial guesses of the first three roots of the equation. Then use the method of bisection to calculate the roots and finally use the solutions to obtain the allowed values of the energy E, in the unit of $\hbar^2/2m$. (20 points)

Q3. $\{(x, y)\}$={(1, 0.54030); (1.1, 0.45360); (1.2, 0.363236); (1.3, 0.26750); (1.4, 0.16997)}. For this given data, find $f(1.27)$ using Lagrange interpolation. (10 points)

Q4. Calculate the integral numerically for $f(x) = x, [0, 1.0]$; $f(x) = x^2, [0, 1.0]$; $f(x) = \sin(x), [0, \pi]$ both using trapezoidal and Simpson's 1/3 rule for intervals N=2, 4, 6 ...
Define error as relative error abs(numerical-analytical)/analytical and plot the error as a function of the number of interval N for both the processes. Confirm from the plot that is the behaviour you expect from theoretical understanding of the methods.
Make two separate plots for two different methods, each of the two plots should contain the results for all the four functions. (20 points)