

**PHYS 7411 Spring 2015**  
**Computational Physics**  
**Homework 1**

**Due by class Wednesday 4 February 2015**

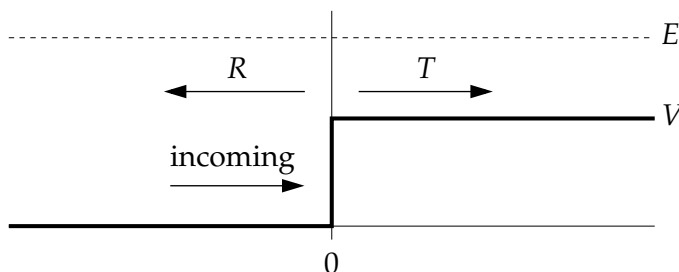
(Any late assignments will be penalized in the amount of 25% per day late. Any copying of computer programs will be penalized with no credit.)

**Exercise 1: Another ball dropped from a tower**

A ball is dropped from a tower of height  $h$  with initial velocity zero. Write a program that asks the user to enter the height in meters of the tower and then calculates and prints the time the ball takes until it hits the ground, ignoring air resistance. Use your program to calculate the time for a ball dropped from a 100 m high tower.

**Exercise 2: Quantum potential step**

A well-known quantum mechanics problem involves a particle of mass  $m$  that encounters a one-dimensional potential step, like this:



The particle with initial kinetic energy  $E$  and wavevector  $k_1 = \sqrt{2mE}/\hbar$  enters from the left and encounters a sudden jump in potential energy of height  $V$  at position  $x = 0$ . By solving the Schrödinger equation, one can show that when  $E > V$  the particle may either (a) pass the step, in which case it has a lower kinetic energy of  $E - V$  on the other side and a correspondingly smaller wavevector of  $k_2 = \sqrt{2m(E - V)}/\hbar$ , or (b) it may be reflected, keeping all of its kinetic energy and an unchanged wavevector but moving in the opposite direction. The probabilities  $T$  and  $R$  for transmission and reflection are given by

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2}, \quad R = \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2.$$

Suppose we have a particle with mass equal to the electron mass  $m = 9.11 \times 10^{-31}$  kg and energy 10 eV encountering a potential step of height 9 eV. Write a Python program to compute and print out the transmission and reflection probabilities using the formulas above.

**Exercise 3: The Madelung constant**

In condensed matter physics the Madelung constant gives the total electric potential felt by an atom in a solid. It depends on the charges on the other atoms nearby and their locations. Consider for instance solid sodium chloride—table salt. The sodium chloride crystal has atoms arranged on a cubic lattice, but with alternating sodium and chlorine atoms, the sodium ones having a single positive charge  $+e$  and the chlorine ones a single negative charge  $-e$ , where  $e$  is the charge on the electron. If we label each position

on the lattice by three integer coordinates  $(i, j, k)$ , then the sodium atoms fall at positions where  $i + j + k$  is even, and the chlorine atoms at positions where  $i + j + k$  is odd.

Consider a sodium atom at the origin,  $i = j = k = 0$ , and let us calculate the Madelung constant. If the spacing of atoms on the lattice is  $a$ , then the distance from the origin to the atom at position  $(i, j, k)$  is

$$\sqrt{(ia)^2 + (ja)^2 + (ka)^2} = a\sqrt{i^2 + j^2 + k^2},$$

and the potential at the origin created by such an atom is

$$V(i, j, k) = \pm \frac{e}{4\pi\epsilon_0 a \sqrt{i^2 + j^2 + k^2}},$$

with  $\epsilon_0$  being the permittivity of the vacuum and the sign of the expression depending on whether  $i + j + k$  is even or odd. The total potential felt by the sodium atom is then the sum of this quantity over all other atoms. Let us assume a cubic box around the sodium at the origin, with  $L$  atoms in all directions. Then

$$V_{\text{total}} = \sum_{\substack{i, j, k = -L \\ \text{not } i=j=k=0}}^L V(i, j, k) = \frac{e}{4\pi\epsilon_0 a} M,$$

where  $M$  is the Madelung constant, at least approximately—technically the Madelung constant is the value of  $M$  when  $L \rightarrow \infty$ , but one can get a good approximation just by using a large value of  $L$ .

Write a program to calculate and print the Madelung constant for sodium chloride. Use as large a value of  $L$  as you can, while still having your program run in reasonable time—say in a minute or less.

#### Exercise 4: The semi-empirical mass formula

In nuclear physics, the semi-empirical mass formula is a formula for calculating the approximate nuclear binding energy  $B$  of an atomic nucleus with atomic number  $Z$  and mass number  $A$ :

$$B = a_1 A - a_2 A^{2/3} - a_3 \frac{Z^2}{A^{1/3}} - a_4 \frac{(A - 2Z)^2}{A} + \frac{a_5}{A^{1/2}},$$

where, in units of millions of electron volts, the constants are  $a_1 = 15.67$ ,  $a_2 = 17.23$ ,  $a_3 = 0.75$ ,  $a_4 = 93.2$ , and

$$a_5 = \begin{cases} 0 & \text{if } A \text{ is odd,} \\ 12.0 & \text{if } A \text{ and } Z \text{ are both even,} \\ -12.0 & \text{if } A \text{ is even and } Z \text{ is odd.} \end{cases}$$

- Write a program that takes as its input the values of  $A$  and  $Z$ , and prints out the binding energy for the corresponding atom. Use your program to find the binding energy of an atom with  $A = 58$  and  $Z = 28$ . (Hint: The correct answer is around 490 MeV.)
- Modify your program to print out not the total binding energy  $B$ , but the binding energy per nucleon, which is  $B/A$ .
- Now modify your program so that it takes as input just a single value of the atomic number  $Z$  and then goes through all values of  $A$  from  $A = Z$  to  $A = 3Z$ , to find the one that has the largest binding energy per nucleon. This is the most stable nucleus with the given atomic number. Have your program print out the value of  $A$  for this most stable nucleus and the value of the binding energy per nucleon.

- d) Modify your program again so that, instead of taking  $Z$  as input, it runs through all values of  $Z$  from 1 to 100 and prints out the most stable value of  $A$  for each one. At what value of  $Z$  does the maximum binding energy per nucleon occur? (The true answer, in real life, is  $Z = 28$ , which is nickel. You should find that the semi-empirical mass formula gets the answer roughly right, but not exactly.)

### Exercise 5: Binomial coefficients

The binomial coefficient  $\binom{n}{k}$  is an integer equal to

$$\binom{n}{k} = \frac{n!}{k!(n-k)!} = \frac{n \times (n-1) \times (n-2) \times \dots \times (n-k+1)}{1 \times 2 \times \dots \times k}$$

when  $k \geq 1$ , or  $\binom{n}{0} = 1$  when  $k = 0$ .

- a) Using this form for the binomial coefficient, write a user-defined function `binomial(n,k)` that calculates the binomial coefficient for given  $n$  and  $k$ . Make sure your function returns the answer in the form of an integer (not a float) and gives the correct value of 1 for the case where  $k = 0$ .
- b) Using your function write a program to print out the first 20 lines of “Pascal’s triangle.” The  $n$ th line of Pascal’s triangle contains  $n + 1$  numbers, which are the coefficients  $\binom{n}{0}$ ,  $\binom{n}{1}$ , and so on up to  $\binom{n}{n}$ . Thus the first few lines are

```
1 1
1 2 1
1 3 3 1
1 4 6 4 1
```

- c) The probability that an unbiased coin, tossed  $n$  times, will come up heads  $k$  times is  $\binom{n}{k}/2^n$ . Write a program to calculate (a) the total probability that a coin tossed 100 times comes up heads exactly 60 times, and (b) the probability that it comes up heads 60 or more times.

### Exercise 6: Prime numbers

The program in Example 2.8 is not a very efficient way of calculating prime numbers: it checks each number to see if it is divisible by any number less than it. We can develop a much faster program for prime numbers by making use of the following observations:

- a) A number  $n$  is prime if it has no prime factors less than  $n$ . Hence we only need to check if it is divisible by other primes.
- b) If a number  $n$  is non-prime, having a factor  $r$ , then  $n = rs$ , where  $s$  is also a factor. If  $r \geq \sqrt{n}$  then  $n = rs \geq \sqrt{n}s$ , which implies that  $s \leq \sqrt{n}$ . In other words, any non-prime must have factors, and hence also prime factors, less than or equal to  $\sqrt{n}$ . Thus to determine if a number is prime we have to check its prime factors only up to and including  $\sqrt{n}$ —if there are none then the number is prime.
- c) If we find even a single prime factor less than  $\sqrt{n}$  then we know that the number is non-prime, and hence there is no need to check any further—we can abandon this number and move on to something else.

Write a Python program that finds all the primes up to ten thousand. Create a list to store the primes, which starts out with just the one prime number 2 in it. Then for each number  $n$  from 3 to 10 000 check whether the number is divisible by any of the primes in the list up to and including  $\sqrt{n}$ . As soon as you find a single prime factor you can stop checking the rest of them—you know  $n$  is not a prime. If you find no prime factors  $\sqrt{n}$  or less then  $n$  is prime and you should add it to the list. You can print out the list all in one go at the end of the program, or you can print out the individual numbers as you find them.

### Exercise 7: Recursion

A useful feature of user-defined functions is *recursion*, the ability of a function to call itself. For example, consider the following definition of the factorial  $n!$  of a positive integer  $n$ :

$$n! = \begin{cases} 1 & \text{if } n = 1, \\ n \times (n - 1)! & \text{if } n > 1. \end{cases}$$

This constitutes a complete definition of the factorial which allows us to calculate the value of  $n!$  for any positive integer. We can employ this definition directly to create a Python function for factorials, like this:

```
def factorial(n):
    if n==1:
        return 1
    else:
        return n*factorial(n-1)
```

Note how, if  $n$  is not equal to 1, the function calls itself to calculate the factorial of  $n - 1$ . This is recursion. If we now say “`print(factorial(5))`” the computer will correctly print the answer 120.

- a) We encountered the Catalan numbers  $C_n$  previously in Exercise 2.7 on page 46. With just a little rearrangement, the definition given there can be rewritten in the form

$$C_n = \begin{cases} 1 & \text{if } n = 0, \\ \frac{4n - 2}{n + 1} C_{n-1} & \text{if } n > 0. \end{cases}$$

Write a Python function, using recursion, that calculates  $C_n$ . Use your function to calculate and print  $C_{100}$ .

- b) Euclid showed that the greatest common divisor  $g(m, n)$  of two nonnegative integers  $m$  and  $n$  satisfies

$$g(m, n) = \begin{cases} m & \text{if } n = 0, \\ g(n, m \bmod n) & \text{if } n > 0. \end{cases}$$

Write a Python function `g(m, n)` that employs recursion to calculate the greatest common divisor of  $m$  and  $n$  using this formula. Use your function to calculate and print the greatest common divisor of 108 and 192.

Comparing the calculation of the Catalan numbers in part (a) above with that of Exercise 2.7, we see that it’s possible to do the calculation two ways, either directly or using recursion. In most cases, if a quantity can be calculated *without* recursion, then it will be faster to do so, and we normally recommend taking this route if possible. There are some calculations, however, that are essentially impossible (or at least much more difficult) without recursion.