Computational Physics Lab

(PH49012)

Spring-2021, IIT KGP

Assignment 06

Q1. Write a program to calculate an approximate value for the integral $\int_0^2 (x^4 - 2x + 1)\mathrm{d}x$ using Simpson's method with 100 slices. (10 points)

Q2. We consider the 1-D motion of a particle of mass m in a time independent potential $V(x)$. The fact that the energy E will be conserved allows us to integrate the equation of motion and obtain a solution in closed form. We consider a particular case of SHM where the particle is in bound motion between two points a and b where $V(a) = E$ and $V(b) = E$ and $V(x) < E$ for $a < x < b$. The time period of the oscillation T is given by:

$$T = \int_a^b \frac{\sqrt{2}\mathrm{d}x}{\sqrt{E - V(x)}}$$

Consider a particle with $m = 1\mathrm{Kg}$ in the potential $V(x) = \frac{1}{2}kx^2$ with $k = 4\ \mathrm{Nm}^{-1}$

(a) Numerically calculate the time period of oscillation by integrating the equation with Simpson method and check this against the expected value. The integrand will diverge at the limits. So, the limit has to be redefined as $(b - \epsilon)$ in place of b. Note, numerically obtained value of T will diverge for very low values of ϵ. Make a log-log plot of ϵ vs. T. Then choose a suitable value of ϵ that will provide a reasonably accurate value of T.

(b) Verify that T does not depend on the amplitude of oscillation. (10+10 points)

Q3. Write a program to find out the root of the following function by using Bisection and Newton-Raphson method.

$$f(x) = x^3 - x^2 + 2$$

. For Bisection method: use range [-5,5] to get the solution. Put the number of iterations and initial guess as comment within your code. (10+10 points)

Q4. Heat capacity of a solid:
Debye's theory of solids gives the heat capacity of a solid at temperature T to be

$$C_v = 9V\rho k_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2}\mathrm{d}x,$$

where V is the volume of the solid, ρ is the number density of atoms, k_B is Boltzmann's constant, and θ_D is the so-called *Debye temperature*, a property of solids that depends on their density and speed of sound.

(a) Write a python function cv(T) that calculates C_v for a given value of the temperature, for a sample consisting of 1000 cubic centimeters of solid aluminum, which has a number density of $\rho = 6.022 \times 10^{28}\mathrm{m}^{-3}$ and a Debye temperature of $\theta_D = 428\mathrm{K}$. Use Gaussian quadrature to evaluate the integral, with $N = 50$ sample points.

(b) Use your function to make graph of the heat capacity as a function of temperature from $T = 5\mathrm{K}$ to $T = 500\mathrm{K}$ (15+05 points)

Q5. Quantum uncertainty in the harmonic oscillator:
In units where all the constants are 1, the wavefunction of the nth energy level of the one-dimensional quantum harmonic oscillator—i.e., a spinless point particle in a quadratic potential well—is given by

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} \mathrm{e}^{-x^2/2} H_n(x),$$

for $n = 0...\infty$, where $H_n(x)$ is the nth Hermite polynomial. Hermite polynomials satisfy a relation somewhat similar to that for the Fibonacci numbers, although more complex:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$

The first two Hermite polynomials are $H_0(x) = 1$ and $H_1(x) = 2x$.

(a) Write a user-defined function H(n,x) that calculates $H_n(x)$ for given x and any integer $n \geq 0$. Use your function to make a plot that shows the harmonic oscillator wavefunctions for $n = 0, 1, 2$ and 3, all on the same graph, in the range $x = -4$ to $x = 4$.

(b) The quantum uncertainty in the position of a particle in the nth level of a harmonic oscillator can be quantified by its root-mean-square position $\sqrt{\langle x^2 \rangle}$, where

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 \mathrm{d}x$$

Write a program that evaluates the integral using Gaussian quadrature on 100 points, then calculates the uncertainty (i.e., the root-mean-square position of the particle) for a given value of n. Use your program to calculate the uncertainty for $n = 5$. You should get an answer in the vicinity of $\sqrt{\langle x^2 \rangle} = 2.3$

Hint: You may perform a change of variable to deal with the infinite limit e.g.,

$$\int_0^{\infty} f(x)\mathrm{d}x = \int_0^1 \frac{1}{(1-z)^2} f\left(\frac{z}{1-z}\right) \mathrm{d}z$$

(10+20 points)

Reference: Q4 and Q5 are taken from Computational Physics by Mark Newman

Simpson's method:

$$I(a,b) \simeq \frac{1}{3}h \left[f(a) + f(b) + 4 \sum_{\text{k=1,3...}}^{N-1} f(a+kh) + 2 \sum_{\text{k=2,4...}}^{N-2} f(a+kh) \right]$$

Gaussian quadrature:

$$\int_a^b f(x)\mathrm{d}x \simeq \sum_{k=1}^{N} w_k f(x_k)$$
