PHYS6350 (Computational Physics)

Problem Set 2

Due:

Fri, Feb 24, 2023, end of the day

Instructions:

Send via Teams (preferably) or email. Should include code (or, where applicable, note) which solves the problems and, where applicable, plots and/or annotations. The preferred languages are Python/Jupyter notebook/C++ while other choices may be accepted on an individual basis.

Problem 2.1: Lambert W function

The Lambert W function $W(x)$ is defined as the solution to the following equation

$$W(x)\,e^{W(x)} = x\ ,$$

and appears in a number of physical applications, such as the Wien's displacement constant or the equation of state of excluded volume model.

a) Write a program to calculate $W(x)$ in range $x = 0...6$. Plot the results (or output in a tabular format).

b) Calculate $W'(x)$ in range $x = 0...6$ using numerical differentiation. Plot the results (or output in a tabular format).

c) Derive the following analytic expression for $W'(x)$,

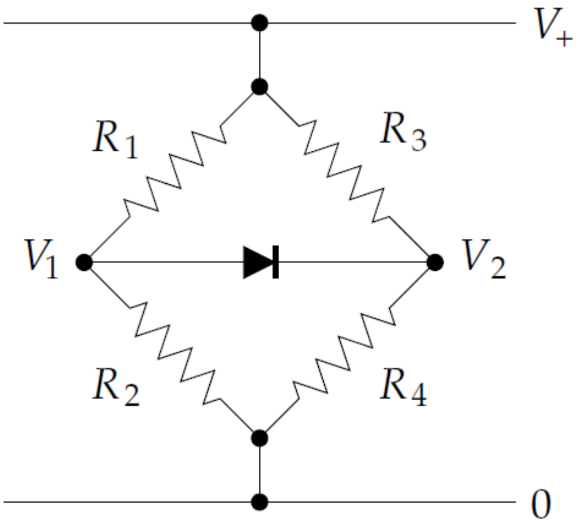
$$W'(x) = \frac{W(x)}{x[1 + W(x)]},$$

and use it to verify the accuracy of the numerical derivative.

Problem 2.2: Nonlinear circuits

This is Exercise 6.17 from M. Newman "Computational Physics"

Consider the following simple circuit, a variation on the classic Wheatstone bridge:



The resistors obey the normal Ohm law, but the diode obeys the diode equation:

$$I = I_0(e^{V/V_T} - 1),$$

where V is the voltage across the diode and I_0 and V_T are constants.

a) The Kirchhoff current law says that the total net current flowing into or out of every point in a circuit must be zero. Applying the law to voltage~V_1 in the circuit above we get

$$\frac{V_1 - V_+}{R_1} + \frac{V_1}{R_2} + I_0\left[e^{(V_1-V_2)/V_T} - 1\right] = 0.$$

Derive the corresponding equation for voltage V_2.

b) Solve the two nonlinear equations using your favorite method (Newton, Broyden, relaxation) for the voltages V_1 and V_2 with the conditions

$$V_+ = 5\,\mathrm{V},$$
$$R_1 = 1\,\mathrm{k\Omega}, \qquad R_2 = 4\,\mathrm{k\Omega}, \qquad R_3 = 3\,\mathrm{k\Omega}, \qquad R_4 = 2\,\mathrm{k\Omega},$$
$$I_0 = 3\,\mathrm{nA}, \qquad V_T = 0.05\,\mathrm{V}.$$

c) The electronic engineer's rule of thumb for diodes is that the voltage across a (forward biased) diode is always about 0.6 volts. Confirm that your results agree with this rule.

Problem 2.3: Heat capacity of a solid

Adapted from Exercise 5.9 from M. Newman "Computational Physics"

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.

Write a code 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 $\theta_D = 428$ K.

a) Use adaptive rectangle rule to calculate $C_V(T)$. Explain why we should use it over the Romberg method.

b) Use Gaussian quadrature to calculate $C_V(T)$.

c) Use the two evaluations to make a graph of the heat capacity as a function of temperature from $T = 5$ K to $T = 500$ K.

Note: It is ok to use arbiratry units for $C_V(T)$, just make sure that the shape of the $C_V(T)$ curve is correct

Problem 2.4: The Stefan-Bolztmann constant

This is Exercise 5.12 from M. Newman "Computational Physics"

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

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

Here $\hbar$ is Planck's constant over 2π, c is the speed of light, and k_B is Boltzmann's constant.

a) Show that the total energy per unit area radiated by a black body is

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

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

c) 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.