NUMERICAL INTEGRALS AND DERIVATIVES

Homework 3: DUE ON FRIDAY 21ST AT 11:59 PM

Problem 1: Heat capacity of a solid

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

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

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.

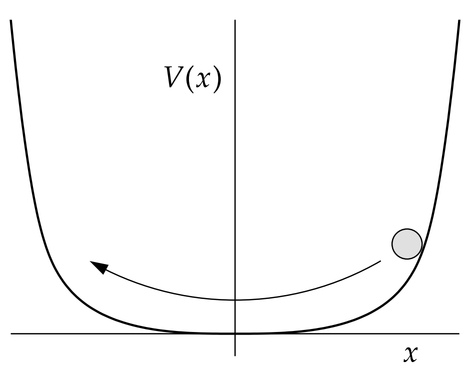
a) Write a Python function `cv(T)` that calculates C_V for a given value of the temperature, for a sample consisting of 1000 cubic centimeters of solid aluminum, which has a number density of $\rho = 6.022 \times 10^{28}\,\text{m}^{-3}$ and a Debye temperature of $\theta_D = 428\,\text{K}$. Use Gaussian quadrature to evaluate the integral, with $N = 50$ sample points. Hint: you can use the function(s) defined in `gaussxw.py` (from our class exercises).

b) Use your function to make a graph of the heat capacity as a function of temperature from $T = 5\,\text{K}$ to $T = 500\,\text{K}$.

Problem 2: Period of an anharmonic oscillator

The simple harmonic oscillator crops up in many places. Its behavior can be studied readily using analytic methods and it has the important property that its period of oscillation is a constant, independent of its amplitude, making it useful, for instance, for keeping time in watches and clocks.

Frequently in physics, however, we also come across anharmonic oscillators, whose period varies with amplitude and whose behavior cannot usually be calculated analytically. A general classical oscillator can be thought of as a particle in a concave potential well. When disturbed, the particle will rock back and forth in the well:



The harmonic oscillator corresponds to a quadratic potential $V(x) \propto x^2$. Any other form gives an anharmonic oscillator. (Thus there are many different kinds of anharmonic oscillator, depending on the exact form of the potential.)

One way to calculate the motion of an oscillator is to write down the equation for the conservation of energy in the system. If the particle has mass m and position x, then the total energy is equal to the sum of the kinetic and potential energies thus:

$$E = \tfrac{1}{2}m\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 + V(x).$$

Since the energy must be constant over time, this equation is effectively a (nonlinear) differential equation linking x and t.

Let us assume that the potential $V(x)$ is symmetric about $x = 0$ and let us set our anharmonic oscillator going with amplitude a. That is, at $t = 0$ we release it from rest at position $x = a$ and it swings back towards the origin. Then at $t = 0$ we have $\mathrm{d}x/\mathrm{d}t = 0$ and the equation above reads $E = V(a)$, which gives us the total energy of the particle in terms of the amplitude. When the particle reaches the origin for the first time, it has gone through one quarter of a period of the oscillator. By rearranging the equation above for $\mathrm{d}x/\mathrm{d}t$ and then integrating with respect to t from 0 to $\frac{1}{4}T$, it can be shown that the period T is given by

$$T = \sqrt{8m}\int_0^a \frac{\mathrm{d}x}{\sqrt{V(a) - V(x)}}.$$

a) Suppose the potential is $V(x) = x^4$ and the mass of the particle is $m = 1$. Write a Python function that calculates the period of the oscillator for given amplitude a using Gaussian quadrature with $N = 20$ points, then use your function to make a graph of the period for amplitudes ranging from $a = 0$ to $a = 2$.

b) You should find that the oscillator gets faster as the amplitude increases, even though the particle has further to travel for larger amplitude. And you should find that the period diverges as the amplitude goes to zero. How do you explain these results?

Problem 3: The Stefan–Boltzmann constant

The Planck theory of thermal radiation tells us that in the (angular) frequency interval ω to $\omega + \mathrm{d}\omega$, a black body of unit area radiates electromagnetically an amount of thermal energy per second equal to $I(\omega)\,\mathrm{d}\omega$, where

$$I(\omega) = \frac{\hbar}{4\pi^2c^2}\frac{\omega^3}{(\mathrm{e}^{\hbar\omega/k_BT} - 1)}.$$

Here $\hbar$ is Planck's constant over 2π, c is the speed of light, and k_B is Boltzmann's constant. Integrating over frequency, it can be shown that the total energy per unit area radiated by a black body is

$$W = \frac{k_B^4T^4}{4\pi^2c^2\hbar^3}\int_0^\infty \frac{x^3}{\mathrm{e}^x - 1}\,\mathrm{d}x.$$

a) Write a program to evaluate the integral in this expression. Explain what method you used, and how accurate you think your answer is.

b) Even before Planck gave his theory of thermal radiation around the turn of the 20th century, it was known that the total energy W given off by a black body per unit area per second followed Stefan's law: $W = \sigma T^4$, where σ is the Stefan–Boltzmann constant. Use your value for the integral above to compute a value for the Stefan–Boltzmann constant (in SI units) to three significant figures. Check your result against the known value, which you can find in books or on-line. You should get good agreement.

Problem 4: 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

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

for $n = 0 \ldots \infty$, 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 $x = 4$. Hint: There is a function `factorial` in the `math` package that calculates the factorial of an integer.

b) Make a separate plot of the wavefunction for $n = 30$ from $x = -10$ to $x = 10$. Hint: If your program takes too long to run in this case, then you're doing the calculation wrong—the program should take only a second or so to run.

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

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 \, dx.$$

Write a program that evaluates this integral using Gaussian quadrature on 100 points and 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 $\sqrt{\langle x^2 \rangle} = 2.3$.

Problem 5: Electric field of a charge distribution

Suppose we have a distribution of charges and we want to calculate the resulting electric field. One way to do this is to first calculate the electric potential ϕ and then take its gradient. For a point charge q at the origin, the electric potential at a distance r from the origin is $\phi = q/4\pi\epsilon_0 r$ and the electric field is $\mathbf{E} = -\nabla\phi$.

a) You have two charges, of $\pm 1\,\mathrm{C}$, $10\,\mathrm{cm}$ apart. Calculate the resulting electric potential on a $1\,\mathrm{m} \times 1\,\mathrm{m}$ square plane surrounding the charges and passing through them. Calculate the potential at $1\,\mathrm{cm}$ spaced points in a grid and make a visualization on the screen of the potential using a density plot.

b) Now calculate the partial derivatives of the potential with respect to x and y and hence find the electric field in the xy plane. Make a visualization of the field also. This is a little trickier than visualizing the potential, because the electric field has both magnitude and direction. One way to do it might be to make two density plots, one for the magnitude, and one for the direction, the latter using the "`hsv`" color scheme, which is a rainbow scheme that passes through all the colors but starts and ends with the same shade of red, which makes it suitable for representing things like directions or angles that go around the full circle and end up where they started. A more sophisticated visualization might use `matplotlib`'s `quiver` function, drawing a grid of arrows with direction and length chosen to represent the field.