Università di Pisa
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Dispense di Algoritmi di Spettroscopia

Giovanni Moruzzi

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Contents

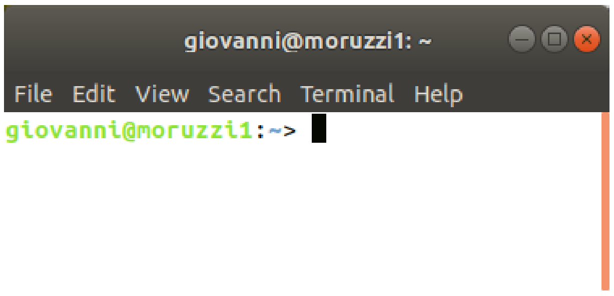
Chapter 1

Python Basics and the Interactive Mode

1.1 Using the Command Line

When you start writing your own computer programs it can be useful, even if not mandatory, to interact with your computer via the *command line*. Since nowadays the overwhelming majority of the computer users ignore even the existence of the command line, we discuss it briefly in this section.

In order to use the command line you start by opening a window, sometimes called *terminal*, *shell* or *console*, in the computer monitor. The terminal contains a *command prompt* comprising a sequence of characters indicating readiness to accept commands. The actual prompt is different from one operating system to another, and some operating systems allow you to customize it. In the rest of this book the prompt will be represented by the two-character sequence `$>`. The command prompt literally prompts the user to take action. Figure 1.1 shows a typical terminal, and its prompt, on Ubuntu Linux. Terminals of other operating systems look similar. A simple way to open a terminal under Linux is pressing `Ctrl+Alt+T` (pressing the keys `Ctrl`, `Alt` and `T` simultaneously on the keyboard).



```
giovanni@moruzzi1:~>
```

Figure 1.1 A Linux terminal. Here the prompt is the sequence `giovanni@moruzzi1:~>`

If you are using macOS, the `Terminal` app is in the `Utilities` folder in `Applications`. To open it, either open your `Applications` folder, then open `Utilities` and double-click on `Terminal`, or press `Command-spacebar` to launch `Spotlight` and type ”Terminal,” then double-click the search result.

Under Windows you can open a terminal by clicking the `Start` button, typing `cmd` and pressing the <Enter> key.

The command line on a terminal was the primary means of interaction with most computer systems in the mid-1960s. In those times the “terminal” initially consisted of a teleprinter, later replaced by a keyboard and cathode-ray monitor. The command line continued to be used throughout the 1970s and 1980s on personal computer systems including MS-DOS, CP/M and Apple DOS, the “terminal” being replaced by a “terminal emulator”, a window on the computer monitor where you could type your commands. The interface between your commands and the computer actions is usually implemented with a *command line shell*, a program that accepts commands as text input and converts commands into appropriate operating system functions.

Once you have opened a terminal you can start typing commands, hitting <Enter> at the end of each. Each operating system has its own list of native commands, and you can add your personal commands. For instance, if you type "`ls -l`" in a Linux or Mac terminal, you will get the list of the contents of the current directory. The same result is obtained by typing "`dir`" in a Windows terminal. In this context you don't need to learn the whole lists of available commands for your operating system: when the command line is needed, we shall tell you what to type.

1.2 Installing Python

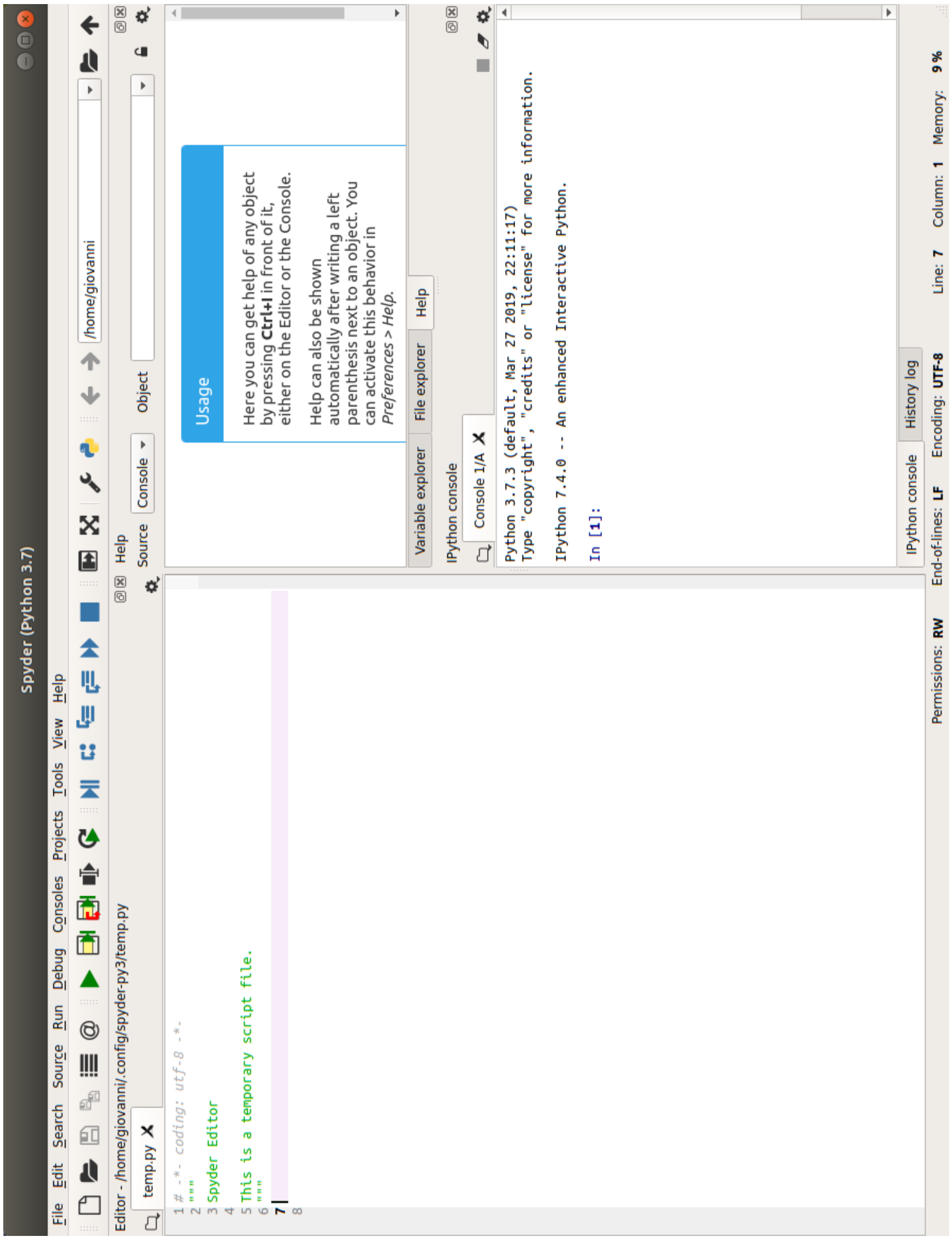
1.2.1 General

Obviously, in order use Python you must have Python (we shall use the Python 3 version) installed in your computer. The Ubuntu and Debian distributions of Linux come with both Python 2 and Python 3 already installed by default, thus you can skip the following Subsections 1.2.2 and 1.2.3 if you use Ubuntu or Debian. If you have Windows or macOS (previously Mac OS X and later OS X) you will probably need to install Python 3. In this case Subsections 1.2.2 and 1.2.3 tell you how to do it.

However, even if you are a Linux user, you might be interested in using Python in an *integrated development environment* (IDE) rather than through the command line in a terminal (particularly if Section 1.1 has scared you!) An IDE is a software application that provides comprehensive facilities to computer programmers for software development. An IDE normally consists of a source-code editor for typing your program code, build automation tools, and a debugger. By *build automation* we mean the combined processes of compiling computer source code into binary code, packaging binary code, and running automated tests. A very good option for Python is Anaconda, a free and open-source distribution of the Python and R programming languages for scientific computing. Anaconda is available for Linux, Windows and macOS, and you can easily download it from their site

`https://www.anaconda.com/distribution/`

whatever your operating system. Choose the Python 3 version for your operating system, and follow the download instructions on your browser. Installing Anaconda automatically installs also a version of Python, thus, if Anaconda is your choice, you can skip Subsections 1.2.2 and 1.2.3 even if you are a Windows or Mac user. Once Anaconda is installed, launch Spyder 3, and you obtain the window shown in Fig. 1.2. The Spyder window is divided into three rectangular subwindows: the left subwindow is an editor for typing programs, or *scripts*, see Chapter 2; the lower-right subwindow is a console where you can use Python interactively, as discussed in this chapter starting from Section 1.3. An alternative good IDE is IDLE (Integrated Development and Learning Environment), which is also available for Windows, Linux and macOS. However, in the present book we shall discuss only Spyder and the command-line terminal


Spyder (Python 3.7)
File Edit Search Source Run Debug Consoles Projects Tools View Help
/home/giovanni
Editor - /home/giovanni/.config/spyder-py3/temp.py
temp.py
Help
Source Console Object
Variable explorer File explorer Help
IPython console
Console 1/A
IPython console History log

```
# -*- coding: utf-8 -*-
"""
Spyder Editor

This is a temporary script file.
"""
```

Usage

Here you can get help of any object by pressing **Ctrl+I** in front of it, either on the Editor or the Console.

Help can also be shown automatically after writing a left parenthesis next to an object. You can activate this behavior in *Preferences > Help*.

```
Python 3.7.3 (default, Mar 27 2019, 22:11:17)
Type "copyright", "credits" or "license" for more information.

IPython 7.4.0 -- An enhanced Interactive Python.

In [1]:
```

Permissions: **RW** End-of-lines: **LF** Encoding: **UTF-8** Line: **7** Column: **1** Memory: **9 %**

Figure 1.2 The Spyder3 integrated development environment.

1.2.2 Downloading Python for Windows

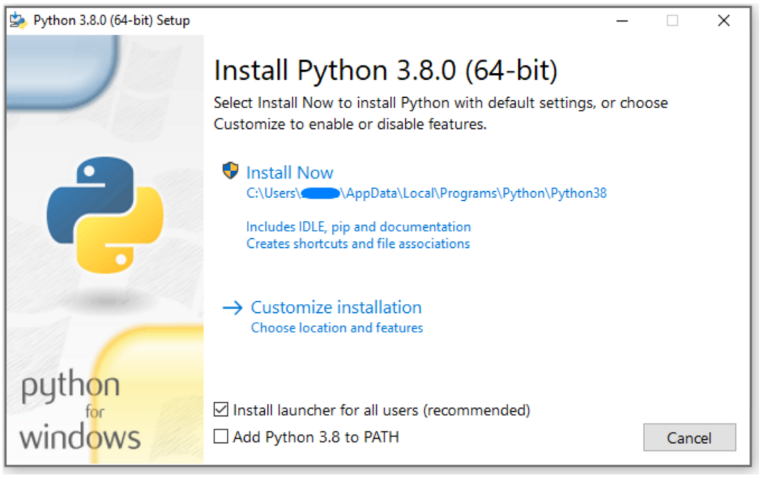
Step 1: Download the Python 3 Installer

Open a browser window and navigate to the Download page for Windows at python.org. Underneath the heading at the top that says Python Releases for Windows, click on the link for the Latest Python 3 Release - Python 3.x.x. Scroll to the bottom and select either Windows x86-64 executable installer for 64-bit or Windows x86 executable installer for 32-bit.

Step 2: Run the Installer

Once you have chosen and downloaded the installer of your choice, simply run it by double-clicking on the downloaded file. You should see a dialog similar to Fig. 1.3 on your computer monitor.

Then just click `Install Now`. This will download Python 3, the *pip* Python package manager and Python documentation. That should be all there is to do. A few minutes later you should have a working Python 3 installation on your Window system.


Python 3.8.0 (64-bit) Setup

Install Python 3.8.0 (64-bit)

Select Install Now to install Python with default settings, or choose Customize to enable or disable features.

Install Now
C:\Users\[redacted]\AppData\Local\Programs\Python\Python38

Includes IDLE, pip and documentation
Creates shortcuts and file associations

→ Customize installation
Choose location and features

☑ Install launcher for all users (recommended)
☐ Add Python 3.8 to PATH

Figure 1.3 Python installer for Windows.

1.2.3 Downloading Python for macOS

In the following, the symbol `$>` stands for the command prompt on the terminal, while a backslash (\) will mean that a long single command, that actually you must type in a single line, has been split into two lines to fit the page.

Step 1: Confirm your Python version

Although Python 2 is installed by default on Apple computers, Python 3 is not. You can confirm this by typing in Terminal

```
$> python --version
Python 2.7.15
```

To check if Python 3 is already installed try running the command

```
$>python3 --version.
```

Most likely you will see an error message, but it is worth checking. Even if you have a version of Python 3, we want to be on the most recent release, which is 3.7.0 at this point in 2018.

Step 2: Install Xcode and Homebrew

It is advisable to use the package manager Homebrew to install Python 3. Homebrew depends on Apples Xcode package, so run the following command to install it

```
$> xcode-select --install
```

Click through all the confirmation commands (Xcode is a large program so this might take a while to install depending on your internet connection).
Next, install Homebrew with the following (long) command:

```
/usr/bin/ruby -e "\$(curl␣-fsSL␣\
https://raw.githubusercontent.com/Homebrew/install/master/install)"
```

Note: You can also find this command on the homepage of the Homebrew website. It is easier to copy and paste rather than typing, since its a long command.

To confirm that Homebrew installed correctly, run this command:

```
$> brew doctor
```

Your system is ready to brew.

Step 3: Install Python 3

To install the latest version of Python, run the following command:

```
$> brew install python3
```

Now let's confirm which version was installed:

```
$> python3 --version
Python 3.7.0
```

To open a Python 3 shell from the command line type `python3`:

```
$> python3
Python 3.7.0 (default, Jun 29 2018, 20:13:13)
{[Clang 9.1.0 (clang-902.0.39.2)]} on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

When you want to exit, type `exit()` and then Return, or `Ctrl-D` (press the Control and D keys at the same time).

1.3 Using Python in Interactive Mode

Once you have installed Python in your computer, or a friend has installed it for you, you have the two possibilities discussed above:

1. You can open a terminal and access Python through the command line, provided that Section 1.1 did not scare you.

2. You can start using Python through an IDE, here we shall consider Spyder.

Python programs, or Python commands, are executed by an interpreter. There are two ways of using Python: i) the *interactive mode*, which we discuss in the rest of the present chapter, and ii) Python programs (also called *Python scripts*), which we shall discuss in the rest of the book.

When working in the interactive mode you type Python commands one by one (or small groups of commands, as we shall see below) at the Python prompts, and Python immediately interprets what you wrote and executes your commands. This is what you must do according to your choice between command-line terminal or Spyder IDE,

1. If you choose the command line in a terminal, you start the Python interactive mode by simply typing `python3`, and pressing `<Enter>`, at the command prompt. Immediately after entering the interactive mode you see something like this on your monitor

   ```
   $> python3
   Python 3.5.2 (default, Nov 17 2016, 17:05:23)
   [GCC 5.4.0 20160609] on linux
   Type "help", "copyright", "credits" or "license" for more\
   information.
   >>>
   ```

   Obviously some of what you see above will change according the Python version installed in your computer and to your operating system. The back slash (\) at the end of the fourth line means that the whole line was too long to fit in the page of the book, so it was split and continued below. The symbol >>> in the last line is the *Python prompt*, prompting you to enter your first Python command.

2. Alternatively, if you choose Anaconda and Spyder, the interactive mode is available in the bottom-right subwindow of Fig. 1.2, called the *IPython* console (IPython stands for "Interactive Python"). You type your first Python command at the prompt "`In [1]:`".

The advantage of the interactive mode is that you can immediately see how Python reacts to your commands, and discover possible errors immediately. On the other hand, the interactive mode becomes uncomfortable when you write long codes, that are better handled by Python *scripts*, to be introduced in Chapter 2.

This is what you see if you type, for instance, "`print('Hello World!!!')`" at the Python prompt in the terminal

```
>>> print('Hello World!!!')
Hello World!!!
>>>
```

while this is what you see in the IPython console of Spyder

```
In [1]: print('Hello World!!!')
Hello World!!!

In [2]:
```

`print()` is a command (actually, a *function*, to be discussed in Section 2.2) that tells Python to print the content of the parentheses (the *argument* of the function). The single quotes (`'`) tell Python to interpret their content as a sequence of printable characters (a *string*) to be printed as they are, not as a *variable* (see Section 1.4). A string can also be delimited by double quotes, `"also this is a` `string"`: single quotes and double quotes are fully equivalent in Python. The final prompts, `>>>` in the terminal, and `In [2]:` in the IPython console, tell you that Python is waiting for your next command. In the examples of the rest of this chapter we shall show only the terminal prompt ">>>", if you use Spyder this will be replaced by the prompt "`In [n]`", where `n` is a progressive natural number.

Python in interactive mode can be used as a desktop calculator, for instance:

```
>>> 15+16
31
>>>_+9
40
>>>
```

the underscore (`_`) in the command `_+9` means that 9 must be added to the previous result. This works only in interactive mode, not in scripts.

1.4 Variables

1.4.1 Variable Types

In computer programming, a variable is a memory storage location associated to a symbolic name (its *identifier*), which contains some quantity of information (the variable *value*). Differently from other programming languages, Python variables do not need explicit declaration to reserve memory space. The memory allocation (or *variable declaration*) occurs automatically the first time the variable appears at the left of an equal sign (=), which serves as *assignment operator*. In other words, the equal sign assigns values from its right side to the variable at its left side. When choosing the name for a new variable remember that

1. The name of a variable must begin with a letter (a-z, A-Z) or underscore (_).

2. The following characters of the name can be letters, numbers or underscores.

3. Variable names are *case sensitive*, for instance, `cat`, `Cat` and `CAt` are three different variables.

4. Variable names can have any (reasonable) length.

5. There are reserved words, or *keywords*, used by Python to define the syntax and structure of the Python language. You cannot use keywords as variable names.

The first time a variable is used, it must appear at the left side of an assignment operation. The assignment first reserves space for the variable in the computer memory, then copies what is at the right side of the = sign into the variable storage location. Successive assignments involving the same variable only change its previous value, keeping its memory location.

Python variables belong to five standard data types:

1. Numbers
2. Strings
3. Lists
4. Tuples

5. Dictionaries

Numbers can be *integers* like `10`, *long integers* like `51924361L`, *floats* like `132.57`, and *complex* like `13.2+2.5j` (`j` standing for the imaginary unit). We have already met strings in Section 1.3: strings are sequences of characters enclosed in quotation marks. As mentioned above, both pairs of single quotes and pairs of double quotes are allowed: `'platypus'` and `"platypus"` are equivalent. Lists and tuples are discussed in Section 1.10, dictionaries in Section 1.14, below. In this section we handle strings and numbers. For example you can type

```
>>> counter=100          # An integer assignment
>>> mass=10.0            # A floating point
>>> velocity=15.22       # A floating point
>>> name="John"          # A string

>>> print(name)
John
>>> print(mass*velocity)
152.20000000000002
>>> print(format(mass*velocity,"10.3f"))
152.200
>>> momentum=mass*velocity
>>> print(momentum)
152.20000000000002
```

You have to type only what follows the Python interpreter prompts (>>>), while all the lines not starting with prompts are printed by Python automatically. Note the presence of *rounding errors*. This is due to the fact that all numbers, integers or float, are stored in binary form in a computer memory. While this does not give problems with integers, you must remember that binary fractions only terminate if the denominator has 2 as the only prime factor. Thus, most rational numbers (and all irrational numbers) need an infinite number of bits for an exact binary representation. However, obviously, only a finite number of bits is available for storing a variable, and this leads to rounding errors. This is the reason for the apparently strange value of the product `mass*velocity`. Often a *formatted output* leads to a more "aesthetic" result (see Section 1.15). Here, the command `print(format(mass*velocity,"10.3f"))` tells Python to print the result as a 10 *character* number, with 3 digits after the decimal point. The 10 *characters* include all digits before and after the decimal point, leading blanks, the decimal point itself and, in the case of a negative number, the minus sign (see Section 1.15).

As in most other programming languages the asterisk, or star, sign (`*`) is used for multiplication (see Section 1.5 below). In Python, the hash symbol (#) and everything that follows it in a same line are considered a comment, and are ignored in the program execution. A multiline comment is delimited by triple quotes

```
'''
this is a multiline
comment
'''
```

also triple double quotes `"""` work as comment delimiters.

1.4.2 Variable-Type Conversion

Sometimes it is necessary to perform conversions between the built-in variable types, in order to manipulate values in a different way. To convert between variable types you simply use the type name as a function. In addition, Python provides several built-in functions to perform special kinds of conversions. All of these functions return a new object representing the converted value. The most relevant examples follow.

Conversions between Integers and Floats

When you type a sequence of digit not containing a decimal point, Python interprets it as an integer. This will be often what you wish, but you might need your number stored in memory as a float. The conversion is achieved through the function `float()`, this is how it works

```
>>> x=35
>>> xf=float(x)
>>> print(x,xf)
35 35.0
```

here the variable `x` is stored in memory as an integer, `xf` as a float. Conversion from float to integer is achieved through the function `int()`

```
>>> y=48.9
>>> yi=int(y)
>>> print(y,yi)
48.9 48
```

note that this conversion does not round `y` to the nearest integer: the function `int()` simply cuts off the decimal point and the following digits. If what you want is *rounding to the nearest integer*, you can simply add 0.5 to the float

```
>>> yr=int(y+0.5)
>>> print(yr)
49
```

Remember that you must add −0.5 if the float to be rounded is negative.

```
>>> y=-15.8
>>> yr1=int(y+0.5)
>>> yr2=int(y-0.5)
>>> print(y,yr1,yr2)
-15.8 -15 -16
```

Conversions between Numbers and Strings

A string is a sequence of characters. Thus, for instance, the two consecutive characters `35` might be stored in the computer memory as an integer, as a float, or as a string comprising the two characters `'3'` and `'5'`. As we have seen above, the command `x=35` assigns the value 35 to the integer variable `x`. This can be converted to a string variable, say `xs`, by the `str()` function:

```
>>> x=35
>>> xs=str(x)
>>> xs
'35'
```

```
>>> print(xs)
35
```

note that, when you simply type `xs` in Python interactive mode, Python prints the string in quotes, while the string is printed without quotes by the command `print(xs)`. However, see the effect of the format type `r` on the `print()` function in Subsection 1.15.3. Converting an integer to a string can be useful, for instance, for counting its digits through the `len()` function

```
>>> x=23457439
>>> xs=str(x)
>>> print(len(xs))
8
```

Conversion of strings to integers is done by the `int()` function, from string to floats by the `float()` function, for instance

```
>>> xs='542'
>>> xi=int(xs)
>>> xf=float(xs)
>>> print(xs,xi,xf)
542 542 542.0
```

If a string contains a character that is not a digit, a decimal point, a leading minus or plus sign, or leading and/or trailing blanks, it cannot be converted into a number, and Python will report an error

```
>>> xs='543f'
>>> x=int(xs)
Traceback (most recent call last):
File "<stdin>", line 1, in <module>
ValueError: invalid literal for int() with base 10: '543f'
```

Here, and in following Python error messages, `File "<stdin>"` means that the error was found in the *standard input*, i.e., in what you typed from the computer keyboard. Analogously, `"<stdout>"` stands for *standard output* , which is the computer monitor.

1.5 Arithmetic Operators

The basic arithmetic operators that can be applied to numeric variables are

$+$	addition	$2.5 + 3.0 = 5.5$	$-$	subtraction	$2.5 - 3.0 = -0.5$
$*$	multiplication	$2.5 * 3.0 = 7.5$	/	division	$2.5/2 = 1.25$
//	floor division	$7//2 = 3;\ -7//2 = -4$	%	modulus	$11\%3 = 2$
$**$	exponentiation	$11 * *2 = 121$			

Note that the *floor* of -3.5 is -4, since $-4 < -3.5$.

1.6 Assignment operators

Apart from the already discussed = operator, other assignment operators are obtained by combining the basic arithmetic operators with the = operator as follows

`+=`	`c+=a`	is equivalent to	`c=c+a`	`-=`	`c-=a`	is equivalent to	`c=c-a`
`*=`	`c*=a`	is equivalent to	`c=c*a`	`/=`	`c/=a`	is equivalent to	`c=c/a`
`%=`	`c%=a`	is equivalent to	`c=c%a`	`**=`	`c**=a`	is equivalent to	`c=c**a`
`//=`	`c//=a`	is equivalent to	`c=c//a`				

For instance, you can type

```
>>> a=8
>>> b=3
>>> b+=a
>>> print(a,b)
8 11
>>>
```

1.7 Comparison and Logical Operators

The comparison operators are

>	greater than	<	less than	==	equal to
! =	not equal to	>=	greater than or equal to	<=	less than or equal to.

The result of a comparison is a Boolean value, denoted by either *True* or *False* in Python. For instance you can type

```
>>> print('10>15 is ',10>15)
10>15 is  False
```

Note that here the `print()` function has two arguments, the first being the string `'10>15 is '`, which is printed *as is*, the second being the expression `10>15`, without quotes, which is evaluated to *False* before being printed.

The logical operators are

`and`	True if both the operands are true
`or`	True if either of the operands is true
`not`	True if operand is false (complements the operand)

for instance

```
>>> x=10
>>> y=15
>>> z=20
>>> print('x==y is ',x==y)
x==y is  False
>>> print('not x==y is ',not x==y)
not x==y is  True
>>> print(x!=y and y!=z)
True
>>> print(x<y or y>z)
True
```

1.8 Python Packages and the `import` Statement

We have already met a few Python built-in functions, like `print()`, `int()`, `float()`, ..., that we can use as soon as we enter Python's interactive mode. Python comes with a huge number of such predefined function which, apart from saving us the time of writing the functions ourselves (see Section 2.2), have the further, important advantage that they are optimized and stored in machine language, so that they are executed much faster than user-defined code. This is one of the strengths of Python. The number of Python predefined functions is so large that it would not be convenient to have all of them always automatically accessible. The functions are thus grouped into separate *modules*, which, in turn, may be grouped into *packages*, and one must import them from their respective packages before use. This is done with the `import` statement. The packages from which we shall import functions more often are called `math` (mathematical functions), `numpy` (the *numerical* package), `scipy` (the *scientific* package), and `matplotlib` (the plotting package). Packages `scipy` and `matplotlib` are further divided into subpackages. As an example, suppose that you need the square root of 5. If, after entering the interactive mode, you simply type `sqrt(5)` you get an error message

```
>>> sqrt(5)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
NameError: name 'sqrt' is not defined
```

because the function `sqrt()` does not belong to the set of automatically available Python functions: you must import it from `math` (or from `numpy`) before use. For this you have the following three possibilities:

```
>>> import math as mt
>>> mt.sqrt(5)
2.23606797749979
```

here we have imported the whole `math` package under the name `mt`, and from now on we have access to all `math` functions by preceding their names with the prefix "`mt.`". Obviously you can replace the name `mt` with any name of your choice, provided you use it consistently in your following commands. After importing you can access any other `math` function, for instance you can type

```
>>> mt.cos(mt.pi)
-1.0
```

and get the cosine of π, `mt.pi` being the value of π stored in the `math` package (usually 3.141592653589793). Another import possibility is

```
>>> from math import sqrt
>>> sqrt(5)
2.23606797749979
>>> cos(pi)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
NameError: name 'cos' is not defined
>>>
```

here we have imported *only* the function `sqrt()` from `math`, and we can used it without prefix. All other `math` functions have not been imported, therefore, for instance, the function `cos()` is not defined. You can use this method to import as many functions as you wish simultaneously, for instance

```
>>> from math import sqrt,cos,sin
>>> print(sqrt(5),cos(0),sin(0.3))
2.2360679775 1.0 0.295520206661
```

Finally we can type

```
>>> from math import *
>>> sqrt(5)
2.2360679774997898
>>> cos(pi)
-1.0
```

where the asterisk (`*`) stands for "everything". This command imports everything from `math`, and gives us access to all `math` functions without prefixes. However, this method is discouraged because it can lead to name collisions if used for more packages in the same session, or if a predefined variable of the imported package has the same name as one of your variables. The functions defined in `math` are listed in Appendix A, as well as the packages of the cmath module, comprising the definitions of the complex functions.

Other packages, like `numpy` and `scipy`, comprise huge numbers of functions and definitions each, and we cannot list them all in the present book. You can easily find the complete lists on the internet. Remember that often the same function is defined in different packages.

1.9 Conditional Statements

The comparison and logical operators usually appear in *conditional statements*. Conditional statements are vital in any programming language: they are needed whenever, starting from a given point of the program, we must follow different algorithms depending on whether, at that point, a condition evaluates to *True* or *False*. Conditional statements are written through the `if`, `elif` and `else` statements, which operate as you would expect from their names, `elif` standing for *else if*. This is a simple example

```
>>> from math import sqrt
>>> x=-5
>>> if x>0:
...     print("x is positive")
...     print(sqrt(x))
... elif x<0:
...     print("x is negative")
...     print(sqrt(-x))
... else:
...     print("x is zero")
...     print(0)
...
x is negative
2.2360679775
>>>
```

Note that all conditional statements end with a colon "`:`", and that the lines to be executed if the condition is true (the *conditioned* commands) are indented by the same amount of space with respect to the conditional statement. You can use spaces or tabs for indentation, but you are advised not to mix them: use only tabs, or only spaces, according to your taste. Now to the code. At the first prompt we import the function `sqrt()` from the `math` package. At the second prompt we create a variable `x` to which we assign a negative value. Starting from the third prompt we build an `if-elif-else` sequence that determines what to do if `x` is greater than, smaller than, or equal to 0. If `x` is greater than zero the two indented lines following the condition "`if x>0:`" are executed, and the rest of the code is ignored. If `x` is *not* greater than zero, the `elif` (*else if*) condition is checked, and if the condition is met, the `elif` conditioned code (the two following lines, indented relative to the statement "`elif x<0:`") are executed, and the following code is skipped. If neither the `if` nor the `elif` conditions are met, the code conditioned by `else` is executed. In an `if, elif, else` sequence there may be only one `if` (and there *must* be one!), there may be any number of `elif` conditions (including zero), and only one, or zero final `else`.

1.10 Lists and Tuples

A *list* is a a set of values (items), which is written as a sequence of comma-separated items between square brackets. The items in a list need not be of the same type.

Creating a list can be done by typing different comma-separated values between square brackets. For example

```
>>> list1 = ['physics', 'chemistry', 1997, 2000]
>>> list2 = [1, 2, 3, 4, 5 ]
>>> list3 = ["a", "b", "c", "d"]
>>> print(list2 ,list3)
[1, 2, 3, 4, 5] ['a', 'b', 'c', 'd']
>>> print(list3[1])
b
>>> list2[3]=10
>>> print(list2)
{[1, 2, 3, 10, 5]}
>>> list2=['cat','platypus']
>>> print(list2[1])
platypus
>>>
```

Similar to string indices, list indices start at 0, and lists can be sliced, concatenated and so on. Single list elements are accessed by indexing, like `list2[3]` above.

A *tuple* is a sequence of immutable Python objects. Tuples are sequences, just like lists. The relevant difference between tuples and lists is that a tuple, and its elements, cannot be changed. Syntactically, a tuple is declared by typing its comma-separated items between parentheses (round brackets, which, however, are not mandatory in the declaration), whereas lists use square brackets (which are mandatory). Thus you can create a tuple simply by typing different comma-separated variables, within parentheses or not.

```
>>> tuple1=4,5,6
>>> tuple2=('meerkat','walrus','carpenter')
>>> print(tuple1)
(4, 5, 6)
>>> print(tuple2[0])
meerkat
>>> tuple2[2]='elephant'
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: 'tuple' object does not support item assignment
>>>
```

As stated above, changing a tuple is not allowed. However, it is possible to convert lists to tuples, and tuples to lists, analogously to what can be done between different number types or strings. For instance

```
>>> animals=list(tuple2)
>>> animals[2]='elephant'
>>> print(animals)
['meerkat', 'walrus', 'elephant']
>>>
```

here the elements of `tuple2` are copied into the list `animals`, which, being a list, is not immutable. If, eventually, we type

```
1 >>> tuple2=tuple(animals)
2 >>> tuple2
3 ('meerkat', 'walrus', 'elephant')
4 >>>
```

we see that, apparently, we have changed the tuple! Actually, Line 1 has destroyed the original tuple and created a new one with the same name, comprising the elements of the list `animals`.

1.11 List Methods

Python *methods* are functions that belong to Python objects. In Chapter 8 we shall meet methods belonging to instances of a *class*, here we consider methods belonging to list instances. Python includes the following *list methods*, that can change list instances (lists)

`append()`	`index()`	`remove()`
`count()`	`insert()`	`reverse()`
`extend()`	`pop()`	`sort()`

All above methods do what you can expect from their names, here are examples of how they operate

```
>>> animals=["cat","dog","goose"]
>>> animals.append("meerkat")
>>> animals
['cat', 'dog', 'goose', 'meerkat']
>>> animals.count("goose")
1
>>> animals.insert(2,"duck")
>>> animals
['cat', 'dog', 'duck', 'goose', 'meerkat']
>>> animals.insert(0,"bear")
>>> animals
['bear', 'cat', 'dog', 'duck', 'goose', 'meerkat']
>>> animals.index('dog')
2
>>> animals.index("snail")
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
```

```
ValueError: 'snail' is not in list
>>> popped=animals.pop()
>>> popped
'meerkat'
>>> animals
['bear', 'cat', 'dog', 'duck', 'goose']
>>>animals.reverse()
>>> animals
['goose', 'duck', 'dog', 'cat', 'bear']
>>> animals2=["meerkat","elephant","penguin"]
>>> animals.extend(animals2)
>>> animals
['goose', 'duck', 'dog', 'cat', 'bear', 'meerkat', 'elephant',\
'penguin']
>>> animals.sort()
>>> animals
['bear', 'cat', 'dog', 'duck', 'elephant', 'goose', 'meerkat',\
'penguin']
>>>
```

Method `append()` appends a new element at the end of the list, `count()` returns the number of times the argument occurs in the list, `extend()` appends another list at the end of the list, `index(obj)` returns the lowest index of `obj` in the list (remember that indices start from 0), `insert(index,obj)` inserts `obj` at position `index`, `pop()` returns the last item of the list and erases it from the list, `remove(obj)` removes `obj` from the list, `reverse()` reverses the list order and `sort()` sorts the list elements.

1.12 Lists and the = Assignment Operator

1.12.1 Copying Lists

Some care must be taken when using the = assignment operator with lists:

```
>>> a=[3,4,5,6]
>>> print(a)
[3, 4, 5, 6]
>>> b=a
>>> print(b)
[3, 4, 5, 6]
>>> a[0]=127
print('a=',a,'b=',b)
a= [127, 4, 5, 6] b= [127, 4, 5, 6]
>>>
```

The first statement creates a list comprising the numbers 3, 4, 5 and 6 as elements, and the variable `a` points to it. The statement `b=a` makes `b` point to exactly the same memory location as `a`. Thus, when the first element of the list is changed by the statement `a[0]=127`, the change affects both `a` and `b`. If you want to handle two independent lists, you must proceed this way

```
>>> a=[3,4,5,6]
>>> b=a.copy()
>>> a[0]=127
>>> print('a=',a,'b=',b)
a= [127, 4, 5, 6] b= [3, 4, 5, 6]
```

The method `.copy()` makes `b` point to an independent list, initially identical to the list pointed to by `a`, but any subsequent change to `a` does not affect `b`, and vice versa. Another possibility is

```
a=[3,4,5,6]
>>> b=a[:]
>>> a[0]=10
>>> print('a=',a,'b=',b)
a= [10, 4, 5, 6] b= [3, 4, 5, 6]
>>>
```

When in doubt, you can use the `id()` function, which returns the "identity" of its argument. An object identity is an integer unique for the given object, which remains constant during the object lifetime

```
>>> a=[3,4,5,6]
>>> b=a
>>> c=a.copy()
>>> print(id(a),id(b),id(c))
140402853321544 140402853321544 140402912014856
>>>
```

As stated above, the statement `b=a` makes `b` point to the same memory location as `a`, thus `b` and `a` have the same *identity*, while `c` points to an independent copy of `a`, thus its *identity* is different.

1.12.2 Copying the Elements of Lists and Tuples

It is possible to use the = assignment operator to copy the values of the elements of lists and tuples to separate variables in a single command. For instance, if you type

```
>>> a=[10,20,30]
>>> x1,x2,x3=a
>>> print(x2)
20
>>>
```

the variables `x1`, `x2` and `x3` are assigned the values of the three elements of the list `a`. The number of comma-separated values on the left-hand side **must** equal the number of elements of the list, or tuple, on the right-hand side, otherwise Python will report an error

```
>>> x4,x5=a
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: too many values to unpack (expected 2)
>>>
```

As we know from Section1.10, the use of parentheses is optional when assigning a tuple. Thus in the following code

```
>>> x1,x2,x3=15,'walrus',25
>>> print(x1,x2,x3)
15 walrus 25
%>>>
```

the first command can be considered both as a tuple unpacking or as a multiple assignment.

A list can comprise any number of elements, including 0 (empty list) and 1 (single-element list). Some care must be taken when unpacking a single-element list:

```
1 >>> a=[15]
2 >>> b=a
3 >>> c,=a
4 >>> print(b)
5 [15]
6 >>> print(c)
7 15
8 >>>
```

The first command creates the list a, comprising the single element 15. The command b=a does not copy the single element of a to a single variable b, rather, it makes b point to the same memory location as a, as we saw in Subsection 1.12.1. In order to copy the only element of a into a variable c we need the command at Line 3, c,=a. The comma after c tells Python that we are extracting the elements of the list a, the absence of further variables after the comma tells that the list comprises a single element.

1.13 Slicing Lists and Strings

When you have a list, a tuple or an array it is possible to extract or modify specific sets of sub-elements without recurring to the loops that we shall encounter in Section 1.16. For instance, consider the list

```
a=[0,1,2,3,4,5,6,7,8,9,10,11,12]
```

and assume that you need a list b comprising the first 6 elements of a. This is how to do it in Python

```
>>> b=a[:6]
>>> b
[0, 1, 2, 3, 4, 5]
>>>
```

this command generates a new list b comprising a *slice* of a containing its first 6 elements. You can also type

```
>>> c=a[3:8]
>>> c
[3, 4, 5, 6, 7]
>>> d=a[4:]
>>> d
[4, 5, 6, 7, 8, 9, 10, 11, 12]
>>>
```

copying into c the *slice* of a from element number 3 (remember that the first element of the list is element number 0) up to, but not including, element number 8. For d we obtain the slice of the elements from the fifth (labeled by number 4) to the end. The lower and upper limits of the slice are separated by a colon inside the square brackets. The default values are 0 for the lower limit, and the whole list for the upper limit. Thus, b=a[:] copies the whole list a into b, as seen at the end of Section 1.12. Slicing can use a third argument (separated by a second colon), corresponding to a *step*. For instance

```
>>> a[::3]
[0, 3, 6, 9, 12]
>>>
```

here we have simply printed out the result, without storing it in a new variable. What we have got is a sublist of every third element of the list, starting from element 0 up to the last element. We can also use all the three arguments, for instance if we type

```
>>> a[1:11:2]
[1, 3, 5, 7, 9]
>>>
```

we select every second element (the third slicing argument is 2) starting from element number 1 (the second element of the list, specified by the first slicing argument), up to, but not including element number 11, specified by the second slicing argument.

Slicing of strings is perfectly analogous to slicing of lists:

```
>>> str='once upon a time'
>>> str[5:9]
'upon'
>>> str[::2]
'oc pnatm'
>>> str[::-1]
'emit a nopu ecno'
>>>
```

In the last case a negative step means going backwards, considering the string (or the list) as extended cyclically, and what we get is the string in reverse order.

Slicing can also be used to modify selected elements of lists. For instance, if we type

```
>>> thislist=[3,6,9,12,15,18,21]
>>> thislist[::3]=[24,96,168]
>>> thislist
[24, 6, 9, 96, 15, 18, 168]
>>>
```

every third element of `thislist` has been replaced by an element of the list `[24,96,68]`. It is important that the number of elements selected by slicing the list on the left hand side must exactly match the number of elements of the list at the right, otherwise Python reports an error

```
>>> thislist[::3]=[3,12,21,85]
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: attempt to assign sequence of size 4 to extended slice\
of size 3
>>>
```

1.14 Dictionaries

A Python dictionary is an unordered collection of items. Each dictionary item is a pair consisting of a *key* and a *value*, with the requirement that the keys must be unique within one dictionary. The key and value of a dictionary item are separated by a colon (`:`), different items (different pairs) are separated by commas. A dictionary is created by writing its items within braces

```
>>> MyDict={'gatto':'cat','cane':'dog','ornitorinco':'platypus'}
>>> print(MyDict['cane'])
dog
>>>
```

a value of the dictionary `MyDict` can be retrieved by indexing `MyDict` with the corresponding key in square brackets. An alternative way of creating a dictionary is through the `dict()` function. For instance:

```
>>> MyOtherDict=dict(Katze='cat',Hund='dog',Schnabeltier='platypus')
>>> MyOtherDict
{'Katze': 'cat', 'Hund': 'dog', 'Schnabeltier': 'platypus'}
>>> print(MyOtherDict['Katze'])
'cat'
>>>
```

In this case the arguments of the `dict()` function are written within parentheses, as usual for functions. Keys are not written within quotes, each *key* is separated by the corresponding *value* by an equal sign (=) rather than by a colon (:).

A new dictionary item is added by simply assigning it

```
>>> MyDict['ape']='bee'
>>> print(MyDict)
{'ape': 'bee', 'ornitorinco': 'platypus', 'cane': 'dog',\
'gatto': 'cat'}
>>>
```

A dictionary item can be removed with the `del` statement

```
>>> del MyDict['ornitorinco']
>>> print(MyDict)
{'ape': 'bee', 'cane': 'dog', 'gatto': 'cat'}
>>>
```

you can modify an existing item by reassigning it

```
>>> MyDict['cane']='hound'
>>> print(MyDict)
{'ape': 'bee', 'cane': 'hound', 'gatto': 'cat'}
>>>
```

Dictionary values have no restrictions: a dictionary item can be any arbitrary Python object, either a standard object or a user-defined object. However, the same is not true for the keys: duplicate keys are not allowed, and keys are immutable. This means that you can use strings, numbers or tuples as dictionary keys, but not, for instance, lists.

1.15 The `print()` Function and Formatting

We have already met the `print()` function with single and multiple arguments of different types (integer and float numbers, strings, lists, ...) in the previous sections of this chapter. Its purpose is to print its arguments on the terminal. Note that in interactive mode the value of any variable can also be printed by simply typing its name at the Python prompt, as we have seen in many previous examples. Here follows an example of the use of the `print()` function

```
>>> animal='platypus'
>>> num=4.5
>>> print(animal,num,27,4/3)
platypus 4.5 27 1.3333333333333333
>>>
```

Often we need a more refined way of printing, which, for instance, allows us to control the number of digits printed after the decimal point for a float number like 4/3. Or we might want to align the decimal points of numbers printed in successive lines. All this, and more, is achieved through *formatted printing*. For this Python offers two possibilities.

1.15.1 Old Style

The old style format is very similar to the C/C++ format, for instance:

```
>>> from math import sqrt
>>> num=15/7
>>> print('the square root of %.5f is %.5f'%(num,sqrt(num)))
the square root of 2.14286 is 1.46385
>>>
```

The string `'the square root of %.5f is %.5f'` appearing as argument of the `print()` function at the third line is a *format string*. A format string, written within quotes like all strings, is printed by the `print()` function on the terminal as is, character by character, except for the *placeholders* it may contain. Placeholders are substrings beginning with the `%` character, here we have two of them, both in the form `%.5f`. The format string is followed by a *string modulo operator*, represented by a `%` character, which couples the format string to a following tuple. The tuple, `(num,sqrt(num))` in our case, comprises the values to be inserted at the locations of the placeholders. Thus, the number of elements of the tuple must equal the number of placeholders in the format string. The general syntax for a placeholder is

`%[flags][width][.precision]type`

The parts within square brackets are optional, while the leading `%` and the type are mandatory. In the case of `%.5f` neither *flags* nor *width* are given, while the *precision*, `.5`, requires 5 digits after the decimal point. The *type* `f` indicates that the tuple elements to be printed are float numbers. The following lines show how formatted printing can be used for aligning numbers of successive lines

```
>>> print("%5d%10.5f\n%5d%10.5f"%(11,sqrt(11),1525,sqrt(1525)))
   11   3.31662
 1525  39.05125
>>>
```

here the placeholder `%5d` requires 5 characters of width for an integer number (*type* `d`), while the placeholder `%10.5f` requires a *width* of 10 characters (characters include the decimal point, and, for a negative number, the minus sign), with 5 digits after the decimal point (*precision*) for a float number (type `f`). When the width is specified, the numbers are right-justified within the reserved space (10 characters in the case of `%10.5f`), with trailing blanks added at the left in order to complete the width. The newline code `\n` in the format inserts a *new line* command, thus splitting the output into two consecutive lines.

1.15.2 New Style

Also the new-style format makes use of a format string as argument of the `print()` function. But the format string is not coupled to a tuple of variables via the string modulo operator. Rather, the `.format()` method (we recall that a Python *method* is a function belonging to the object preceding the dot) is applied to the format string. The format string still has placeholders for the variables to be inserted. The syntax of the placeholders is similar to the old-style syntax, but the percent character, `%`, is replaced by a colon character, `:`, and placeholders are written within braces. This is an example

```
>>> x=1525
>>> print("the square root of {:5d} is {:10.5f}".format(x,sqrt(x)))
the square root of 1525 is   39.05125
>>>
```

The new-style allows us to use optional positional parameters before the colons in the placeholders, so that the format arguments can be written in any order

```
>>> x=1525
>>> print("the square root of {a:5d} is {b:10.5f}".format(b=sqrt(x),a=x))
the square root of 1525 is   39.05125
```

where `a` and `b` are positional parameters. Any number of positional parameters is allowed. Positional parameters also make multiple use of a single variable possible:

```
>>> print("{k:.2f}, or, more precisely, {k:.10f}".format(k=17/13))
1.31, or, more precisely, 1.3076923077
```

1.15.3 Format Types and Flags

These are the meanings of the conversion types appearing in the format placeholders

`d`	signed integer decimal	`f`	floating point decimal format
`i`	signed integer decimal	`F`	floating point decimal format
`o`	unsigned octal	`g`	same as `e` or `f`, see below
`x`	unsigned hexadecimal (lower case)	`G`	same as `E` or `F`, see below
`X`	unsigned hexadecimal (upper case)	`c`	single character
`e`	floating point exponential (lower case)	`r`	string
`E`	floating point exponential (upper case)	`s`	string

Types `d`, `i`, `o`, `x` and `X` refer to integer numbers. Types `d` and `i` print signed integers in decimal format, and are fully equivalent. Type `o` prints unsigned integers in octal format, while types `x` and `X` print unsigned numbers in hexadecimal format, `x` prints the hexadecimal digits A-F in lower case, `X` prints the same hexadecimal digits in upper case. This is an example

```
>>> print("{a:d}  {a:o}  {a:x}  {a:X}".format(a=254))
254  376  fe  FE
>>>
```

Note that $3 \times 8^2 + 7 \times 8 + 6 = 254$, and $15 \times 16 + 14 = 254$. Types `e`, `E`, `f`, `F`, `g` and `G` are for float numbers. A placeholder `{:w.pe}`, or `{:w.pE}`, `w` being the required *width* and `p` the required *precision*, causes the corresponding number to be printed in *scientific notation* , i.e., in the form $x \times 10^n$, where n is an integer, and x is a real number such that $1 \leqslant |x| < 10$. A placeholder `{:w.pf}` prints the number in normal float representation. For instance

```
>>> print("{b:10.4f}␣{b:10.4e}␣{b:10.4E}".format(b=1527.42))
 1527.4200 1.5274e+03 1.5274E+03
>>>
```

The width includes the characters needed for the decimal point, the minus sign if the number is negative, and, in the case of scientific notation, also the exponent. The only difference between `e` and `E` types is the case of the letter `e` (`E`). There is no difference between `f` and `F`. Type `g` (`G`) is equivalent to type `e` (`E`) if the exponent is greater than −4 or less than *p*, equivalent to `f` (`F`) otherwise. See the following two examples

```
>>> print("{a:15.5f}{a:15.5e}{a:15.5g}".format(a=5000/3))
     1666.66667    1.66667e+03         1666.7
>>> print("{a:15.5f}\{a:15.5e}{a:15.5g}".format(a=5e-5/3))
        0.00002    1.66667e-05     1.6667e-05
>>>
```

Type `c` prints a single character, and accepts an integer (ASCII or UTF-8 character encoding) as format argument

```
>>> for i in range(65,70):print("{:c}".format(i))
...
A
B
C
D
E
>>>
```

Here we have used a `for` loop, to be discussed in Section 1.16. Types `r` and `s` refer to strings.

```
>>> print("{:s}".format("Have␣a␣good␣day!"))
Have a good day!
>>> print("{!r}".format("Have␣a␣good␣day!"))
'Have␣a␣good␣day!'
>>>
```

Note that the string is printed within quotes if you use the `r` code, and that the `r` code must be preceded by an exclamation mark, `!`, rather than by a colon, `:`.

1.16 Loops

Loops are extremely important in computer programming. Python has two types of loops: the `for` and the `while` loop.

1.16.1 The `for` Loop

It is important to realize that the Python `for` loop behaves differently from the `for` loop of other programming languages, notably C/C++. For using the Python `for` loop you must first have a sequence of elements, for instance a list or a tuple, and the `for` loop iterates over the elements of the sequence. This is an example

```
>>> flowers=["rose","cyclamen","daisy","tulip"]
>>> for x in flowers:
```

```
...         print(x)
...
rose
cyclamen
daisy
tulip
>>> from math import sqrt
>>> numbers=[533,712,925]
>>> for x in numbers:
...         print("{:10.4f}".format(sqrt(x)))
...         print("this␣was␣the␣square␣root␣of␣{:10.4f}".format(x))\
...
   23.0868
this was the square root of   533.0000
   26.6833
this was the square root of   712.0000
   30.4138
this was the square root of   925.0000
>>>
```

The declaration of a `for` loop must terminate with a colon (`:`), and all commands of the loop must be indented, for instance by a `tab`, or by an arbitrary, but fixed number of spaces, relatively to the line of the loop declaration. In interactive mode, the command sequence of a `for` loop (or of a `while` loop) is terminated by typing an unindented empty line. The iteration sequence of a `for` loop can be provided by the `range()` function, which accepts up to three arguments

```
>>> for x in range(5):
...         print(x)
...
0
1
2
3
4
>>> for x in range(6,10):
...         print(x)
...
6
7
8
9
>>> for x in range(6,12,3):
...         print(x)
...
6
9
>>>
```

Note that the `range()` function is zero-based, thus, `range(5)` generates the list of the first 5 integer numbers $[0, 1, \ldots 4]$, while the expression `range(`n_1`,`n_2`)` generates the list of the $n_2 - n_1$ integers $[n_1, n_1 + 1, \ldots, n_2 - 1]$. Finally, in the case of three arguments, `range(`n_1`,`n_2`,`n_3`)`, the third argument is interpreted as the constant spacing between successive numbers of the list. The last number of the list is the highest number smaller than n_2. This behavior is anologous to the behavior of slicing that we met in Section 1.13

It is also important to remember that the `range()` function is *not* part of the `for` syntax. Rather, `range()` is a built-in Python function that creates a number list. The number list is created *before* the loop is executed, and it cannot be changed during the loop execution. Thus, for instance, if you type

```
>>> a=3
>>> for i in range(a):
...         print(i)
...         if i==0:
...         a=10
...
0
1
2
>>> print(a)
10
>>>
```

the loop iterates over the list `[0,1,2]` in spite of the fact that the value of `a` is changed at the first iteration. However, the `for` loop can be interrupted by a `break` statement, as discussed in Subsection 1.16.3 below.

Another important built-in Python function, particularly useful when associated to a `for` loop, is `enumerate()`. It allows us to loop over a sequence and have a simultaneous automatic counter. Here is an example of its use

```
>>> flowers=[rose,cyclamen,daisy,tulip]
>>> for i,x in enumerate(flowers):
...     print(i,x)
...
0 rose
1 cyclamen
2 daisy
3 tulip
>>>
```

It is also possible to have the counter starting from any given integer value, by adding an optional argument to `enumerate()`

```
>>> for i,x in enumerate(flowers,15):
...     print(i,x)
...
15 rose
16 cyclamen
17 daisy
18 tulip
>>>
```

Obviously, variables `i` and `x` are available for any possible use in the loop commands.

1.16.2 The `while` Loop

A `while` loop iterates as long as a specified Boolean condition is true. For example:

```
>>> i=5
>>> while i<=8:
...     print(i)
...     i+=1
...
5
6
7
8
>>>
```

Here the variable `i` is set equal to 5 before the loop begins. The loop is iterated till *i* is smaller than, or equal to 8, each iteration prints the value of `i`, then increments it by 1.

1.16.3 Breaking a Loop

A loop can be interrupted by a `break` statement. For instance, we might write for a `for` loop

```
>>> for j in range(10):
...     if j>3:
...         break
...     print(j)
...
0
1
2
3
>>>
```

The `break` is executed when the condition `j>3` is met. Note the double indentation before the `break` command: an indentation relative to the loop, plus an indentation relative to the `if` statement. The `print(j)` line has a single indentation, since it is part of the loop, but it is not conditioned by the `if` statement.

The `break` statement has an interesting application in the `while` loop:

```
>>> count=0
>>> while True:
...     print(count)
...     count+=1
...     if count>2:
...         break
...
0
1
2
>>>
```

Here the Boolean condition for the `while` loop is always true by definition, being the Boolean constant *True* itself. Thus, the loop would go on forever if it did not contain the `break` condition.

1.16.4 The `continue` Statement

The `continue` statement is used to skip the part of the loop (either `for` or `while`) that follows it, without interrupting the loop itself, but passing to the following iteration. For instance, the following code skips all odd numbers, printing only the even ones

```
>>> for i in range(5):
...     if i%2>0:
...         continue
...     print(i)
...
0
2
4
```

If the condition `i%2>0` is met, i.e., if the remainder of the division of `i` by 2 is greater than zero (`i` is odd), the print function is skipped, and the next iteration is started.

1.17 Operations with Matrices and Vectors

1.17.1 Lists and Arrays

In a sense, a vector is a list of numbers, and a matrix is a list of lists of numbers, so, we can write

```
>>> v1=[1,2,3]
>>> v2=[4,5,6]
>>> a1=[[1,2,3],[4,5,6],[7,8,9]]
>>> a2=[[9,8,7],[6,5,4],[3,2,1]]
>>> print(v1)
[1, 2, 3]
>>> print(a1)
[[1, 2, 3], [4, 5, 6], [7, 8, 9]]
```

However, we get a surprise if we add two *such* vectors, or two *such* matrices,

```
>>> print(v1+v2)
[1, 2, 3, 4, 5, 6]
>>> print(a1+a2)
[[1, 2, 3], [4, 5, 6], [7, 8, 9], [9, 8, 7], [6, 5, 4], [3, 2, 1]]
```

the surprise being due to the fact that, when two Python *lists* are added, the result is a new list comprising the elements of both lists. If we want the usual mathematical operations on matrices and vectors, we need `numpy.array` objects instead of lists. Thus, first we must import `numpy`, then declare vectors and matrices as `numpy.arrays`

```
>>> import numpy as np
>>> v1=np.array([1,2,3])
>>> v2=np.array([4,5,6])
>>> a1=np.array([[1,2,3],[4,5,6],[7,8,9]])
>>> a2=np.array([[9,8,7],[6,5,4],[3,3,1]])
>>> print(a1)
[[1 2 3]
 [4 5 6]
 [7 8 9]]
>>> a1
array([[1, 2, 3],
       [4, 5, 6],
       [7, 8, 9]])
>>> print(v1+v2)
```

```
[5 7 9]
>>> print(a1+a2)
[[10 10 10]
 [10 10 10]
 [10 11 10]]
>>> print(a1+v1)
[[2 4 6]
 [5 7 9]
 [8 10 12]]
```

Note the output difference after typing `print(a1)` and simply typing `a1`: in the latter case, the word `array()` appears, and commas are printed between row elements. Adding two arrays leads to the expected result if the two arrays have the same dimensions. However it is possible to add a matrix and a vector, an operation not allowed in usual matrix algebra, provided that the number of columns of the matrix equals the number of elements of the vector. The vector elements are added to the corresponding elements of each matrix row.

This is a first step into matrix algebra, but we still get a surprise if we multiply two arrays by using the usual `*` multiplication operator, met in Section 1.5

```
>>> print(v1*v2)
[ 4 10 18]
>>> print(a1*a2)
[[ 9 16 21]
 [24 25 24]
 [21 24  9]]
>>> print(a1*v1)
[[ 1  4  9]
 [ 4 10 18]
 [ 7 16 27]]
```

what we get is actually an *element by element multiplication* (sometimes called *Hadamard product*), as shown above. Note that the `*` multiplication of a matrix by a vector multiplies the elements of each row of the matrix by the corresponding elements of the vector. It is also possible to obtain a Hadamard element by element division, using either the / operator or the `numpy.divide()` function

```
>>> np.divide(v1,v2)
array([ 0.25,  0.4 ,  0.5 ])
>>> print(v1/v2)
[ 0.25  0.4   0.5]
```

Note that the `numpy` package contains also many mathematical functions, sharing the names with the `math` functions. If you apply these `numpy` functions to *scalar* quantities, their behavior is analogous to the behavior of their `math` counterparts, with a possible difference in precision

```
>>> import numpy as np
>>> import math as mt
>>> print(mt.sqrt(5),np.sqrt(5))
2.23606797749979 2.2360679775
>>> print(mt.sin(mt.pi/4),np.sin(np.pi/4))
0.7071067811865475 0.707106781187
```

But there is an important difference: the `numpy` mathematical functions can take *arrays*, or lists, as arguments , while the `math` functions can't,

```
>>> a=[5,6,7,8]
>>> np.sqrt(a)
array([ 2.23606798,  2.44948974,  2.64575131,  2.82842712])
>>> mt.sqrt(a)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: must be real number, not list
```

We shall see the importance of the `numpy` mathematical functions in Chapter 3, where we shall discuss how to plot functions. As an example, consider the following commands

```
>>> import numpy as np
>>> x=np.arange(0,3.6,0.5)
>>> x
array([ 0. ,  0.5,  1. ,  1.5,  2. ,  2.5,  3., 3.5 ])
>>> y=np.sin(x)
>>> y
array([ 0.        ,  0.47942554,  0.84147098,  0.99749499,  0.90929743,\
        0.59847214,  0.14112001, -0.35078323])
```

Command `x=np.arange(0,3.6,0.5)` generates an array `x` of floats ranging from 0.0 to 3.5, which we could use as abscissae of a plot. Command `y=np.sin(x)` generates an array `y` such that each of its elements is the sine of the corresponding element of `x`. Thus, the elements of `y` can be used as ordinates of our plot.

1.17.2 Slicing out Rows and Columns from a Matrix

Slicing out a row from a matrix is obvious:

```
>>> a1=np.array([[1,2,3],[4,5,6],[7,8,9]])
>>> a1
array([[1, 2, 3],
       [4, 5, 6],
       [7, 8, 9]])
>>> row0=a1[0]
>>> row0
array([1, 2, 3])
>>> row1=a1[1]
>>> row1
array([4, 5, 6])
```

Slicing out a column is slightly less obvious:

```
>>> column0=a1[:,0]
>>> column0
array([1, 4, 7])
>>> column2=a1[:,2]
>>> column2
array([3, 6, 9])
```

note the comma before the index.

1.17.3 Arrays and Matrix Arithmetics

If what we want is the usual row-by-column matrix multiplication we must use the `numpy.dot()` function, which performs the scalar (or *dot*) product of two arrays. A few examples follow

```
>>> c=np.dot(v1,v2)
>>> print(c)
32
>>> a3=np.dot(a1,a2)
>>> print(a3)
[[ 30  27  18]
 [ 84  75  54]
 [138 123  90]]
>>> v3=np.dot(a1,v1)
>>> print(v3)
[14 32 50]
>>> v4=np.dot(v1,a1)
>>> print(v4)
[30 36 42]
```

Once we have an array `a` we can use the function `numpy.tile()` to obtain a new array by repeating `a` a given number of times

```
>>> from numpy import tile
>>> a=[1,2,3,4]
>>> b=tile(a,3)
>>> b
array([ 1,  2,  3,  4,  1,  2,  3,  4,  1,  2,  3,  4])
>>> c=[[1,2],[3,4]]
>>> d=tile(c,3)
>>> d
array([[1, 2, 1, 2, 1, 2],
       [3, 4, 3, 4, 3, 4]])
```

the second argument of `tile()` giving the number of repetitions. Note that we built `a` and `c` as *lists*, but `b` and `d` are *arrays*. We can obtain a matrix from a vector, or, more generally, a final array of higher dimension than the start array, by using a tuple as second argument of `tile()`:

```
>>> c=tile(a,(len(a),1))
>>> c
array([[ 1,  2,  3,  4],
       [ 1,  2,  3,  4],
       [ 1,  2,  3,  4],
       [ 1,  2,  3,  4]])
```

the first item of the tuple `(len(a),1)` telling how many rows the matrix will have (here we are generating a square matrix), and the second how many times the array `a` is repeated in each row, here only once.

1.17.4 Further Matrix Operations

Transpose

We can transpose a matrix by using the `.transpose()` method:

```
d=c.transpose()
>>> d
array([[ 1,  1,  1,  1],
              [ 2,  2,  2,  2],
              [ 3,  3,  3,  3],
              [ 4,  4,  4,  4]])
```

The same result can be obtained by typing

```
>>> d=c.T
```

the `.T` operator being a shorthand for the `.transpose()` operator. Finally, we can generate a symmetric matrix `e` by typing, for instance

```
>>> e=d*a
>>> e
array([[ 1,  2,  3,  4],
       [ 2,  4,  6,  8],
       [ 3,  6,  9, 12],
       [ 4,  8, 12, 16]])
```

where $e_{ij} = a_i a_j$, since the `*` product multiplies each element of each row of `d` by the corresponding element of `a`, as discussed in Subsection 1.17.1. Analogously, we can generate a skew-symmetric matrix `f` by typing, for instance

```
>>> f=d-a
>>> f
array([[ 0, -1, -2, -3],
       [ 1,  0, -1, -2],
       [ 2,  1,  0, -1],
       [ 3,  2,  1,  0]])
```

where $f_{ij} = a_i - a_j$, since the `-` operator subtracts the elements of `a` from the corresponding elements of each row of `d`. Obviously, all the above operations can be obtained also by using nested `for` or `while` loops. For instance, our skew-symmetric matrix can be generated by the nested loops

```
>>> d=np.empty([len(a),len(a)])
>>> for i in range(len(a)):
...     for j in range(len(a)):
...         d[i,j]=a[i]-a[j]
...
```

where the `numpy.empty()` function returns a new array of given dimensions, without initializing the entries. Note that the function `numpy.empty()` has a single argument, which must be a tuple if a multidimensional array is needed. The matrix elements are then initialized by the nested loops. A more efficient way of writing the nested loops could be

```
>>> d=np.zeros([len(a),len(a)])
>>> i=0
>>> while i<len(a):
...     j=0
...     while j<i:
...         d[i,j]=a[i]-a[j]
...         d[j,i]=-d[i,j]
...         j+=1
...     i+=1
...
```

where the function `numpy.zeros()` returns a new array of given dimensions whose elements are all zero. As for function `numpy.empty()`, the single argument of `numpy.zeros()` must be a tuple if what we want is a multidimensional array. The skew symmetry of the matrix is exploited in order to skip the calculation of the diagonal elements and not to repeat the off-diagonal calculations twice. However, it is important to remember that Python array-manipulation functions are pre-compiled and optimized, thus they run much faster than the loops that a user can write in Python.

Sum the Elements over a Given Axis

Function `numpy.sum()` sums the elements of an array over a given axis.

```
>>> a=np.array([[1,2,3],[4,5,6],[7,8,9]])
>>> a
array([[1, 2, 3],
       [4, 5, 6],
       [7, 8, 9]])
>>> np.sum(a,axis=0)
array([12, 15, 18])
>>> np.sum(a,axis=1)
array([ 6, 15, 24])
```

axis 0 is the horizontal axis, parallel to the matrix rows, and axis 1 is the vertical axis, parallel to the matrix columns. Note that the argument `axis=0` in the `sum()` function indicates that columns are added, leaving a single, collapsed row. This can seem misleading when working with two-dimensional arrays (matrices), since `axis=0` means that sums are performed column-wise. However, this is the most straightforward definition when working with three- or higher-dimensional arrays.

Trace

The *trace* of a matrix is calculated by the `numpy.trace()` operator

```
>>> np.trace(a)
15
>>>
```

Determinant and Inverse

The *determinant* of a matrix is calculated by the `numpy.linalg.det()` operator, while the *inverse* of a matrix is evaluated by the `numpy.linalg.inv()` function

```
>>> a=np.array([[1,3,3],[3,2,1],[18,16,14]])
>>> a
array([[ 1,  3,  3],
       [ 3,  2,  1],
       [18, 16, 14]])
>>> np.linalg.det(a)
-23.999999999999993
>>> b=np.linalg.inv(a)
>>> b
array([[-0.5       , -0.25      ,  0.125     ],
       [ 1.        ,  1.66666667, -0.33333333],
       [-0.5       , -1.58333333,  0.29166667]])
>>> np.dot(a,b)
```

```
array([[  1.00000000e+00,   8.88178420e-16,   0.00000000e+00],
       [  0.00000000e+00,   1.00000000e+00,   5.55111512e-17],
       [  0.00000000e+00,   0.00000000e+00,   1.00000000e+00]])
>>>
```

Note the effects of rounding.

Diagonalization

The diagonalization of a matrix can be performed by the function `numpy.linalg.eig()`, which returns a tuple consisting of a vector and an array. The vector contains the eigenvalues in arbitrary order, while the array contains the corresponding eigenvectors, organized in a matrix, one eigenvector per column. The eigenvectors are normalized so their Euclidean norms are 1. An example of the use of `numpy.linalg.eig()` follows

```
1  >>> import numpy as np
2  >>> a=np.array([[1,2,3,4],[2,2,4,8],[3,4,5,6],[4,9,6,8]])
3  >>> a
4  array([[1, 2, 3, 4],
5         [2, 2, 4, 8],
6         [3, 4, 5, 6],
7         [4, 9, 6, 8]])
8  >>> eigval,eigvec=np.linalg.eig(a)
9  >>> eigval
10 array([19.53241835, -4.10596077, -0.56799313,  1.14153556])
11 >>> eigvec
12 array([[ 0.27701336,  0.18643609, -0.90273601, -0.26017229],
13        [ 0.45869181,  0.75119053,  0.15881403,  0.32137161],
14        [ 0.47236893,  0.02548963,  0.39903646, -0.80179608],
15        [ 0.69980927, -0.63269633, -0.0248134 ,  0.43145535]])
16 >>> np.dot(a,eigvec[:,0])
17 array([ 5.41074085,  8.95936022,  9.22650759, 13.66896747])
18 >>>
```

In the above example, Line 8 unpacks the output of `numpy.linalg.eig()`, storing the eigenvalues of the matrix `a` defined at Line 2 in the array `eigval`, and the eignevectors in the array `eigvec`. Line 16 multiplies matrix `a` by its first eigenvector (the first column of `eigvec`), sliced out of `eigvec`, see Section 1.13 on slicing. The result shown in Line 17 is the first eigenvector itself multiplied by the first eigenvalue (19.53241835). We can check this by typing the command

```
>>> np.dot(eigvec[:,0],eigval[0])
array([ 5.41074086,  8.95936024,  9.2265076 , 13.66896746])
```

which multiplies the first eigenvector by the first eigenvalue.

1.18 Exiting Interactive Mode

We exit from the Python interactive mode by typing either `quit()` (the parentheses are mandatory, in order to tell the interpreter that we are referring to a function), or Ctrl-D at the Pythonprompt.

Chapter 2

Python Scripts

2.1 Scripts

A Python script is an ASCII file containing your Python code, that you can write with your favorite text editor (provided that you use it in plain text mode) and store in the computer memory. Python reads the file as a whole, and then executes its commands, rather than reading and executing the lines you type one by one, as it does when you work in interactive mode. Scripts have some important advantages over the interactive mode: for instance you do not have to retype a long code that you use in separate work sessions, and you can easily change a line of code without retyping all the rest. It is customary, and convenient, to give script files names with a final "`.py`" extension, for instance `myprogram.py`. Once you have typed and saved a script, you can run it simply by typing

```
python3 myprogram.py
```

The command `python3` followed by a file name does not enter the interactive mode, but reads the file, interprets and executes it. In Linux, an alternative is making your script file directly executable. For this, the first line of your file must be

```
#!/usr/bin/env python3
```

which states that the file must be handled by the python3 interpreter. The file, once written, is made executable by typing

```
chmod +x myprogram.py
```

on the terminal, where `chmod` stands for "change mode" (change the *access permissions*) in Unix-like operating systems, and `+x` stand for "add the *execute* permission". Obviously, you must replace `myprogram.py` by the actual name of your script! Once the script is made executable, you run it simply by typing its name

```
myprogram.py
```

An executable script is executed also if you type `python3 myprogram.py`. In fact python3, if called directly, interprets the first line, beginning with a hash sign (`#`), as a comment, and ignores it. If you are using Python 2 instead of Python 3, it is convenient to add a second "commented" line to the file

```
#coding: utf8
```

this tells the interpreter to use the more complete UTF-8 character encoding rather than plain ASCII characters. Python 3 uses UTF-8 encoding by default.

As an example, let us write a script that evaluates the prime factors of an integer number. We can call the script `factorize.py`. As we already know, a hash symbol (#) followed by any character sequence is considered as a comment and ignored by Python. Thus, you can omit all the lines comprising only a hash symbol when you copy the file. We have inserted them only to separate code parts visually, in order to make the script more "human understandable". Further, if you copy this script, or any script listed in the rest of this book, you should *not* type the numbers at the beginning of each line: they are *not* part of the code. We have inserted them only to identify the lines in the code discussion.

Listing 2.1 factorize.py

```
 1  #!/usr/bin/env python3
 2  import math
 3  import time
 4  from sys import argv
 5  #
```

We import the libraries *math* and *time*, and the list `argv` from the library *sys*. We shall see in the following why we need this stuff.

```
 6  num = argv[1]
 7  start = time.time()
 8  #
```

Variable `argv` is a list of strings comprising everything that you typed in the command line when calling the script, including the script name. Thus, if we typed, for instance
`factorize.py 3512`
element `argv[0]` contains the string '`factorize.py`', and `argv[1]` contains the string '`3512`'. The second string, `argv[1]`, is copied into the variable `num` at Line 6. Only `num` will be used by our program. At Line 7, the function `time.time()` returns the time in seconds elapsed since a platform-dependent starting instant, as a floating point number. The starting instant (*time origin*) for Unix and Unix-like systems is January 1st, 1970, at 00:00:00 (UTC). In any case, the actual time origin is not relevant: we are interested only in the *time difference* between the start and the end instants of the execution of our program, in order to know how long the program runs.

```
 9  n=int(num)
10  print("digits:␣{:d}".format(len(num)))
11  #
```

At line 9 the string `num` (the UTF-8 string '3512' in our case) is converted into the integer variable `n`, which shall be used for computation. Line 10 counts the number of digits in the number to be factorized (4 in our case), and prints it on the terminal. Note that the symbol ␣ stands for a space (a blank).

```
12  sqnf=int(math.ceil(math.sqrt(float(n))))
13  #
14  factors = []
15  #
```

Line 12 stores in `sqnf` the maximum integer which can be a prime factor of `n`, i.e., the smallest integer greater than $\sqrt{n}$. Line 14 creates the empty list `factors`, that we shall fill with the prime factors of our number.

```
16  while n%2==0:
17      factors.append(2)
18      n=n//2
19      sqnf=int(math.ceil(math.sqrt(float(n))))
20  #
```

The `while` loop 16-18 stores 2 into `factors` if `n` is even. In this case `n` is replaced by its half, and Line 19 replaces `sqnf` by the value of the new largest possible remaining prime factor. The procedure is iterated as long as the resulting `n` is even, and each time a copy of the number 2 is stored into `factors`.

```
21 i=3
22 while i<=sqnf:
23   while n%i==0:
24     factors.append(i)
25     n=n//i
26     sqnf=int(math.ceil(math.sqrt(float(n))))
27   i+=2
28 #
```

Line 21 assigns the integer value 3 to `i`. Lines 22-27 are two `while` *nested loops*: the loop 23-26 is nested inside the loop 22-27. The loop of lines 23-26 is analogous to the loop 16-19, with 2 replaced by the successive odd numbers `i` generated at line 27, belonging to the external `while` loop. Of course, not all odd numbers are primes!!! But, if an odd number `i` is not prime, `n` has already been divided by the prime factors of `i`, and is no longer divisible by `i`. Thus, checking divisibility by all odd numbers is, in a sense, a more or less unavoidable waste of time, but does not lead to errors. Number `i` is stored into `factors` as long as `i` divides `n`.

```
29 if n!=1:
30   factors.append(n)
31 #
```

Now we are out of all factorizing loops. If the last value of `n` is different from 1, it must be a prime number, and must be stored into `factors`.

```
32 print(factors)
33 elapsed = time.time() - start
34 print("elapsed␣time:␣{:f}␣s\n".format(elapsed))
```

Line 32 prints the list `factors`, i.e., the list of the prime factors of the initial value of `n`. Line 33 stores the time elapsed during the program execution into the variable `elapsed`, which is printed on the terminal at line 34.

Thus, if you type, for instance `factorize.py 3512` at the terminal prompt, you get

```
$>factorize.py 3512
digits:  4
[2, 2, 2, 439]
elapsed time:  0.000120 s
```

the second line (first *output* line) tells you that you are factorizing a 4-digit integer, the third line gives you the actual factorization, $3512 = 2^3 \times 439$, and the last line tells you that the computer needed 1.2×10^{-4} s for computation. Obviously the factorization time is strongly computer-dependent! It is interesting to experiment with integers of different size on the same computer:

```
$>factorize.py 3891252771
digits:  10
[3, 3, 3, 7, 20588639]
elapsed time:  0.001096 s
```

```
$>factorize.py 348961235247715
digits:  15
[5, 131, 532765244653]
elapsed time:  0.118137 s

$>factorize.py 348961223452477159
digits:  18
[1831, 190585048308289]
elapsed time 1.443072 s

$>factorize.py 655449788001142878671 digits:  21
[655449788001142878671]
elapsed time:  3280.387602 s
```

Obviously the simple algorithm presented above can be improved, but the computation time of all known algorithms increases approximately exponentially with the number of digits of the integer to be factorized. For a given number of digits of *n* we observe the longest factorization time if *n* is prime. In the last example above 655 449 788 001 142 878 671 is a prime number.

The security of all current cryptographic algorithms relies on the fact that the factorization of large integers takes a long time.

2.2 Functions

2.2.1 General

As in all programming languages, in Python a function is a block of code that performs a specific task, and that can be called several times by other parts of the program. Python comes with a huge amount of built-in (prewritten, precompiled and optimized) functions, some immediately available, and some packed into separate libraries, organized in *modules* and *packages*, that you must import into your code before use. We have already met the `import` command in several occasions. Some relevant mathematical functions available in Python are listed in Appendix A.

You can also write your own functions to perform specialized tasks. Unlike older high-level programming languages, and as in C/C++, in Python there is no distinction between *functions* and *subroutines*. The code of a Python function begins with a `def` statement and, if it must return values, ends with a `return` statement. The commands in the function definition are not executed as Python first passes over the lines, but only when the function is *called* by another part of the script. A function can have any number of arguments, including zero. A function with zero arguments is the equivalent of what, in other programming languages, is called a *subroutine*.

As a simple example, we can turn script 2.1 into a function coded inside a larger script that checks which of the first 20 natural numbers are prime:

Listing 2.2 FuncFactorize.py

```
#!/usr/bin/env python3
import math
#
```

```
4  def factorize(n):
5     sqnf=int(math.ceil(math.sqrt(float(n))))
6     factors = []
7     while n%2==0:
8        factors.append(2)
9        n=n//2
10    i=3
11    while i<=sqnf:
12       while n%i==0:
13          factors.append(i)
14          n=n//i
15          sqnf=int(math.ceil(math.sqrt(float(n))))
16       i+=2
17    if n!=1:
18       factors.append(n)
19    return factors
20 #
```

Lines 4-19 define the function `factorize()`, which has the single argument `n` (the integer number to be factorized), and outputs the list of the factors of `n`. As stated above, a function can have any number of arguments, and the arguments are not restricted to belong to the same data type, they can be integers, floats, lists, strings, . . . , mixed in any possible way. In the present case we have a single integer argument, and the code of the function is identical to the corresponding code of Script 2.1. Line 19 returns the list of the prime factors of the argument `n`.

```
21 for i in range(2,21):
22    fact=factorize(i)
23    if len(fact)==1:
24       print(i,"is␣prime")
25    else:
26       print(i,fact)
```

The loop at Lines 21-26 is the main part of the script. Line 22 calls function `factorize()` with successive integer numbers `i` as arguments, and the factors of `i` are stored into the list `fact`. Line 23 checks if `fact` has only one element: in this case, `i` is prime, and this is stated by line 24. Otherwise *i* and its prime factors are printed by line 26. The output of the script follows:

```
$>FuncFactorize.py
2 is prime
3 is prime
4 [2, 2]
5 is prime
6 [2, 3]
7 is prime
8 [2, 2, 2]
9 [3, 3]
10 [2, 5]
11 is prime
12 [2, 2, 3]
13 is prime
14 [2, 7]
15 [3, 5]
```

```
16 [2, 2, 2, 2]
17 is prime
18 [2, 3, 3]
19 is prime
20 [2, 2, 5]
```

2.2.2 Local and Global Variables

The variables of a function can be either *local* or *global*. All variables defined inside a function definition are local to the function by default. This means that whatever happens to this variable in the body of the function will have no effect on other variables of the same name outside of the function definition, if they exist. Thus, for instance, the variables `n`, `sqnf` and `factors` in Script 2.2 are local to the function `factorize()`. Line 22 copies the value of the variable `i`, local to the main body of the script, into the variable `n`, local to the function `factorize()`, and, after the function has been called, copies the output of the function (the list `factors`, local to `factorize()`), into the list `fact`, local to the main body of the script. Things can be made clearer by the simple examples discussed below.

In the case of Listing 2.3 the function `func()` prints the square root of the variable *x*, that has not been defined anywhere. Thus, this is the output when the script is called

Listing 2.3 GlobLoc0.py

```
1 #!/usr/bin/env python3
2 import math
3 #
4 def func():
5   print(math.sqrt(x))
6 #
7 func()
```

```
$>GlobLoc0.py
Traceback (most recent call last):
File "./GlobLoc0.py", line 7, in <module>
func()
File "./GlobLoc0.py", line 5, in func
print(math.sqrt(x))
NameError:  name 'x' is not defined
```

Python warns that Line 7 of the script calls the function `func()`, which prints the square root of variable *x* at Line 5, leading to an error because *x* has not been defined anywhere.

Listing 2.4 GlobLoc1.py

```
1 #!/usr/bin/env python3
2 import math
3 #
4 def func():
5   print(math.sqrt(x))
6 #
7 x=5.0
8 func()
```

Listing 2.4 defines the variable *x* at Line 7, thus outside of the definition of `func()`. When Line 8 calls `func()`, Python interprets *x* as a *global* variable defined in the main body of the script because a variable named *x* local to `func()` does not exist. Thus, no error is found, and the square root of 5 is printed in the output, which reads

```
$>GlobLoc1.py
2.23606797749979
```

Finally, Script 2.5 defines both a variable named *x* inside the function definition, at Line 5, and another variable, also named *x*, in the main body of the script, at Line 8. In this case two separate non-interacting variables, both named *x*, one local to the main body and the other local to function `func()`, coexist in the script. The output, when the script is called, is

```
$>GlobLoc2.py
1.7320508075688772
2.23606797749979
```

Line 9 calls `func()`, which, at Line 6, prints the square root of its local variable x, i.e., $x = 3.0$, ignoring the variable x local to the main body of the script. Finally, Line 10, being outside of the function definition, ignores the variables local to the function, and prints the square root of the variable x local to the main body of the script, i.e., $x = 5.0$.

Listing 2.5 GlobLoc2.py

```
1  #!/usr/bin/env python3
2  import math
3  #
4  def func():
5      x=3.0
6      print(math.sqrt(x))
7  #
8  x=5.0
9  func()
10 print(math.sqrt(x))
```

2.3 Reading and Writing Files

Up to now we have passed data to Python by typing values on the keyboard, thus through the *standard input*, and we read the results of Python elaborations on the computer monitor, or *standard output*. This is convenient for small tasks, but is absolutely not convenient for the elaboration of large data sets, as is almost always the case when we are dealing, for instance, with experimental results. When we must elaborate large amounts of data, it is convenient to read data stored in *input files* (this also avoids retyping all the data if our program crashes!), and have the computation results written into other, *output files*.

We start with a simple example. First, we write a text file containing one number per line with our favorite editor, and name it `numdata.txt`. For instance:

```
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0
```

The following simple script reads `numdata.txt` and displays the read data on the terminal

Listing 2.6 ReadFile0.py

```
#!/usr/bin/env python3
#
hnd=open("numdata.txt","r")
num=hnd.readlines()
print(num)
hnd.close()
```

Line 3 opens the file in *read mode*. The name of the file, being a string, must be within quotes. The argument `"r"` stands for *read mode*, meaning that the script can *read*, but not in any way *modify*, the file. The variable `hnd` is the *file handler*, a pointer to the file in the computer memory. All successive operations on the file go through this handler. Line 4 creates the list `num`, where the method `hnd.readlines()` copies all the lines of the file. Line 6 *closes* the file, so that the file is no longer accessible to the script. It is very important to always close a file that has been opened, in order to avoid that it may be corrupted. This is what we see when we run the script

```
$>ReadFile0.py
['2.0\n', '4.0\n', '6.0\n', '8.0\n', '10.0\n', '12.0\n', '14.0\n',
'16.0\n', '18.0\n', '20.0\n', '\n']
```

All items of the list are within quotes because they are interpreted as *strings*, not as *numbers*, and all of them end with a newline sign `\n` because we wrote one number per line. The last `\n` means that we typed a blank line at the end of the file. If we want to elaborate these numbers, we must first convert them to regular floats. The script that follows does the job

Listing 2.7 ReadFile.py

```
1  #!/usr/bin/env python3
2  from math import sqrt
3  #
4  num=[]
5  hnd=open(”numdata.txt”,”r”)
6  while True:
7    buff=hnd.readline()
8    if not buff:
9      break
10   try:
11     num.append(float(buff.strip()))
12   except ValueError:
13     pass
14 hnd.close()
15 #
16 hnd=open(”sqrtdata.txt”,”w”)
17 for i in range(len(num)):
18   hnd.write('{:6.2f}{:12.4f}\n'.format(num[i],sqrt(num[i])))
19 hnd.close()
```

Line 2 imports the function `sqrt()` from `math`, we shall need it for evaluating square roots. Line 4 creates the list `num` where we shall store the numbers read from the file. Line 5 opens the file in read mode. Lines 6-13 define an *infinite* loop for reading the file. We use an infinite loop because we don't know the length of the file before reading it. At each loop iteration, Line 7 copies successive lines of the file into the list `buff`. Note that, while the method `readlines()` encountered in Script 2.6 reads all the lines of the file in a single step, the method `readline()` reads a single line at a time. When the end of the file is reached, `readline()` returns an empty string, which is considered as equivalent to *False* by the `if` statement of line 8. Thus, the loop is interrupted when the end of the file is reached. Lines 10-13 check if it is possible to convert each line into a float number. The method `strip()` strips all blank and newline characters from the beginning and end of each string (thus, for instance, the newline characters `\n` at the end of each line are *stripped*). What remains of each string is converted to a float and appended to the list `num`. If the conversion to float fails (for instance, there is nothing to convert at the last line, which comprises only a `\n` character), a *ValueError* exception is raised, and the `try...except` statement simply skips the action, and nothing is appended to `num`. Line 14 closes the input file, and frees the file handler `hnd`. Line 16 opens an output file named `sqrtdata.txt` in *write mode* (argument `"w"`). Write mode means that a file named `sqrt-data.txt` will be created on the disk if it does not exist already. If a file of that name exists, it will be overwritten, and its previous content will be permanently lost. The loop at lines 16-17 writes lines one by one into the output file, each line comprising a number of the input file and its square root. Finally, line 19 closes the output file. When you run Script 2.7 you don't see anything on the terminal, but a file named `sqrtdata.txt` is created, and you can read it with an editor. This is its content

```
 2.00       1.4142
 4.00       2.0000
 6.00       2.4495
 8.00       2.8284
10.00       3.1623
12.00       3.4641
14.00       3.7417
16.00       4.0000
18.00       4.2426
20.00       4.4721
```

2.4 Calling External Commands from Python Scripts

It is possible to call external (operating-system) commands from Python, and to write Python scripts more or less equivalent to Unix Bash files and Windows batch files. This can be done through methods of the *os* and *subprocess* modules. For instance, line 3 of Listing 2.8 calls the VLC media player, available for Linux, Windows and Mac OSX.

Listing 2.8 Calling VLC Media Player

```
1 #!/usr/bin/env python3
2 import os
3 os.system('vlc')
```

The external command `vlc` is inserted into a string, which is passed as argument to the method `os.system()`.

It is often necessary to pass parameters to an external commands. This is done by inserting the parameters into the string argument. For instance, under Linux, when you wish the list of the contents of a a directory, you can type `ls -latr` in a terminal. Here, `ls` is the command that lists the directory contents. The meanings of the four letters in the option string are: `l`: use a long listing format, `a`: include entries starting with "." ("hidden" files), `t`: sort by modification time, newest first, `r`: reverse order while sorting (i.e., newest last). The result is similar to what you obtain by typing the command `dir` in a Windows terminal.

Listing 2.9 Listing the contents of a directory

```
#!/usr/bin/env python3
import os
os.system('ls -latr')
```

The `os.system()` method can also launch multiple commands separately. This is done by writing each command, with its parameters, in a separate string, and then passing the string commands, joined by vertical bars, "|", as argument to `os.system()`.

Listing 2.10 Calling VLC and Listing a Directory

```
#!/usr/bin/env python3
import os
os.system('ls -latr' | 'vlc')
```

Thus, Listing 2.10 simultaneously lists the contents of the directory and calls the *VLC* media player. Obviously this is of no practical interest whatsoever here, but we shall see later on that this trick can be used, for instance, for performing calculations in parallel on multi-processor computers.

Chapter 3

Plotting with Matplotlib

3.1 Pyplot

Pyplot is a collection of command-style functions that make Matplotlib work like MATLAB. Each pyplot function makes some change to a figure: e.g., creates a figure, creates a plotting area in a figure, plots lines in a plotting area, adds labels (text) to the plot itself or to the horizontal and vertical axes of the figure, ... Successive calls to different *pyplot* functions preserve what done in the figure by the previously called functions, so that the complete figure can be drawn in successive steps.

3.2 Plotting Lists of Numbers

As a first, simple example let us see what happens if we plot a single list of numbers, for instance the list $[1.0, 2.0, 4.0, 8.0, 16.0, 32.0, 64.0]$. We can do this by writing the following listing

Listing 3.1 Plot1List.py

```
1  #!/usr/bin/env python3
2  import matplotlib.pyplot as plt
3  #
4  plt.plot([1.0,2.0,4.0,8.0,16.0,32.0,64.0])
5  plt.show()
```

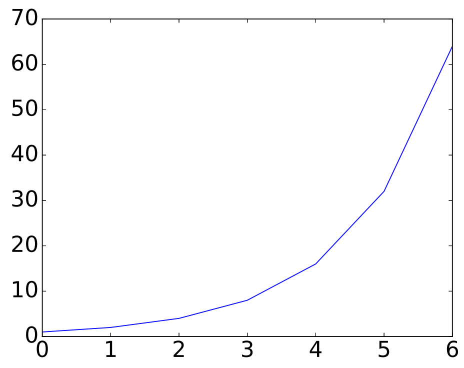


Figure 3.1

Line 2 imports `matplotlib.pyplot` as `plt`. The function `plot()` is called at Line 4, and generates the polyline shown in Fig. 3.1. Note that, if we provide a single list, or array, of numbers to the `plot()` function, *matplotlib* assumes that we are giving a sequence of *ordinates* (y values), and the corresponding x values are generated automatically. The default list of x values has the same length as the list of y values, and comprises successive natural numbers starting with 0. In the present case, this leads to the correct plot, since we are actually plotting $y = 2^x$. In the more general case, we pass `plot()` two lists of equal length, the first of which will be considered as the list of the *abscissae*, and the second as the list of the ordinates of the points to be plotted. The figure will be scaled accordingly. We can also pass an optional third argument which is a *format string* indicating the color and line type of the plot. The default format string is '`b-`', which generates a solid blue line as in Fig. 3.1. Listing 3.2 gives a further example.

Listing 3.2 Plot2Lists.py

```
1 #!/usr/bin/env python3
2 import matplotlib.pyplot as plt
3 #
4 plt.plot([3.0,4.0,5.0,6.0,7.0,8.0],[8.0,16.0,32.0,64.0,128.0,256.0],'ro')
5 plt.show()
```

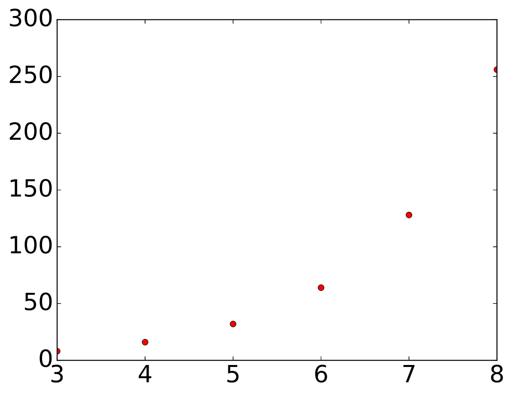


Figure 3.2

Line 4 passes the two *x* and *y* lists to `plot()`, while the third argument, the string `'ro'`, asks for the plot to be represented by red (`r`) circles (`o`). The default value of this argument is `'b-'`, corresponding to a blue (`b`) continuous line (`-`), as in the case of Fig. 3.1. *Matplotlib* is not limited to working with lists: this would be definitely uncomfortable for numeric processing. Rather, we shall normally use *numpy* arrays instead of hand-written lists. In fact, all sequences are converted to numpy arrays internally. Listing 3.3 plots three different lines, with different format styles, in a single command using arrays.

Listing 3.3 multiplot.py

```
1 #!/usr/bin/env python3
2 import matplotlib.pyplot as plt
3 import numpy as np
4 #
5 x=np.arange(0.0,2.0,0.05)
6 plt.plot(x,x,x,np.sqrt(x),'ro',x,x**2,'g^')
7 plt.show()
```

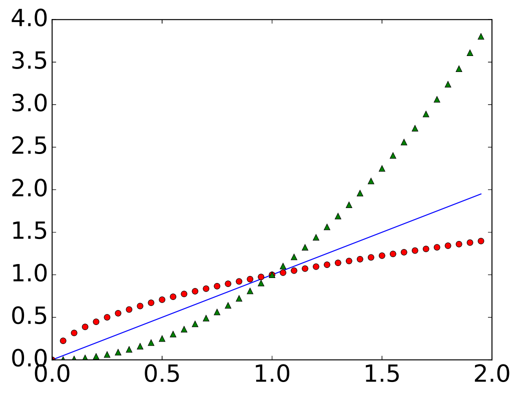


Figure 3.3

Line 5 creates the array `x` comprising the 40 elements $0.0, 0.05, 0.1, \ldots, 1.95$. The first two arguments of the `plot()` function at line 6 plot the array $y = x$ as a function of x, thus resulting in a straight line. No format string is given, consequently the default blue continuous line is used for the plot. The three following arguments, `x`, `np.sqrt(x)` and the format string `'ro'`, plot $y = \sqrt{x}$ as a function of x, using red circles. Finally, the last three arguments `x`, `x**2` and the string `'g^'`, plot $y = x^2$ vs x using green triangles. The three plots are superposed in Fig. 3.3.

3.3 Plotting Functions

We can plot all the functions supplied by, for instance, the *numpy* and *scipy* packages, as well as any user-defined function, by first sampling *x* and *y* coordinates into two `numpy` arrays, and then passing the arrays to `plot()`. As a first example we plot a sine curve using Listing 3.4

Listing 3.4 PlotSin.py

```
1  #!/usr/bin/env python3
2  import numpy as np
3  import matplotlib.pyplot as plt
4  #
5  x = np.arange(0,6.4,0.1);
6  y = np.sin(x)
7  plt.plot(x, y)
8  plt.show()
```

Line 2 imports `numpy`. Line 5 creates the `x` array, comprising the 64 numbers $0, 0.1, 0.2, \ldots, 6.3$. Line 6 creates the `y` array, comprising the 64 values $y_i = \sin(x_i)$. Line 7 creates the plot of y vs x, and line 8 displays the plot on the computer monitor, as shown in Fig. 3.4. The plot can be refined by calling further *pyplot* functions. A slightly modified version of Listing 3.4 follows

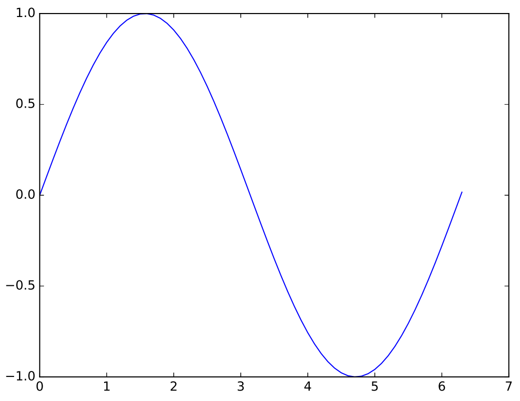


Figure 3.4

Listing 3.5 PlotSinFig2.py

```
1  #!/usr/bin/env python3
2  import numpy as np
3  import matplotlib.pyplot as plt
4  #
5  x = np.arange(0,6.4,0.1);
6  y = np.sin(x)
7  plt.plot(x, y)
8  plt.grid(True)
9  plt.xticks(fontsize=14)
10 plt.yticks(fontsize=14)
11 plt.ylabel(r'$\sin(x)$',fontsize=24)
12 plt.xlabel(r'$x/{\rm rad}$',fontsize=24)
13 plt.tight_layout()
14 plt.savefig('SineGrid.eps',format='eps',\
15    dpi=1000)
16 plt.show()
```

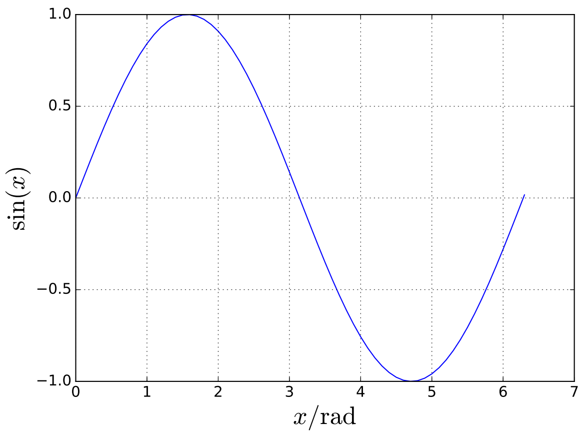


Figure 3.5

Line 8 adds a grid to the plot, Lines 9 and 10 change the default font sizes of the x and y scales of the grid, respectively. Lines 11 and 12 write labels for the y and x axes of the plot, respectively. The labels must be enclosed in single or double quotes (' or "). Labels can be in plain text, but LaTeX text, enclosed between $ signs, can also be used. In this case the text string must be preceded by an *r*. The leading *r* is important: it signifies that the string is a *raw string*, where, for instance, backslashes must not be interpreted as python escapes. Again, the font size of a label can be specified. It is advisable to experiment a little bit with different font sizes at lines 9-13 in order to obtain an aesthetically satisfactory result. Line 13 adjusts the layout of the figure in order to include the grid ticks and labels: as an experiment, see what happens if you move line 13 immediately after line 8, or 9. Line 14-15 creates an Encapsulated PostScript figure named 'SineGrid.eps'. The supported formats for the output figure are *.png*, *.pdf*, *.ps*, *.eps* and *.svg*. The result is shown in Fig. 3.5.

3.4 Multiple Figures

A single Python script can generate a figure comprising more than one separate plots (*subplots*). An example is shown in Listing 3.6

Listing 3.6 SubPlots.py

```
 1 #!/usr/bin/env python3
 2 import matplotlib.pyplot as plt
 3 import numpy as np
 4
 5 def fun1(t,omega,tau,ampl):
 6     y=ampl*np.cos(omega*t)*np.exp(-t/tau)
 7     return y
 8 def fun2(t,omega,omega2,ampl):
 9     y=ampl*np.sin(omega2*t)*np.sin(omega*t)
10     return y
11 #
```

Lines 5-7 and 8-10 define the two functions `fun1(t,omega,tau,ampl)` and `fun2(t,omega, omega2,ampl)`, in mathematical form they are

$$f_1(t,\omega,\tau,A) = A\cos(\omega t)\,\mathrm{e}^{-t/\tau} \quad \text{and} \quad f_2(t,\omega,\omega_2,B) = B\sin(\omega_2 t)\sin(\omega t)\ , \tag{3.1}$$

respectively. These two functions will be plotted in the following.

```
12 omega=32.0
13 omega2=np.pi/2.0
14 tau=1.0
15 ampl=5.0
16 ampl2=10.0
```

Lines 12-16 assign numerical values to parameters of the two functions f_1 and f_2 of (3.1), namely $\omega = 32$, $\omega_2 = \pi/2$, $\tau = 1.0$, $A = 5.0$ and $B = 10.0$.

```
17 t=np.arange(0.0, 2.0, 0.01)
18 s1=fun1(t,omega,tau,ampl)
19 s2=fun2(t,omega,omega2,ampl2)
20 # .......................................
21 plt.figure(figsize=(10,4))
```

Line 17 creates the array `t`, comprising the 200 numbers $[0.00, 0.001, 0.002, \ldots, 0.199]$ that will be used as abscissae for the plots. Lines 18 and 19 create the two arrays `s1` and `s2`, used as ordinates in the plots. Line 21 creates a figure 10 inches wide and 4 inches high. The absolute values (or units) are actually not relevant, since the figure will be scaled both on the computer monitor or in printing, but the width/height ratio **is** relevant.

```
22 # .................................. subplot 1
23 plt.subplot(1,2,1)
24 plt.plot(t,s1)
25 plt.plot(t,ampl*np.exp(-t/tau))
26 plt.grid(True)
27 plt.xticks(fontsize=14)
28 plt.yticks(fontsize=14)
29 plt.ylabel(r'$A\,\cos(\omega t)\,{\rm e}^{-t/\tau}$',fontsize=24)
30 plt.xlabel(r'$t$',fontsize=24)
31 plt.tight_layout()
```

Line 23 creates the first subplot. The arguments 1,2,1 of the function `subplot()` assign 1 row and 2 columns to the complete figure, thus the two subplots will be located side by side on the same row. The last argument, 1, tells that what follows will be drawn in the first (left) subplot. Line 24 plots the array `s1` vs the array `t`, i.e., f_1 vs t. Line 25 adds the plot of the exponential $A\,\mathrm{e}^{-t/\tau}$ vs t. The rest is analogous to lines 8-13 of Listing 3.5. The two superposed plots are shown in the left part of Fig. 3.6

```
32  # ..................................  subplot 2
33  plt.subplot(1,2,2)
34  plt.plot(t,s2)
35  plt.plot(t,ampl2*np.sin(omega2*t))
36  plt.grid(True)
37  plt.xticks(fontsize=14)
38  plt.yticks(fontsize=14)
39  plt.ylabel(r'$B\,\sin(\omega␣t)\,\sin(\omega_2␣t)$',fontsize=24)
40  plt.xlabel(r'$t$',fontsize=24)
41  plt.tight_layout()
42  #
```

Line 33 creates the second subplot, located on the second column of the first (and only) row of the figure, i.e., at the right. Line 34 plots the array `s2` vs the array `t`, i.e., f_2 vs t. Line 35 adds the plot of the low-frequency sine $B\sin(\omega_2 t)$ vs t. Lines 36-41 add grid and axis labels, and adjust the font sizes. The plot is shown in the right part of Fig. 3.6.

```
43  plt.savefig('MultiPlot0.eps',format='eps',dpi=1000)
44  plt.show()
```

A figure in Encapsulated PostScript is created, and the two plots are shown on the computer monitor.

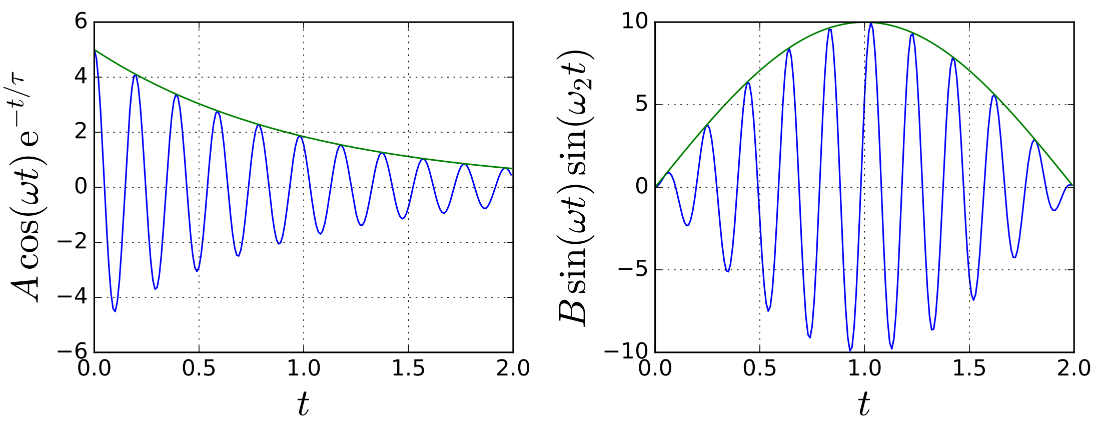


Figure 3.6

3.5 Logarithmic Axis Scales

Pyplot supports not only linear axis scales, but also *logarithmic* and *logit* scales. This can be useful when data span many orders of magnitude. Listing 3.7 gives an example.

Listing 3.7 LogPlot.py

```
1  #!/usr/bin/env python3
2  import matplotlib.pyplot as plt
3  import numpy as np
4  # ................................ functions
5  x=np.arange(1.0,20.5,1.0)
6  y1=x**2
7  y2=np.sqrt(x)
```

Line 5 creates the array `x=` $[1.0, 2.0, \ldots, 20.0]$. Lines 6 and 7 create the arrays `y1` and `y2`, with $y_i^{(1)} = x_i^2$ and $y_i^{(2)} = \sqrt{x_i}$.

```
8  # .....................................
9  plt.figure(figsize=(10,8))
```

Analogous to Line 21 of Listing 3.6. Again, only the width/height ratio of the whole figure is relevant to us.

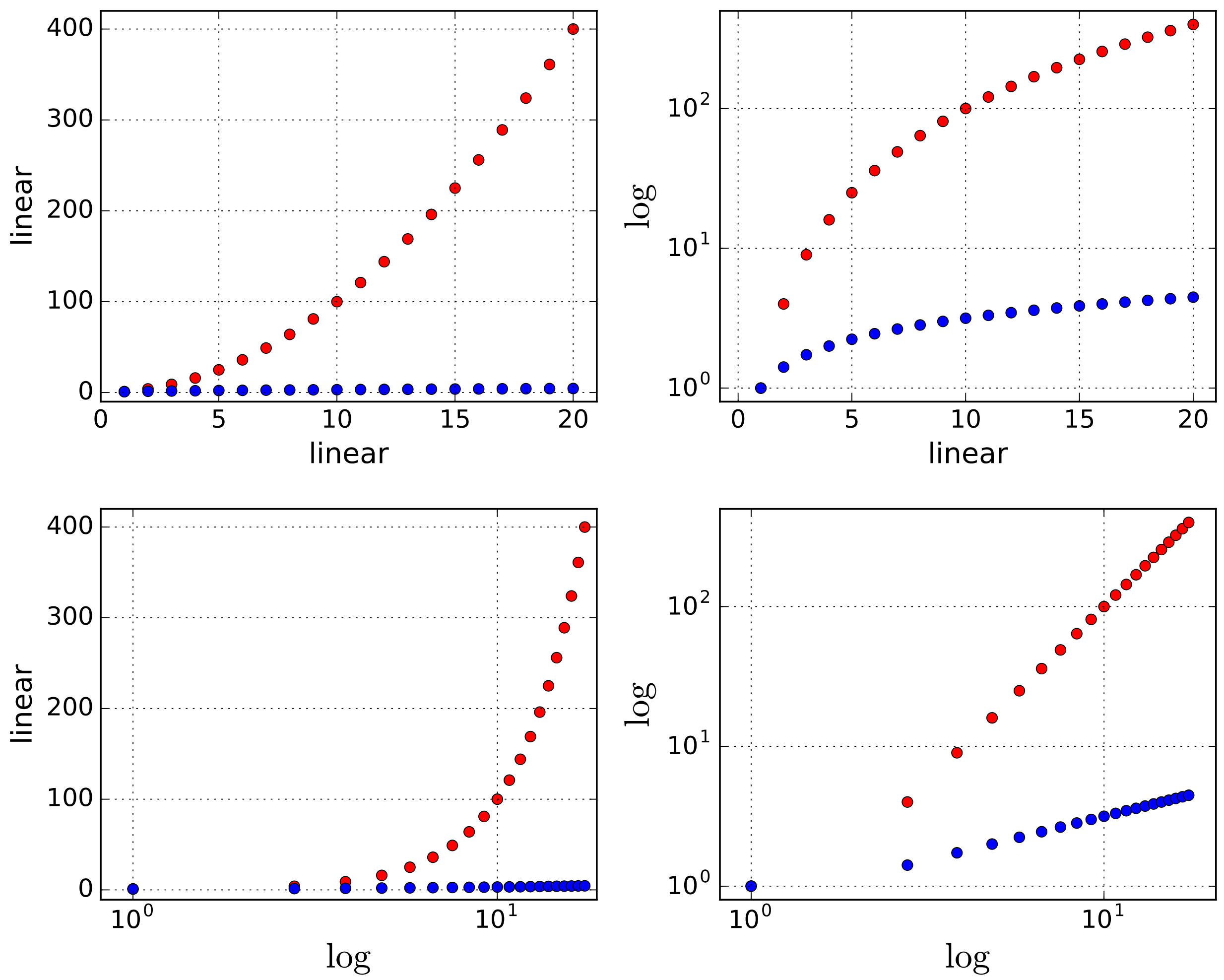


Figure 3.7

```
10 # .................................. subplot 1
11 plt.subplot(2,2,1)
12 plt.plot(x,y1,'ro')
13 plt.plot(x,y2,'bo')
14 plt.grid(True)
15 plt.xticks(fontsize=14)
16 plt.yticks(fontsize=14)
17 plt.xlabel('linear',fontsize=16)
18 plt.ylabel('linear',fontsize=16)
19 plt.tight_layout()
20 plt.ylim(-10,420)
21 plt.xlim(0,21)
```

This is the first of four sublopts, located in the first position, (1, 1) or upper left, of our 2×2 plot array shown in Fig. 3.7. All four plots display the same data, i.e., `y1` vs `x` superposed to `y2` vs `x`. The `y1` data are represented by red circles, the `y2` data by blue circles in all plots. In this first plot both the x and the y scales are linear, and the plot of the square root data results very flat. Lines 20 and 21 set the limits of the x and y values, slightly extending their default values. This is done in order to keep the circles representing the extreme data points within the plot frame. As an experiment, see what happens if you comment out these lines.

```
22 # .................................. subplot 2
23 plt.subplot(2,2,2)
24 plt.plot(x,y1,'ro')
25 plt.plot(x,y2,'bo')
26 plt.grid(True)
27 plt.yscale('log')
28 plt.xticks(fontsize=14)
29 plt.yticks(fontsize=14)
30 plt.xlabel('linear',fontsize=16)
31 plt.ylabel(r'$\log$',fontsize=20)
32 plt.tight_layout()
33 plt.ylim(0.8,500)
34 plt.xlim(-0.8,21)
```

This is the second (upper right) subplot. Line 27 makes the y scale logarithmic, with this choice the plot of the square roots is no longer flat. Remember that, when you use a logarithmic scale, negative and zero coordinate values must be avoided.

```
35 # .................................. subplot 3
36 plt.subplot(2,2,3)
37 plt.plot(x,y1,'ro')
38 plt.plot(x,y2,'bo')
39 plt.grid(True)
40 plt.xscale('log')
41 plt.xticks(fontsize=14)
42 plt.yticks(fontsize=14)
43 plt.xlabel(r'$\log$',fontsize=20)
44 plt.ylabel('linear',fontsize=16)
45 plt.tight_layout()
46 plt.ylim(-10.8,420)
47 plt.xlim(0.8,22)
```

This is the third (lower left) subplot. Line 40 makes the x scale logarithmic, while the y scale is linear.

```
48  # .................................. subplot 4
49  plt.subplot(2,2,4)
50  plt.plot(x,y1,'ro')
51  plt.plot(x,y2,'bo')
52  plt.grid(True)
53  plt.xscale('log')
54  plt.yscale('log')
55  plt.xticks(fontsize=14)
56  plt.yticks(fontsize=14)
57  plt.xlabel(r'$\log$',fontsize=20)
58  plt.ylabel(r'$\log$',fontsize=20)
59  plt.tight_layout()
60  plt.ylim(0.8,500)
61  plt.xlim(0.8,25)
```

This is the fourth (lower right) subplot. Lines 53 and 54 make the scales of both axes logarithmic. The circles representing both data sets lie on straight lines, because we have

$$\log y^{(1)} = \log x^2 = 2\log x \qquad \text{and} \qquad \log y^{(2)} = \log\sqrt{x} = \frac{1}{2}\log x\,. \tag{3.2}$$

```
62  #
63  plt.savefig('LogPlot0.eps',format='eps',dpi=1000)
64  plt.show()
```

3.6 Plotting Field Lines

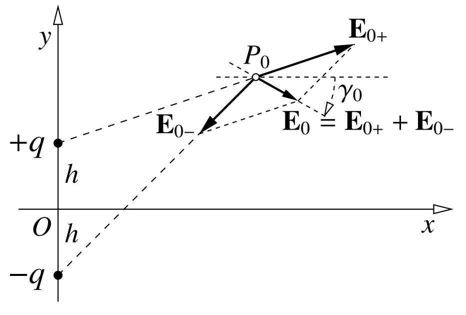


Figure 3.8

In this section we consider how to plot field lines, specifically how to plot the field lines of an electric dipole. Our dipole consists of two charges, $+q$ and $-q$, located at $(0, +h)$ and $(0, -h)$ in a Cartesian reference frame, respectively, as shown in Fig 3.8. Extensions to the field lines generated by more complicated charge configurations should be straightforward. The idea is using a method analogous to the Euler method for solving ordinary differential equations, discussed later on in Section 5.2. In other words, we approximate each field line by a polyline comprising very short line segments of equal length. Each polyline starts from an initial point $P_0 \equiv (x_0, y_0)$, close to, but obviously not coinciding with, one of the two charges $\pm q$ generating the field. Once chosen the start point P_0 of a field line, we evaluate the electric field $\boldsymbol{E}_0$ in it. What is relevant for our method is not the intensity of the field, but only its direction, which forms an angle $\gamma_0 = \arctan(E_{0y}/E_{0x})$ (negative in the case of Fig. 3.8) with the x direction. Once determined the angle γ_0, we choose a small length $\delta\ell$, which will be the common length of all the single line segments forming the polyline approximating the field line. In general, some experimenting on the most convenient value for $\delta\ell$ can be needed. The second vertex of our polyline is the point $P_1 \equiv (x_1, y_1) = (x_0 + \delta\ell\cos\gamma_0, y_0 + \delta\ell\sin\gamma_0)$. The next step is the evaluation of the electric field $\boldsymbol{E}_1$ in P_1 and its angle γ_1 with the x direction, which determines the point P_2. The procedure is iterated for finding the successive vertices P_m of the polyline. We shall stop when the polyline gets to close to the other point charge, or when it exits our intended plotting region. A possible procedure is shown in Listing 3.8.

Listing 3.8 PlotDipoleField.py

```
1  #!/usr/bin/env python3
2  import matplotlib.pyplot as plt
3  import numpy as np
4  # ............................................. charge locations
5  yplus=1.0
6  yminus=-1.0
7  xplus=xminus=0.0
8  rad=0.1
9  lim=30
10 nLin=60
11 plt.axis('off')
```

Quantities `xplus` (`yminus`) and `yplus` (`yminus`) are the *x* and *y* coordinates of the positive (negative) charge of the dipole, in arbitrary units. Quantity `rad` is the radius of a circle around the positive charge $+q$, from where our field lines will start, see Fig. 3.9. We stop the evaluation of a field line when the *x*, or *y* coordinate of the current vertex is greater than `lim`, or smaller than `-lim`. Both `rad` and `lim` are expressed in the same arbitrary units as `xplus`, `xminus`, `yplus` and `yminus`. Quantity `nLin` is the number *n* of field lines starting from the positive charge. Line 11 removes the axes from the figure. You can comment this line out, and see what happens.

```
12 # ................................................... field lines
13 i=0
14 delta=0.05
```

Variable `i` is a counter for the field lines, while `delta` is the length $\delta\ell$ of the line segments.

```
15 while i<nLin:
16   xlist=[]
17   ylist=[]
18   alpha0=i*2*np.pi/float(nLin)
19   x=xplus+rad*np.cos(alpha0)
20   y=yplus+rad*np.sin(alpha0)
21   xlist.append(x)
22   ylist.append(y)
23   while True:
24     alpha=np.arctan2((y-yplus),(x-xplus))
25     beta=np.arctan2((y-yminus),(x-xminus))
26     Eplus =1.0/((x-xplus)**2+(y-yplus)**2)
27     Eminus=-1.0/((x-xminus)**2+(y-yminus)**2)
28     Ex=Eplus*np.cos(alpha)+Eminus*np.cos(beta)
29     Ey=Eplus*np.sin(alpha)+Eminus*np.sin(beta)
30     gamma=np.arctan2(Ey,Ex)
31     x=x+delta*np.cos(gamma)
32     y=y+delta*np.sin(gamma)
33     if x>lim or x<-lim or y>lim or y<0:
34       break
35     xlist.append(x)
36     ylist.append(y)
37   plt.plot(xlist,ylist,'k-',linewidth=0.5)
38   ylist=-np.array(ylist)
```

```
39      plt.plot(xlist,ylist,'k-',linewidth=0.5)
40      i+=1
```

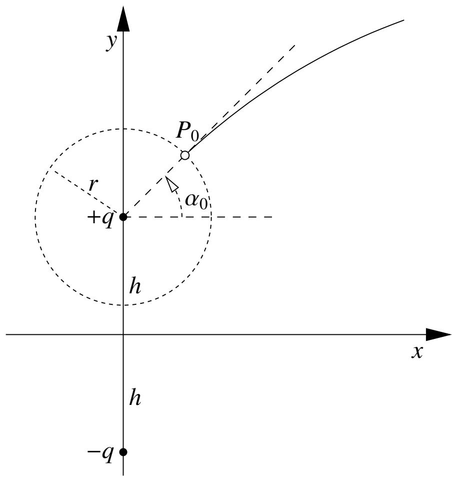


Figure 3.9

Loop 15-40 draws a single field line at each iteration. Lines 16 and 17 create the (initially empty) lists of the x and y coordinates of the vertices of the approximating polyline. Angle `alpha0`, $\alpha_0 = 2\pi i/n$ (n being the number of plotted field lines), defined at Line 18 and shown in Fig. 3.9, determines the position of the start point P_0 of the current field line. All field lines start from points equally spaced on a small circumference of radius `rad` (r in the figure) centered around the positive charge $+q$. The x and y coordinates of P_0 are evaluated at lines 19 and 20, respectively, and inserted into `xlist` and `ylist` at lines 21 and 22. The loop 23-36 evaluates the successive vertices of the field line, P_m, as shown in Fig. 3.10. Variables `alpha` and `beta` at Lines 24 and 25 are the angles α_m and β_m of Fig. 3.10. Lines 26-29 evaluate the x and y components of the electric field $\boldsymbol{E}_m$ at P_m, and Line 30 the angle γ_m that $\boldsymbol{E}_m$ forms with the x axis. Lines 31 and 32 evaluate the coordinates of the successive point of the "field polyline", P_{m+1}. Lines 33 and 34 break the loop if either the x or the y coordinate is out of range. Only positive y coordinates are accepted, since we can exploit the mirror symmetry of the figure about the x axis. Line 37 plots the field line in the upper half-plane $y > 0$. Line 38 changes the signs of `ylist`, and line 39 draws the symmetric field line in the lower half-plane.

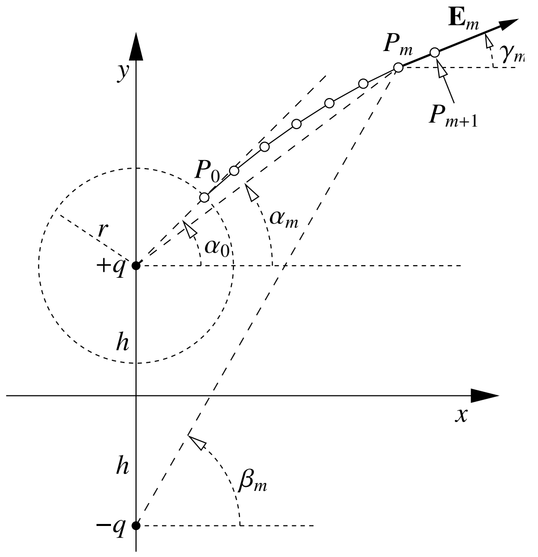


Figure 3.10

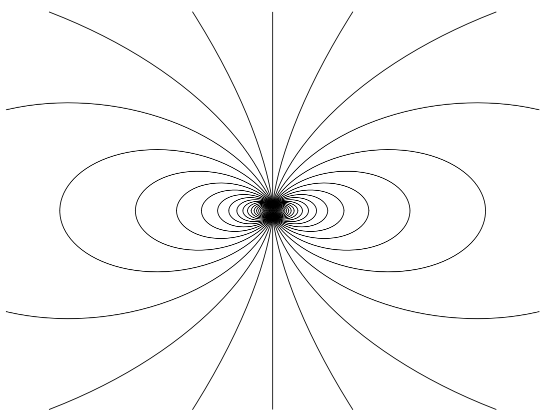


Figure 3.11

```
41  # ............................................................
42  plt.savefig('DipoleField.pdf',format='pdf')
43  plt.show()
```

Line 42 saves the plot into a pdf file named DipoleField.pdf, shown in Fig. 3.11.

3.7 Pyplot Animation

The *matplotlib* library provides the possibility to produce animations on the computer monitor. The easiest way is to use one of the following two animation classes

FuncAnimation: makes an animation by repeatedly calling a provided function `func()`.

ArtistAnimation: this animation uses a fixed set of Artist objects.

In the present context we shall consider the class *FuncAnimation* only, which is of more interest for a physicist. As a simple example, we shall write a script displaying a horizontally translating (panning) plot of an exponentially damped sine curve.

Listing 3.9 SineDecay.py

```
1  #!/usr/bin/env python3
2  #
3  import numpy as np
4  import matplotlib.pyplot as plt
5  import matplotlib.animation as animation
6  #
7  fig,ax=plt.subplots(figsize=(10,6))
8  ax.set(ylim=(-1,1))
9  #
```

Line 7 creates a figure of sizes 10×6 inches with a single subplot `ax`. Line 8 sets the limits of the y axis of the subplot. This is needed to prevent `pyplot` from rescaling the vertical axis of the plot when the amplitude of the plotted function diminishes.

```
10 def func(x):
11     return np.sin(8*x)*np.exp(-0.1*x)
12 #
13 x=np.arange(0,10,0.01)
14 line,=ax.plot(x,func(x))
15 #
```

Lines 10-11 define the function $f(x) = \sin(8x)\,\mathrm{e}^{-0.1x}$, that we are going to plot. Line 13 stores the initial 100 x values at which the function is to be evaluated, namely $[0, 0.01, 0.02, \ldots, 9.99]$, into the list `x`. Line 14 creates the object `line`, belonging to class *matplotlib.lines.Line2D*, in the subplot `ax`. Object `line` has the list `x` as *xdata*, and the list `func(x)` as *ydata*.

```
16 def animate(i):
17     xx=x+i/100
18     line.set_xdata(xx)
19     line.set_ydata(func(xx))
20     ax.set(xlim=(xx[0],xx[999]))
21     return line,
22 #
```

Lines 16-21 define the function `animate()`, which updates the plot at each animation "frame". The function has the single argument `i`, which will be increased by 1 at each animation step. Line 17 creates the list `xx`, whose elements are obtained from the corresponding elements of the original list `x` by adding `i`/100. Lines 18 and 19 update the x and y values of the object `line`, respectively. Line 20 updates the limits of the x axis of the plot. Line 21 returns the object `line`.

```
23  ani=animation.FuncAnimation(fig,animate,interval=20)
24  plt.show()
```

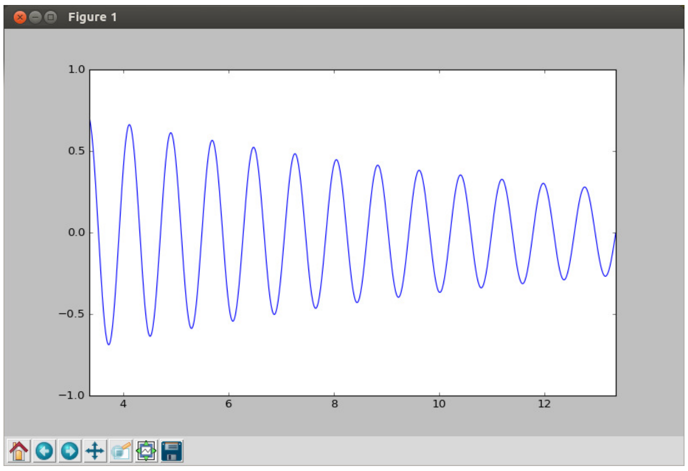


Figure 3.12

At line 23, the function `FuncAnimation()` creates the plot animation by repeatedly calling the function `animate()`. The mandatory arguments of `FuncAnimation()` are two: the figure where to draw, `fig` in our case, and the updating function, here `animate`. Function `FuncAnimation()` has many optional further arguments, here we use only one, namely `interval`, the delay time between consecutive frames in milliseconds, the default value is 200 ms. Here we have chosen a delay of 20 ms. The result is shown in Fig. 3.12. When you actually observe the computer monitor rather than a figure on paper you see the damped sine wave moving toward the left. It is also possible to record the animation into an .mp4 video by inserting the line

`ani.save('test.mp4', fps=30)`

between lines 23 and 24. The first argument of `ani.save()` is the name of the *mp4* file, the second argument is the number of frames per second.

Chapter 4

Numerical Solution of Equations

4.1 Introduction

Solving equations, and systems of equations, of all kinds, both algebraic and transcendental, is a very frequent task in a physicist's life. Very often equations, particularly algebraic nonlinear equations and transcendental equations, have no analytical solutions. In this case we look for *approximate numerical solutions*. Some equations do not even admit solutions at all, but, of course, we shall not deal this case here! However, when tackling equations we must consider the unlucky possibility that its solution simply does not exist. In this chapter we shall consider the numerical solution of equations and systems of equations not involving the derivatives of the unknowns. Ordinary differential equations are left to Chapter 5.

4.2 Systems of Linear Equations

In this section we consider the simplest case: the solution of a system of linear equations. A linear equation is an algebraic equation in which each term is either a constant or the product of a constant and the first power of a single variable. A system of linear equations is a collection of two or more linear equations involving the same set of unknowns. The word *system* indicates that the equations are to be considered collectively, rather than individually. As an example, consider the following system of three equations in the three unknowns x_1, x_2, and x_3

$$\left\{\begin{array}{llll} 3x_1 & -2x_2 & -x_3 & = 2 \\ 2x_1 & -2x_2 & +4x_3 & = 0 \\ -x_1 & +0.5x_2 & -1.5x_3 & = -1 \end{array}\right. \tag{4.1}$$

which can be written, in matrix form,

$$A\boldsymbol{x} = \boldsymbol{b}\,, \quad \text{where} \quad A = \begin{pmatrix} 3 & -2 & -1 \\ 2 & -2 & 4 \\ -1 & 0.5 & -1.5 \end{pmatrix}, \quad \boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \quad \text{and} \quad \boldsymbol{b} = \begin{pmatrix} 2 \\ 0 \\ -1 \end{pmatrix}. \tag{4.2}$$

If we want to solve the system "by hand", we can use one of several methods, for instance *elimination of variables*, *row reduction*, *Cramer's rule*, ...

Python provides the function `numpy.linalg.solve()`, which computes the "exact" solution, $\boldsymbol{x}$, of the linear matrix equation $A\boldsymbol{x} = \boldsymbol{b}$, provided that the determinant of A is different from zero. Listing 4.1 shows how it works

Listing 4.1 LinearSyst.py

```
1 #!/usr/bin/env python3
2 import numpy as np
3 #
4 A=np.array([[3.0,-2.0,-1.0],[2.0,-2.0,4.0],[-1.0,0.5,-1.5]])
5 b=np.array([2.0,0.0,-1.0])
6 x=np.linalg.solve(A,b)
7 print('x␣=',x)
8 bb=np.dot(A,x)
9 print('bb␣=',bb)
```

Line 4 creates matrix `A` as an *array of arrays*: the single subarrays of the argument of the function `array()` are the lines of the matrix A of (4.2). Line 5 stores the vector of the constant terms into the array `b`. Finally, Line 6 solves the equations system by calling `solve()` and stores the solution into the array `x`. Line 7 prints the solution. Line 8 multiplies the matrix `A` by the vector `x` using the function `dot()` and stores the resulting vector into the array `bb`. Line 9 prints the array `bb`, which, if the solution is correct, must equal the array `b`. This is what you see when you run the script

```
$>LinearSyst.py
x = [ 2.00000000e+00 2.00000000e+00 5.55111512e-17]
bb = [ 2.00000000e+00 2.22044605e-16 -1.00000000e+00]
```

Thus $x_1 = 2$, $x_2 = 2$, $x_3 = 0$ is the solution of the system (4.1). Unavoidable rounding errors in numerical methods lead to 5.5×10^{-17} instead of 0 in the solution, and to 2.2×10^{-16} in the check.

4.3 Systems of Nonlinear Equations

We are used to see most equations having both a right-hand side and a left-hand side, but here it is convenient to move all nonzero terms to the left of the equal sign, leaving only a zero at the right side and obtaining an equation of the form

$$f(x) = 0 , \tag{4.3}$$

whose solution, or set of solutions, we are searching. For nonlinear problems a root finding algorithm proceeds by iteration, starting from some approximate trial solution and improving it until some convergence criterion is satisfied. Success strongly depends on having a good first guess for the solution, and this guess usually relies on a detailed analysis of the problem. Whenever possible one should "bracket" the solution, i.e., determine an interval containing the solution. A serious problem can be posed by the existence of multiple solutions, especially if they are close to one another, and/or if they are in even number. If $f(x)$ is a continuous function, a and b are two values such that $a < b$ and $f(a)$ and $f(b)$ have opposite signs, then (4.3) has at least a solution x_1 such that $a < x_1 < b$. But, of course, there might also be any odd number of solutions in the same interval.

For a more thorough discussion of the problem see Chapter 9 of Reference [1].

4.4 Common Methods

The most common methods for the numerical solution of (4.3) are the *bisection method*, the *secant Method*, the *Newton-Raphson Metod* and the *Brent Method*. Here we shall only discuss

1. the bisection method, which relies on the knowledge of the interval where the solution is located, and is very straightforward.

2. The secant method, which also requires that two points are provided, but does not require that the solution is between the two points. Providing such two pints can be interpreted as providing a start point and an initial search step.

A large number of further methods are coded into functions contained in various Python packages, but we cannot discuss all of them here.

4.4.1 Bisection Method

If we have an interval (a, b) such that $a < b$ and $f(a)f(b) < 0$, the *bisection method* cannot fail, obviously provided that $f(x)$ is continuous in the (a, b) interval! This is how it works:

1. evaluate the function $f(c)$ at the midpoint $c = (a + b)/2$;

2. if $f(c) = 0$ the problem is solved, but the probability for this to happen is obviously zero;

3. if $f(c)$ has the same sign as $f(a)$ replace a by c as endpoint of the interval, otherwise replace b by c. The new interval still brackets the solution, but its length is one half of the length of the original interval.

4. Go back to point 1.

At each iteration the interval containing the solution is halved, and we stop when $|a - b| < \varepsilon$, with ε the required accuracy for the solution.

A simple example of an equation which cannot be solved analytically is the following

$$5 + 4x = e^x \ , \quad \text{which we can rewrite as} \quad 5 + 4x - e^x = 0 \ . \tag{4.4}$$

We can use the code of Listing 4.2 in order to check if (4.4) has a solution in the range $0 < x < 10$

Listing 4.2 bisection01.py

```
 1 #!/usr/bin/env python3
 2 from numpy import exp
 3 #
 4 def fun(x):
 5   return 5.0+4.0*x-exp(x)
 6 #
```

Lines 4-5 define the function $f(x) = 5 + 4x - e^x$, whose roots we are searching.

```
 6 #
 7 a=0.0
 8 b=10.0
 9 eps=1.0e-15
10 #
```

Variables `a` and `b` are the endpoints of the investigated interval, and `eps` is the required accuracy on the solution.

```
11  fa=fun(a)
12  fb=fun(b)
13  #
14  if fa*fb>0:
15     print("wrong interval!!!",fa,fb)
16     exit()
17  #
```

Variables `fa` and `fb` are the function values at the endpoints of the interval. If the product `fa*fb` is greater than zero, `fa` and `fb` have the same sign, implying that the function crosses the *x* axis an even number of times (including zero!) in the interval, and the interval is rejected at lines 14-16. Function `exit()` is a standard Python function that causes the script to exit (terminate).

```
18  iter=1
19  while (b-a)>eps:
20     c=(a+b)/2.0
21     fc=fun(c)
22     if fc==0:
23        print("x = ",c)
24        exit()
25     if fc*fa>0:
26        a=c
27        fa=fc
28     else:
29        b=c
30        fb=fc
31     iter+=1
32  #
```

Lines 19-31 are the bisection loop. The midpoint `c` of the interval is evaluated at line 20, and the function value `fc` is evaluated at line 21. At lines 25-30 one of the endpoints of the interval is replaced by the midpoint, so that the interval is halved. At each iteration the counter `iter` is incremented at line 31. The loop stops when the interval width is smaller than `eps`.

```
32  #
33  print("x = ",c)
34  print("accuracy = ",'{:.2e}'.format(b-a))
35  print("f(",c,") =",fun(c))
36  print(iter," iterations needed")
```

Line 33 prints the solution, line 34 the accuracy on the solution, line 35 the function value at the solution, and line 36 the number of iterations.

This is what you observe on the terminal when you run the program

```
$>bisection01.py
x = 2.7800807820516997
accuracy = 4.44e-16
f( 2.7800807820516997 ) = -3.5527136788e-15
55 iterations needed
```

thus, $x = 2.7800807820517000(4)$ is a solution of (4.4). If you widen the search interval at its left, by changing its endpoints at lines 7 and 8 to `a=-10.0` and `b=10.0` you get

```
$>bisection01.py
wrong interval!!!  -35.0000453999 -21981.4657948
```

showing that both $f(a)$ and $f(b)$ are negative. Thus there is an even number of roots in the interval. Since we have already found one root in the right half of the interval $(-10, 10)$, the number of roots cannot be zero, and the interval must contain at least one further root. If we now change the interval endpoints at lines 7 and 8 to the values `a=-10.0` and `b=0.0` we get

```
$>bisection01.py
x = -1.172610558265084
accuracy = 6.66e-16
f( -1.172610558265084 )
= 1.49880108324e-15
55 iterations needed
```

thus, also $x = -1.172610558265084(6)$ is a solution of (4.4). As we have seen, the fact that the (continuous) function has opposite signs at the interval endpoints implies that there is at least one root in the interval, but, in principle, there might be any odd number of roots. Conversely, if $f(a)$ and $f(b)$ have the same sign, this does not necessarily mean that the interval contains no root, there might be an even number of roots. Whenever possible, plotting a function can be of great help in localizing the intervals where its roots are located. Then, the bisection method determines the roots with the required accuracy. Fig. 4.1 shows a plot of our $f(x)$.

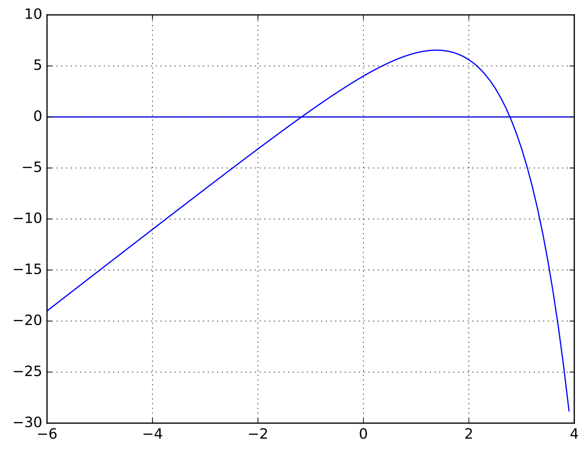


Figure 4.1

4.4.2 The Secant Method

Also the *secant method* requires two start points, let us denote them by x_0 and x_1, possibly both close to the solution x^*. However, this method does not require that the solution lies in the (x_0, x_1) interval. Suppose that we want to find the root of the function $f(x)$ plotted in Fig. 4.2. We start from the two values x_0 and x_1 shown in the figure, and evaluate the values $y_0 = f(x_0)$ and $y_1 = f(x_1)$. Then we draw the straight line passing through the points (x_0, y_0) and (x_1, y_1), which will cross

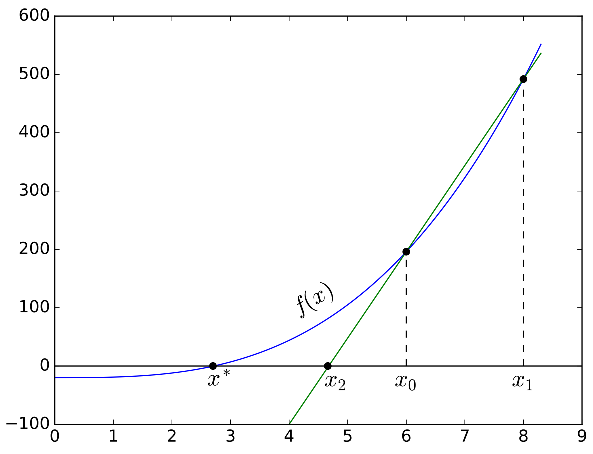


Figure 4.2

the x axis at the point

$$x_2 = x_1 - y_1 \frac{x_1 - x_0}{y_1 - y_0}\,, \tag{4.5}$$

which is closer to the solution x^* than both x_0 and x_1, and evaluate $y_2 = f(x_2)$. Then we proceed by iteration with

$$x_{i+1} = x_i - y_i \frac{x_i - x_{i-1}}{y_i - y_{i-1}}\,. \tag{4.6}$$

The *Newton-Raphson* method is analogous to the secant method, but it requires the first derivative of the function $f(x)$. If we do not have good starting points, the secant method and the Newton-Raphson method can fail, while the bisection method always succeeds if the function has opposite signs at the ends of the initial interval

4.5 Root Finding with the *scipy.optimize* Package

If one has a single-unknown equation, the subpackage *scipy.optimize* provides four root finding functions, based on different algorithms. Each of these algorithms requires the endpoints of an interval in which a root is expected. In general the function `brentq()` is the best choice, but the other three functions may be useful in certain circumstances, or for academic purposes. Listing 4.3 shows a program using `scipy.optimize.bisect()` for finding the positive root of Equation (4.4)

Listing 4.3 optbisect.py

```python
#!/usr/bin/env python3
from numpy import exp
from scipy.optimize import bisect
#
def fun(x):
  return 5.0+4.0*x-exp(x)
#
a=0.0
b=10.0
eps=1.0e-15
#
fa=fun(a)
fb=fun(b)
#
if fa*fb>0:
  print("wrong interval!!!",fa,fb)
  exit()
#
x=bisect(fun,a,b,xtol=eps)
print(x)
```

The three mandatory arguments of `bisect()` are the pointer to the function and the endpoints of the interval containing the root, an optional argument is the required tolerance on the solution. This is what we get on the terminal

```
$>optbisect.py
2.780080782051697
```

Listing 4.4 uses `scipy.optimize.brentq()` leading, obviously, to the same result.

Listing 4.4 optbrent.py

```
#!/usr/bin/env python3
from numpy import exp
from scipy.optimize import brentq
#
def fun(x):
  return 5.0+4.0*x-exp(x)
#
a=0.0
b=10.0
eps=1.0e-15
#
fa=fun(a)
fb=fun(b)
#
if fa*fb>0:
  print("wrong interval!!!",fa,fb)
  exit()
#
x=brentq(fun,a,b,xtol=eps)
print(x)
```

The *scipy.optimize* subpackage provides also root finding algorithms that do not require the end points of an interval containing the solution, but only a good starting point. An example is the function `fsolve()`, used in the following listing.

Listing 4.5 fsolve_demo.py

```
#!/usr/bin/env python3
from numpy import exp
from scipy.optimize import fsolve
#
def fun(x):
  return 5.0+4.0*x-exp(x)
#
xstart=1.0
#
x=fsolve(fun,xstart)
print(x)
```

Here we are finding a root of the same function of Listings 4.3 and 4.4, using $x = 3.0$ as starting value, obtaining the same result. The other root, $x = -1.17261056$, can be obtained by using a different starting point, for instance $x = 1.8$.

4.6 Systems of Nonlinear Equations

4.6.1 Equations Involving only Unknowns

When we have a system of nonlinear equations, it is usually difficult to provide a-priori intervals that contain the solutions for each unknown. Thus it is advisable to use a function like `fsolve()`, which we met in Listing 4.5 of Section 4.5, and whose first argument can actually be a vector of functions rather than a single function. For instance, suppose that we want to solve the system

$$\begin{cases} f_1(x_1,x_2)=0 \\ f_2(x_1,x_2)=0 \end{cases} \quad \text{where} \quad \begin{cases} f_1(x_1,x_2)=4\,x_1+2\,x_2^2-4 \\ f_2(x_1,x_2)=\mathrm{e}^{x_1}+3\,x_1x_2-5\,x_2^3+3\ , \end{cases} \tag{4.7}$$

As start values we assume $x_1^{(0)}=1$ and $x_2^{(0)}=1$. The script follows

Listing 4.6 SystemSolve2.py

```
1  #!/usr/bin/env python3
2  from scipy.optimize import fsolve
3  from numpy import exp
4  #
5  def func(xvect):
6     x1,x2=xvect
7     r1=4*x1+2*x2**2-4
8     r2=exp(x1)+3*x1*x2-5*pow(x2,3)+3
9     return[r1,r2]
```

Lines 5-9 define the function `func()`, which is actually the list of the two functions $f_1(x_1,x_2)$ and $f_2(x_1,x_2)$ of (4.7). The argument `xvect` is actually a list of the two x_1 and x_2 values at which the functions are to be evaluated. Line 6 unpacks `xvect`, while lines 7 and 8 evaluate $f_1(x_1,x_2)$ and $f_2(x_1,x_2)$, respectively, Line 9 returns the list of the two function values.

```
10 xstart=(1,1)
11 sol=fsolve(func,xstart)
12 print("Solution:",sol)
13 #
14 print("Check:",func(sol))
```

Line 10 stores our start values $x_1^{(0)}$ and $x_2^{(0)}$ into `xstart`, line 11 calls `fsolve()` and stores the evaluated solutions for x_1 and x_2 into the list `sol`. Line 12 prints the solutions for x_1 and x_2 and, finally Line 14 prints the corresponding values of $f_1(x_1,x_2)$ and $f_2(x_1,x_2)$. The values of the two functions are expected to be very close to zero. This is what we get when we call `SystemSolve2.py`:

```
$>SystemSolve2.py
Solution:  [ 0.43880303 1.05943095]
Check:  [6.998845947236986 8e-12, -1.4656365010523587e-10]
```

Thus $x_1 = 0.43880303$ and $x_2 = 1.05943095$ are two numerical solutions of the system (4.7). As always with numerical methods, the corresponding values of the two functions are not exactly zero, but very small, namely $f_1(x_1,x_2) \simeq 7.0\times10^{-12}$ and $f_2(x_1,x_2) \simeq -1.5\times10^{-10}$.

If you give wrong start values, `fsolve()` may be unable to converge to a solution. In this case you get the following warning: *the iteration is not making good progress, as measured by the improvement from the last ten iterations*

4.6.2 Equations Involving Unknowns and Parameters

It is often convenient to pass parameter values to a function. For instance, our system 4.7 could be rewritten as

$$\begin{cases} f_1(x_1,x_2)=0 \\ f_2(x_1,x_2)=0 \end{cases} \quad \text{where} \quad \begin{cases} f_1(x_1,x_2)=a_{11}\,x_1+a_{12}\,x_2^2-c_1 \\ f_2(x_1,x_2)=a_{21}\mathrm{e}^{x_1}+a_{22}\,x_1x_2+a_{23}\,x_2^3-c_2\ , \end{cases} \tag{4.8}$$

so that the parameters a_{ij} and c_i can be changed in successive calls to the functions, related to different problems. This is how to do it:

Listing 4.7 SystemSolveParam.py

```
 1  #!/usr/bin/env python3
 2  from scipy.optimize import fsolve
 3  from numpy import exp
 4  #
 5  def func(xvect,params):
 6      x1,x2=xvect
 7      a11,a12,a21,a22,a23,c1,c2=params
 8      r1=a11*x1+a12*x2**2-c1
 9      r2=a21*exp(x1)+a22*x1*x2+a23*pow(x2,3)-c2
10      return[r1,r2]
```

The function `func()` now has two arguments: the list of *unknowns*, `xvect`, and the list of *parameters*, `param`. The function `fsolve()` will solve only for `xvect`, and leave the list `param` unchanged. The variable and parameter lists are unpacked at Lines 6 and 7, respectively. Lines 8 and 9 evaluate the two functions.

```
11  a11=4
12  a12=2
13  a21=1
14  a22=3
15  a23=-5
16  c1=4
17  c2=-3
18  parlist=[a11,a12,a21,a22,a23,c1,c2]
19  xstart=(1,1)
20  sol=fsolve(func,xstart,parlist)
21  print(sol)
```

Lines 11-18 define the parameter values and store them into the list `parlist`. Line 20 passes also the argument `parlist` to `fsolve()`, which now has three arguments, the third being the list of parameters appearing in the functions.

4.7 Integration of Functions

4.7.1 Introduction

The integrals of functions, even of elementary functions, can be computed analytically only in few special cases. In most cases the only choice is the numerical integration, also known as *quadrature*. Obviously, this leaves out the evaluation of indefinite integrals. Here we shall consider methods for the numerical evaluation of an integral of the form

$$I = \int_a^b f(x)\,\mathrm{d}x \tag{4.9}$$

based on adding up the values of $f(x)$ at a sequence of x values within the integration range $[a, b]$.

A rapid survey of some common methods follows.

4.7.2 Rectangular and Trapezoidal Rules

A large class of quadrature rules are based on the division of the integration interval $[a, b]$ into some number n of smaller subintervals, and approximating $f(x)$ by a polynomial of low degree (which is easy to integrate) in each subinterval. For simplicity we shall assume subintervals of equal length

$$\Delta x = \frac{b-a}{n} \,, \tag{4.10}$$

implying the following endpoints for the i-th subinterval

$$a_i = a + i\,\Delta x \,, \quad b_i = a + (i+1)\,\Delta x \,, \quad \text{with} \quad b_i = a_{i+1} \,, \quad \text{and} \quad i = 0, 1, 12, \ldots, n-1 \,. \tag{4.11}$$

The simplest method is to let the approximate function be a constant function (thus, a polynomial of degree zero) within each subinterval, passing through the point

$$\big(x_i, f(x_i)\big) \,, \quad \text{with} \quad x_i = a + (2i+1)\,\frac{\Delta x}{2} = a_i + \frac{\Delta x}{2} \,. \tag{4.12}$$

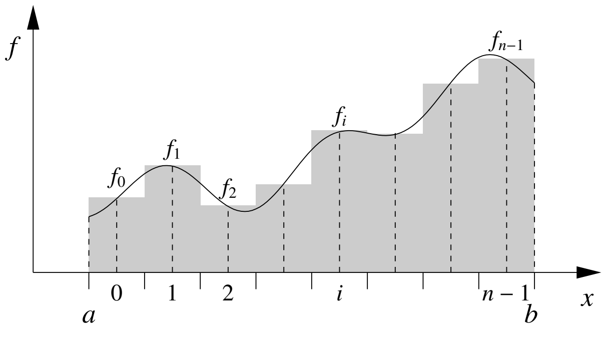


Figure 4.3

This is called the midpoint rule or rectangle rule. The resulting approximation is

$$I = \int_a^b f(x)\,\mathrm{d}x \simeq \Delta x \sum_{i=0}^{n-1} f(x_i) \,, \tag{4.13}$$

which corresponds to approximate the area under the figure curve by the shaded area of Fig. 4.3. The next step is approximating the function by a polynomial of degree one (a straight line) in each subinterval. For this, it is convenient to label $x_0 = a$, $x_n = b$, and $x_i = a_i = b_{i-1}$ for $1 \leqslant i \leqslant n-1$, as in Fig. 4.4. The i-th subinterval has x_i and x_{i+1} as upper and lower limits, respectively, and the corresponding approximating straight line passes through the points $\big(x_i, f(x_i)\big)$ and $\big(x_{i+1},\ f(x_{i+1})\big)$, so that the area below the function curve is approximated by a sum of trapezoids (shaded area in Fig. 4.4). The area of the i-th trapezoid is

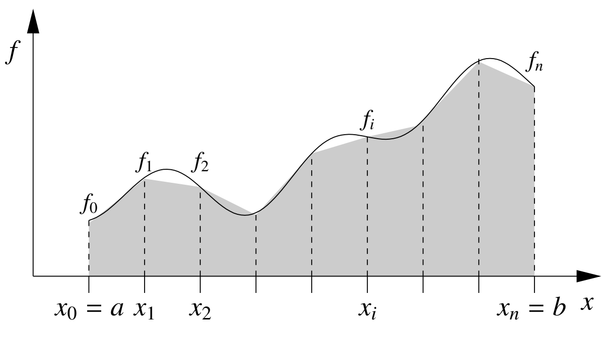


Figure 4.4

$$\frac{f(x_i) + f(x_{i+1})}{2}\,\Delta x \,, \tag{4.14}$$

and the approximation for the integral is

$$\begin{aligned} I &= \int_a^b f(x)\,\mathrm{d}x \\ &\simeq \Delta x \left[\frac{f(x_0) + f(x_n)}{2} + \sum_{i=1}^{n-1} f(x_i) \right] . \end{aligned} \tag{4.15}$$

Note that n function values $f_0 \ldots f_{n-1}$, corresponding to the subinterval midpoints of Fig. 4.3, are involved in (4.13), while $n+1$ function values $f_0 \ldots f_n$, corresponding to the subinterval upper and lower endpoints of Fig. 4.4, are involved in (4.15).

4.7.3 The Simpson Rule

In the next (and, in this context, last) step we approximate the area of a couple of adjacent subintervals by the area below a polynomial of degree two, i.e., a parabolic arc. This is shown for the couple of subintervals between x_{i-1} and x_{i+1} of Fig. 4.5. Thus, the whole integration interval $[a, b]$ must be divided into an even number n of subintervals, and we must have $i = 2m + 1$, with $m = 0, \ldots, (n/2) - 1$. The approximating parabola must pass through the three points (x_{i-1}, f_{i-1}), (x_i, f_i) and (x_{i+1}, f_{i+1}), denoted by the black dots in Fig. 4.5. For each couple of subintervals it is convenient to shift the x origin so that $x_{i-1} = -\Delta x$, $x_i = 0$ and $x_{i+1} = \Delta x$. In this reference frame we write the equation for the parabola as $y = \alpha_i x^2 + \beta_i x + \gamma_i$, and we must have

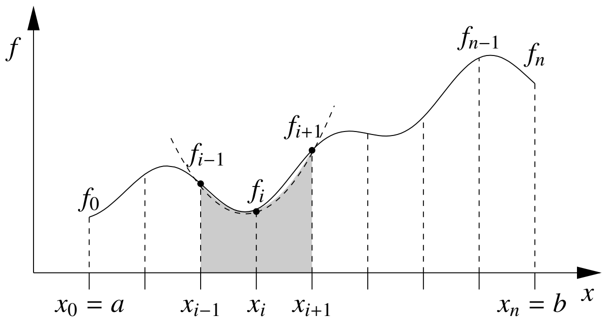


Figure 4.5

$$\begin{aligned} \alpha_i (\Delta x)^2 - \beta_i \Delta x + \gamma_i &= f_{i-1} , \\ \gamma_i &= f_i , \\ \alpha_i (\Delta x)^2 + \beta_i \Delta x + \gamma_i &= f_{i+1} . \end{aligned} \tag{4.16}$$

Solving for α_i, β_i and γ_i we obtain

$$\alpha_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{2(\Delta x)^2} , \quad \beta_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} , \quad \gamma_i = f_i , \tag{4.17}$$

and the area below the parabolic arc is

$$\Delta S_i = \int_{-\Delta x}^{\Delta x} \left(\alpha_i x^2 + \beta_i x + \gamma_i\right) \mathrm{d}x = \left[\alpha_i \frac{x^3}{3} + \beta_i \frac{x^2}{2} + \gamma_i x\right]_{-\Delta x}^{\Delta x} = \left(\frac{1}{3} f_{i-1} + \frac{4}{3} f_i + \frac{1}{3} f_{i+1}\right) \Delta x . \tag{4.18}$$

The approximate integral is thus

$$I \simeq S = \sum_i \Delta S_i = \frac{\Delta x}{3} \left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 4f_{n-1} + f_n\right) . \tag{4.19}$$

4.7.4 The *scipy.integrate.simps* Function

The *scipy.integrate* subpackage provides the `simps()` function discussed in Appendix C.1, which integrates the samplings of a function using the Simpson rule. As a simple example, Listing 4.8 evaluates the integral of the Gaussian function e^{-x^2} between -5 and 5 using `simps()`.

$$\int_{-5}^{5} e^{-x^2} \mathrm{d}x \tag{4.20}$$

Listing 4.8 CheckSimps.py

```python
#!/usr/bin/env python3
import numpy as np
```

```
3 from scipy.integrate import simps
4 #
5 x=np.linspace(-5.0,5.0,31)
6 y=np.exp(-x**2)
7 integ=simps(y,x,even='avg')
8 print(integ)
9 print(np.sqrt(np.pi))
```

Line 5 generates an array x comprising 31 equally spaced numbers between −5 and 5. Line 6 generates an array y such that $y_i = e^{-x_i^2}$ for $i = 0, 1, 2, \ldots, 30$. Line 7 evaluates the variable `integ` which equals the integral (4.20) as evaluated by the Simpson rule. The mandatory arguments of `simps()` are the array y, containing the sampling of the function to be integrated, and the array x, containing the abscissas of the sampling points. The optional argument `even` is active only if the number of sampling points n is even, thus corresponding to an odd number $n - 1$ of subintervals. In this case `even` can have the following three values, corresponding to different behaviors of `simps()`:

- `even='first'` integrate the first $n - 2$ intervals with the Simpson rule, and the last interval with the trapezoidal rule;
- `even='last'` integrate the first interval with the trapezoidal rule and the last $n - 2$ intervals with the Simpson rule;
- `even='avg'` average the results of the above two methods;

Lines 8 and 9 print `integ` and $\sqrt{\pi}$ for a comparison, since we know that

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} . \tag{4.21}$$

This is what we obtain when we run the script

```
$>CheckSimps.py
1.77245385117
1.77245385091
```

References

[1] W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in C, Second Edition*, Cambridge University Press, Cambridge, New York, Victoria, 1992.

Chapter 5

Numerical Solution of Ordinary Differential Equations (ODE)

5.1 Introduction

A differential equation is an equation that contains an unknown function (rather than an unknown value) to be determined, and at least one of its derivatives with respect to an independent variable. If the unknown function depends only on a single independent variable, the differential equation can contain only ordinary derivatives, and it is called an *ordinary differential equation*. On the other hand, if the unknown function depends on several independent variables, and the equation involves partial derivatives of the unknown function instead of ordinary derivatives, the equation is called a *partial differential equation*. In this chapter we are concerned with ordinary differential equations.

A problem involving ordinary differential equations (ODEs) of any order can always be reduced to the study of a system of first-order differential equations. For example the second-order differential equation

$$\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + f(x,y)\,\frac{\mathrm{d}y}{\mathrm{d}x} = g(x,y) \tag{5.1}$$

can be rewritten as the system of two first-order differential equations

$$\begin{aligned}\frac{\mathrm{d}y}{\mathrm{d}x} &= z(x,y)\\ \frac{\mathrm{d}z}{\mathrm{d}x} &= g(x,y) - f(x,y)\,z(x,y)\,,\end{aligned} \tag{5.2}$$

where z is a new unknown function. This is the standard procedure at the basis of the methods for the numerical solution of ODEs. Thus, the generic problem involving ordinary differential equations can be reduced to the study of a system of N coupled first-order differential equations involving N unknown functions y_i, with $i = 1, 2, \ldots, N$, of the form

$$\frac{\mathrm{d}y_i}{\mathrm{d}x} = f_i(x, y_1, \ldots, y_N)\,, \tag{5.3}$$

where the functions $f_i(x, y_1, \ldots, y_N)$ are known. We know that the solutions of differential equations are not completely specified unless appropriate boundary conditions on the y_i are given.

Boundary conditions are divided into two broad categories:

- Initial value problems, where all the y_i are known at some starting value x_0 of the independent variable. In this case it is desired to find the y_i at some final point x_f , or at some discrete list of points (for example, at tabulated intervals).
- In two-point boundary value problems, on the other hand, boundary conditions are specified at more than one x value. Typically, some of the conditions will be specified at the starting point x_0, and the remaining conditions at the final point x_f.

In the following we shall consider the initial value problem up to Section 5.4, while we shall have a look at the (in general more difficult) two-point boundary value problems in Section 5.5.

Most routines for the numerical solution of differential equations are based on the replacement of the differentials $\mathrm{d}y_i$ and $\mathrm{d}x$ appearing in the equations by small, but *finite*, steps Δy_i and Δx: they are thus called *finite-difference methods*. After the replacement, the equations are multiplied by Δx, thus leading to algebraic first-order formulas for the change in the functions Δy_i when the independent variable x is increased by one *step* Δx. At the limit of very small stepsizes a good approximation of the differential equation is obtained. The simplest implementation of this procedure is Euler's method, which is conceptually very important, but not recommended for practical use. However, all more refined methods rely on Euler's method as a starting point.

5.2 Euler and Runge-Kutta Methods

If we wish to solve numerically the differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x,y) \ , \tag{5.4}$$

with the initial condition $y(x_0) = y_0$, the Euler method, which is the simplest method, provides a table of values y_n and x_n, obtained by the recursive formulas

$$x_{n+1} = x_n + \Delta x \ , \quad y_{n+1} = y_n + f(x_n, y_n)\,\Delta x \ + O(\Delta x^2) \ , \tag{5.5}$$

where usually the spacing Δx is kept constant. The main disadvantage of this formula is that it is unsymmetrical: it advances the solution by a step Δx, but uses derivative information only at one end (the beginning) of the step. The error per step is of the order of Δx^2.

An improvement to the Euler method is the second-order Rung-Kutta method [nth order means that the error per step is of order $O(\Delta x^{n+1})$], defined by the sequence

$$\Delta y^{(1)} = f(x_n, y_n)\,\Delta x \ , \tag{5.6}$$

$$\Delta y^{(2)} = f\left(x_n + \frac{1}{2}\Delta x,\ y_n + \frac{1}{2}\Delta y^{(1)}\right)\Delta x \ , \tag{5.7}$$

$$y_{n+1} = y_n + \Delta y^{(2)} + O\left(\Delta x^3\right) \ , \tag{5.8}$$

where the Euler method of (5.6) is used to extrapolate the midpoint of the interval $(x_n + \Delta x/2,\ y_n + \Delta y^{(1)}/2)$ where we evaluate the derivative used for the more accurate $\Delta y^{(2)}$ value of (5.7).

But the most often used formula is the fourth-order Runge-Kutta method, which proceeds as follows

$$\Delta y^{(1)} = f(x_n, y_n)\,\Delta x\,, \tag{5.9}$$

$$\Delta y^{(2)} = f\left(x_n + \frac{1}{2}\Delta x,\ y_n + \frac{1}{2}\Delta y^{(1)}\right)\Delta x\,, \tag{5.10}$$

$$\Delta y^{(3)} = f\left(x_n + \frac{1}{2}\Delta x,\ y_n + \frac{1}{2}\Delta y^{(2)}\right)\Delta x\,, \tag{5.11}$$

$$\Delta y^{(4)} = f\left(x_n + \Delta x,\ y_n + \Delta y^{(2)}\right)\Delta x\,, \tag{5.12}$$

$$y_{n+1} = y_n + \frac{\Delta y^{(1)}}{6} + \frac{\Delta y^{(2)}}{3} + \frac{\Delta y^{(3)}}{3} + \frac{\Delta y^{(4)}}{6} + O\left(\Delta x^5\right)\,, \tag{5.13}$$

Thus the derivative is evaluated four times at each step: once at the initial point, twice at trial midpoints, and once at a trial endpoint, and the final y increment is evaluated as a weighted average of the four $\Delta y^{(i)}$ values. Consequently, the fourth-order Runge-Kutta method is superior to the second-order method if it can use a step at least twice as large achieving at least the same accuracy. This is very often the case, but not always.

5.3 The *scipy.integrate.odeint* Function

The `scipy.integrate.odeint()` function integrates a system of ordinary differential equations of the type (5.3) using *lsoda* from the FORTRAN library *odepack*. It solves the initial value problem for stiff or non-stiff systems of first order ODE's. We shall use it in the form
`y=odeint(f,y0,x,args=(params,))`
where `f(y,x0)` evaluates the derivative of `y` at `x0`, `y0` is an array containing the initial conditions on `y`, `x` is the sequence of x points at which `y` should be evaluated. The initial value point should be the first element of this sequence. Argument `args` is a tuple containing extra arguments to pass to the function. Things are probably made clearer by the example of Section 5.4.

5.4 Large-Amplitude Pendulum

The equation of motion for a simple pendulum without friction is

$$\ell^2 m \frac{\mathrm{d}^2\vartheta}{\mathrm{d}t^2} = -\ell m g \sin\vartheta\,, \quad \text{which reduces to} \quad \frac{\mathrm{d}^2\vartheta}{\mathrm{d}t^2} = -\frac{g}{\ell}\sin\vartheta\,, \tag{5.14}$$

where ℓ is the length of the pendulum, m its mass, $\ell^2 m$ its moment of inertia with respect to the pivot O of Fig. 5.1, and $\ell m g \sin\vartheta$ the torque of the gravity force $m\mathbf{g}$ with respect to the pivot. Equation (5.14) has no anlytical solution, but in the case of small oscillation amplitudes one can approximate $\sin\vartheta \simeq \vartheta$, obtaining the well known equation for the classical harmonic oscillator

$$\frac{\mathrm{d}^2\vartheta}{\mathrm{d}t^2} = -\frac{g}{\ell}\vartheta\,, \tag{5.15}$$

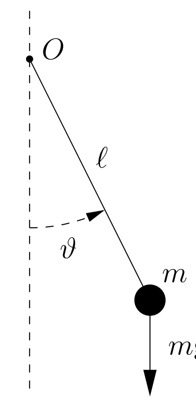


Figure 5.1

as found in any introductory Physics book. Here, however, we are interested in the numerical solution of the more general equation (5.14). The solution can be obtained by running the following script

Listing 5.1 PlotPendulum.py

```
 1 #!/usr/bin/env python3
 2 #coding: utf8
 3 import numpy as np
 4 from scipy.integrate import odeint
 5 import matplotlib.pyplot as plt
 6 #
 7 def dydt(y0,t, params):
 8     theta,omega = y0
 9     GdivL,=params
10     derivs = [omega,-GdivL*np.sin(theta)]
11     return derivs
12 #
```

Lines 7-11 define the function `dydt()` required as first argument by `odeint()`. The arguments of `dydt()` are the array of initial conditions `y0`, the array of times `t` at which the derivatives are required, and the array of additional parameters `params` needed for evaluating the derivatives. We want to solve the second-order differential equation (5.14), which, according to (5.2), can be rewritten as the system of two first-order differential equations

$$\begin{aligned}\frac{\mathrm{d}\vartheta}{\mathrm{d}t} &= \omega \\ \frac{\mathrm{d}\omega}{\mathrm{d}t} &= -\frac{g}{l}\sin\vartheta\,. \end{aligned} \tag{5.16}$$

Line 8 copies the initial values for θ and ω from the array `y0`. Line 9 copies our only parameter, `GdivL` corresponding to the ratio g/l, from the single-element array `params`, see Subsection 1.12.2. Line 10 builds the list `derivs`, comprising the time derivative of ϑ (simply ω), and the time derivative of ω, given by the second of (5.16). The function returns `derivs` at Line 11.

```
13 theta0=np.pi/2.0
14 omega0=0.0
15 y0=[theta0,omega0]
16 #
17 GdivL=4.9
18 params=[GdivL]
19 Omega=np.sqrt(GdivL)
20 period=2.0*np.pi/Omega
21 #
```

Lines 13-14 fix the initial conditions of the pendulum motion: the pendulum starts from a horizontal position, $\vartheta(0) = \pi/2$, with zero angular velocity, $\omega(0) = 0$. The initial conditions are stored in the array `y0` at line 15. The only parameter needed by the function `dydt()` is the ratio g/ℓ, defined at line 17 and stored into the list `params` at line 18. A pendulum length $\ell = 2$ m is assumed, with $g = 9.8$ m/s^2. Variable `Omega` at line 19 is the angular frequency for the small amplitude (harmonic) oscillations, $\Omega = \sqrt{g/\ell}$, while `period` at line 20 is the oscillation period of the purely harmonic oscillator, $T = 2\pi/\Omega$, i.e., $T \simeq 2.838$ s in our case.

```
22 t=np.linspace(0.0,period,101)
23 ThetaHar=theta0*np.cos(Omega*t)
```

```
24  #
25  sol=odeint(dydt,y0,t,args=(params,))
26  theta=sol[:,0]
27  plt.plot(t,theta,'k')
28  plt.plot(t,ThetaHar,'k--')
```

Array `t`, defined at line 22, comprises the times, in seconds, at which $\vartheta(t)$ and $\omega(t)$ are to be evaluated, from $t = 0$ s up to $t = 2.838$ s. A total of 101 equally spaced times, corresponding to 100 time intervals, are requested in the interval $0 \leqslant t \leqslant T$. Line 23 evaluates the angular position $\vartheta_{\text{harmonic}}$, at the same times, of a hypothetical pendulum following a purely harmonic motion with angular frequency Ω, for comparison to our large-amplitude case. At line 25 function `odeint` solves the system (5.16) numerically at the times specified by the list `t`, with the initial conditions specified by the list `y0`. The parameter g/ℓ is passed by the list `params` [see Appendix C.2 for the arguments of `odeint()`]. The solutions are stored into the matrix `sol`. Line 26 copies the ϑ_i values at the required instants from matrix `sol` into the vector `theta`. Column `sol(:,1)` comprises the angular velocity values ω_i at the same instants. Line 27 plots the large-amplitude pendulum positions, using a black (`'k'`) solid line, while line 28 plots the harmonic positions using a dashed black line (`'k--'`).

```
29  plt.axhline(linewidth=1, color='k')
30  plt.rcParams.update({'font.size': 18})
31  plt.grid()
32  plt.xlabel(r'$t$/s', fontsize=22)
33  plt.ylabel(r'$\vartheta$/rad',fontsize=22)
34  plt.text(2.25,1.0,'Harmonic',fontsize=16,rotation=65)
35  plt.text(2.25,0.4,'Large Amplitude',fontsize=16,rotation=65)
36  plt.tight_layout()
37  plt.savefig('LargAmpl00.pdf',format='pdf',dpi=1000)
38  plt.show()
```

Line 29 plots a horizontal black line corresponding to the $\vartheta = 0$ axis of the plot. Line 30 sets the font size for the plot. Line 31 draws a grid. Lines 32 and 33 label the horizontal and vertical axes, respectively. Line 34 writes a text into the figure at $x = 2.25, y = 1.0$, rotated by 65 degrees, which labels the curve for the harmonic motion. Line 35 does the same for the curve corresponding to the large-amplitude-pendulum motion, The fontsize values at lines 30, 32, 33, 34 and 35 are best determined by trial and error, in order to obtain the best result for Fig. 5.2. The same is true for the rotation angles at lines 34 and 35. Line 36 forces the figure to include the axis labels. Line 37 saves the result into a pdf figure, in our case Fig. 5.2. Line 38 shows the plot on the monitor. If you wish to tabulate $\vartheta(t)$, the last lines of the code can be changed as follows

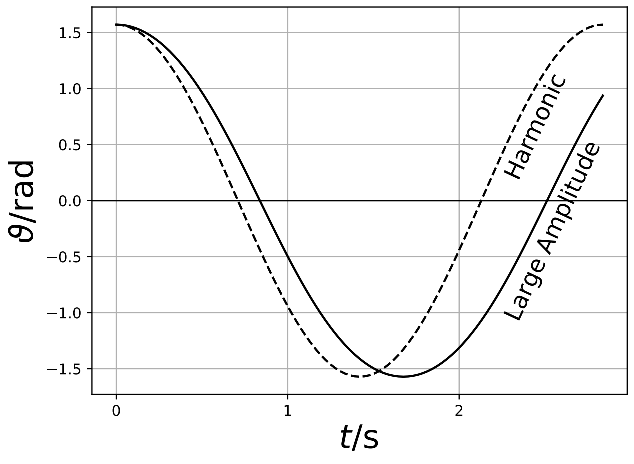


Figure 5.2

```
36  plt.tight_layout()
37  plt.savefig('LargAmpl00.pdf',format='pdf',dpi=1000)
38  hnd=open("large_amplitude.txt",'w')
39  i=0
```

```
40 hnd.write('␣␣i␣␣␣␣sec␣␣␣␣theta␣␣␣harmonic\n\n')
41 while i<len(theta):
42   hnd.write('{:3d}{:8.3f}{:8.3f}{:8.3f}\n'.format(i,t[i],theta[i],ThetaHar[i]))
43   i+=1
44 hnd.close()
45 plt.show()
```

i	sec	theta	harmonic
0	0.000	1.571	1.571
1	0.028	1.569	1.568
2	0.057	1.563	1.558
3	0.085	1.553	1.543
4	0.114	1.539	1.521
5	0.142	1.521	1.494
6	0.170	1.500	1.460
7	0.199	1.474	1.421
8	0.227	1.445	1.376
9	0.255	1.411	1.326
10	0.284	1.374	1.271

Table 5.1

Line 38 creates the file `large_amplitude.txt` in `write` mode (`'w'`), and associates it to the *file handler* `hnd`. Line 38 sets the counter `i` to zero, line 39 writes the table headers into the table, and the loop 40-42 writes the single lines of the table, inserting the index `i` in column 0, the time `t[i]` in column 1, the large-amplitude angular position $\vartheta(t)$ in column 2, and the "harmonic" angular position $\vartheta_{\text{harmonic}}(t)$ in column 3. Line 43 closes the file containing the table. The first few lines of the resulting table are shown in Table 5.1.

The file `large_amplitude.txt` can now be opened and read by any editor, or opened in `read` mode by another Python script using the code
`hnd=open(large_amplitude.txt,'r')`
then the single lines can be read with `hnd.readline()`.

5.5 The Shooting Method

The differential equation of Section 5.4 was second-order because Newton's second law involves a second-order derivative. We know that the general solution of an nth-order differential equation contains n arbitrary independent constants of integration, and in the case of our pendulum we arbitrarily chose two initial conditions, namely the initial position $\vartheta(0) = \pi/2$ and the initial angular velocity $\dot{\vartheta} = \omega = 0$.

We conclude this chapter considering two problems involving second-order ordinary differential equations where we are interested in solutions determined by the conditions at two boundaries, one initial and one final condition. Both problems involve quantum mechanics and the time-independent one-dimensional Schrödinger equation, which involves the second-order derivative with respect to the space coordinate.

5.5.1 The Finite Square Well

Our first example is a simple one-dimensional problem which, in spite of being simple, has no analytical solution: the *finite square well*. In this problem a particle of mass m is confined to a box of width $2x_0$ which has finite potential walls of height V_0, as shown in Fig. 5.3. Denoting the particle position by x, we can choose a coordinate system where the potential energy of the particle can be written as

$$V(x) = \begin{cases} 0 & \text{if} \quad |x| \le x_0 \, , \\ V_0 & \text{if} \quad |x| > x_0 \, . \end{cases} \tag{5.17}$$

The time-independent Schrödinger equation for the particle is thus

$$\left(V(x) - \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\psi(x) = E\psi(x) \; , \tag{5.18}$$

which can be rewritten

$$\left(V_0 H(|x| - x_0) - \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\psi(x) = E\psi(x) \; , \tag{5.19}$$

where E is the energy eigenvalue, and $H(x)$ is the Heaviside step function, defined as $H(x) = 0$ if $x < 0$, and $H(x) = 1$ if $x > 0$. We have a discrete spectrum of bound states for eigenvalues $E_n < V_0$, and a continuous spectrum of free states with eigenvalues $E > V_0$. Here we are interested only in bound states. Both for bound and free states, the wavefunction has three different mathematical expressions, depending on whether the particle is at the left of the box, inside the box or at the right of the box:

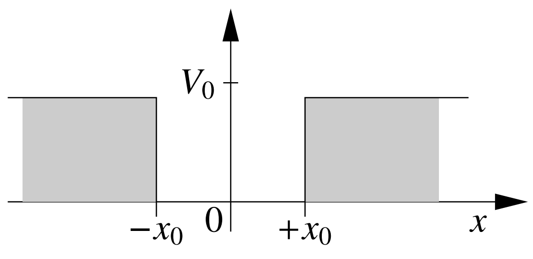


Figure 5.3

$$\psi(x) = \begin{cases} \psi_a(x) \; , & \text{if} \quad x < -x_0 \; , \\ \psi_b(x) \; , & \text{if} \quad -x_0 < x < x_0 \; , \\ \psi_c(x) \; , & \text{if} \quad x > x_0 \; . \end{cases} \tag{5.20}$$

For both bound and free states the solutions inside the well, i.e., for $-x_0 < x < x_0$, where the potential energy is zero, have the form

$$\psi_b(x) = A\sin(kx) + B\cos(kx) \; , \quad \text{with} \quad k = \frac{\sqrt{2mE}}{\hbar} \; , \tag{5.21}$$

where A and B are two constants to be determined. The solutions for bound states ($E_n < V_0$) outside of the well have the form

$$\begin{aligned} &\psi_a(x) = C\,\mathrm{e}^{\alpha x} \; , \\ &\psi_c(x) = D\,\mathrm{e}^{-\alpha x} \; , \quad \text{both with} \quad \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \; , \end{aligned} \tag{5.22}$$

where C and D are two further constants to be determined, and we are disregarding the solutions diverging for $x \to -\infty$ or $x \to \infty$. With our coordinate choice the potential energy $V(x)$ is an even function, therefore our eigenfunctions must be either even or odd functions of x, implying that either $A = 0$ and $C = D$ (even functions), or $B = 0$ and $C = -D$ (odd functions). Finally, a wave function $\psi(x)$ and its first derivative $\mathrm{d}\psi(x)/\mathrm{d}x$ must be continuous everywhere, including at $x = \pm x_0$, where the potential $V(x)$ is discontinuous. This implies that the logarithmic derivative

$$\frac{\mathrm{d}\ln[\psi(x)]}{\mathrm{d}x} = \frac{1}{\psi(x)}\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} \tag{5.23}$$

must be continuous at $x = \pm x_0$. Therefore we must have

$$\begin{aligned}
\text{even:} \quad & -\frac{kB\sin(kx_0)}{B\cos(kx_0)} = -\frac{\alpha C\,\mathrm{e}^{-\alpha x_0}}{C\,\mathrm{e}^{-\alpha x_0}} \quad \Rightarrow \quad \tan(kx_0) = \frac{\alpha}{k} \quad \Rightarrow \quad \tan\left(\frac{\sqrt{2mE}}{\hbar}x_0\right) = \sqrt{\frac{V_0 - E}{E}}\,, \\
\text{odd:} \quad & \frac{kB\cos(kx_0)}{B\sin(kx_0)} = -\frac{\alpha C\,\mathrm{e}^{-\alpha x_0}}{C\,\mathrm{e}^{-\alpha x_0}} \quad \Rightarrow \quad \cot(kx_0) = -\frac{\alpha}{k} \quad \Rightarrow \quad \cot\left(\frac{\sqrt{2mE}}{\hbar}x_0\right) = -\sqrt{\frac{V_0 - E}{E}}\,.
\end{aligned} \tag{5.24}$$

The above conditions cannot be satisfied by arbitrary values of the particle energy E. Only certain energy values (the energy eigenvalues), which solve one of the (5.24) for E, are allowed. Thus the energy levels of the particle such that $E < V_0$ are discrete, and the corresponding eigenfunctions are bound states. Equations (5.24) cannot be solved analytically, and the values of E for which they hold must be found numerically. A possibility is to write them in the form $f(E) = 0$, with, for instance,

$$f(E) = \tan\left(\frac{\sqrt{2mE}}{\hbar}x_0\right) - \sqrt{\frac{V_0 - E}{E}} \tag{5.25}$$

for the even case, and then use one of the numerical root-finding algorithms discussed in Chapter 4 to determine the allowed values of E.

In the following we prefer to consider another numerical method, which will provide both the energy eigenvalues and the discretization of the eigenfunctions of the finite square well.

For this it is convenient to write (5.19) in terms of dimensionless quantities. We start by dividing (5.19) by V_0, obtaining

$$\frac{\hbar^2}{2mV_0}\frac{\mathrm{d}^2\psi_n(x)}{\mathrm{d}x^2} = \left[(H(|x| - x_0) - \frac{E_n}{V_0}\right]\psi_n(x)\,, \tag{5.26}$$

where we are numbering the eigenfunction $\psi_n(x)$ and the energy eigenvalues E_n because we are dealing with a discrete spectrum. Then we introduce the first dimensionless variable

$$\xi = \frac{x}{\alpha}, \quad \text{such that} \quad x = \alpha\xi\,, \tag{5.27}$$

where $\alpha = \hbar/\sqrt{2mV_0}$ has the dimensions of a length, and obtain

$$\frac{\mathrm{d}^2\psi_n(\xi)}{\mathrm{d}\xi^2} = \left[H(|\xi| - \xi_0) - \frac{E_n}{V_0}\right]\psi_n(\xi)\,, \quad \text{where} \quad \xi_0 = \frac{x_0}{\alpha} = \frac{\sqrt{2mV_0}}{\hbar}x_0\,. \tag{5.28}$$

If we introduce the further dimensionless quantities $W_n = E_n/V_0$, corresponding to the energy eigenvalues measured in units of the well depth V_0, our final equation is

$$\frac{\mathrm{d}^2\psi_n(\xi)}{\mathrm{d}\xi^2} = \left[H(|\xi| - \xi_0] - W_n\right]\psi_n(\xi)\,. \tag{5.29}$$

As discussed in Section 5.1, the second-order differential equation (5.29) is equivalent to the following system of two first-order ordinary differential equations (ODE)

$$\begin{aligned}
\frac{\mathrm{d}\psi_n(\xi)}{\mathrm{d}\xi} &= \chi_n \\
\frac{\mathrm{d}\chi_n(\xi)}{\mathrm{d}\xi} &= \left[H(|\xi| - \xi_0] - W_n\right]\psi_n(\xi)\,,
\end{aligned} \tag{5.30}$$

which we shall use for the numerical solution. If an eigenvalue W_n, and the corresponding initial values for $\psi_n(0)$ and $\chi_n(0)$, were known, solving the system (5.30) numerically would provide the discretization of the functions $\psi_n(\xi)$ and $\chi_n(\xi) = \mathrm{d}\psi_n(\xi)/\mathrm{d}\xi$. In the present case the potential is even, thus the eigenfunctions $\psi_n(\xi)$ are either even, with $\chi_n(0) = \mathrm{d}\psi_n(0)/\mathrm{d}\xi = 0$, or odd, with $\psi_n(0) = 0$. The eigenfunction corresponding to the ground state, $\psi_0(\xi)$, is even, and the eigenfunctions ψ_n, with $n > 0$, corresponding to the higher energy levels, are alternatively odd (n odd), and even (n even). If $\psi_n(\xi)$ is an eigenfunction of the Hamiltonian, so is $z\psi_n(\xi)$, with z any complex number. Thus we are allowed to assume the initial conditions

$$\begin{aligned} &\psi_n(0) = 1\,, \qquad &&\chi_n(0) = 0\,, \qquad &&\text{for } n \text{ even,} \\ &\psi_n(0) = 0\,, \qquad &&\chi_n(0) = 1\,, \qquad &&\text{for } n \text{ odd.} \end{aligned} \tag{5.31}$$

Obviously, numerical integration with these initial conditions does not lead to a normalized wavefunction, however, once the wavefunction is found, we can easily evaluate the normalization factor. But we must still determine the correct values of the eigenvalues W_n.

5.5.2 The Shooting Method

The *shooting method* is a method for solving boundary value problems by reducing them to the solution of initial value problems. Roughly speaking, we *shoot out* trajectories in different directions by changing the initial values, until we find the trajectory reaching the desired boundary value. For instance, we know that in our case, the boundary conditions for a bound state are

$$\lim_{\xi\to\pm\infty} \psi_n(\xi) = 0\,. \tag{5.32}$$

These conditions are fulfilled if we insert the conditions (5.31) and the correct value for W_n into the system (5.30), and perform the numerical integration of the ODE system from $\xi = 0$ to $\xi = +\infty$ (actually, up to a sufficiently large value of ξ). We don't need the integration from $\xi = 0$ to $\xi = -\infty$ because of the symmetry of the problem. But, if the value of W_n inserted into (5.30) is not correct, we get a wavefunction $\psi(\xi)$ diverging for $|\xi| \to \infty$. For instance, if we assume $\xi_0 = 10$ in (5.30), the ground state eigenvalue is

$$W_0 = 0.02037903954499\ldots \tag{5.33}$$

(we shall see in the following how this value can be obtained). Fig. 5.4 shows the behavior of $\psi(\xi)$ up to $\xi = 30$. If we insert a slightly different value, say $W_0 \pm \delta W$, with $\delta W = 5 \times 10^{-10}$, we see that $\psi(\xi)$ diverges with increasing ξ. In this case we have $\lim_{\xi\to\infty}\psi(\xi) = -\infty$ for $W_0 - \delta W$, and $\lim_{\xi\to\infty}\psi(\xi) = +\infty$ for $W_0 + \delta W$. Obviously a computer does not deal with real

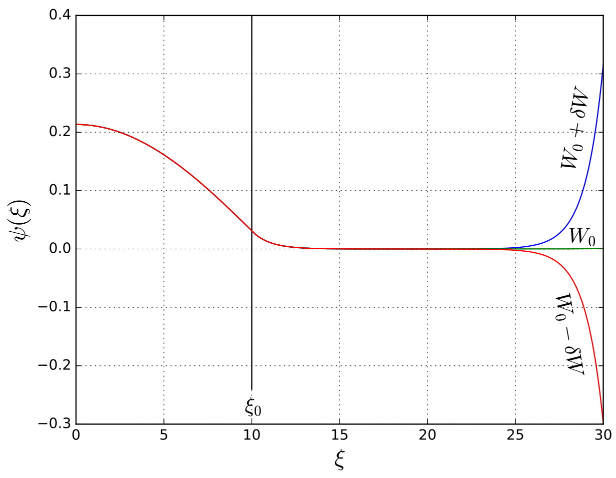


Figure 5.4 Numerical integrations of the ODE system (5.30), assuming the correct normalized energy eigenvalue W_0 (black line), and the slightly different values $W_0 - \delta W$ (red line) and $W_0 + \delta W$ (blue line), with $\delta W/W_0 \simeq 2.5 \times 10^{-8}$. Incorrect values of W_0 lead to divergence at high ξ.

numbers, but all our values, including (5.33), are affected by truncation errors. This means that we observe a divergence of ψ also for our "correct" value of W_0, provided that we go up to sufficiently high ξ values. It is a matter of the precision we require, compatibly with the number of bits used by the computer for storing numbers. In our case the shooting method works as follows:

1. Not knowing the exact value of W_0, we start by inserting an educated guess $W_0^{(0)} < W_0$ into (5.30). Then we integrate our ODE system up to a sufficiently high value $\xi_{\max}$ of ξ, where we expect $\psi(\xi_{\max})$ to be practically zero. In the present case we know that the energy of our particle must be greater than zero, so, we start from $W_0^{(0)} = 0$. The numerical integration will provide a discretized wavefunction $\psi_0^{(0)}(\xi)$, with $\psi_0^{(0)}(\xi_{\max})$ different from zero and usually very large in absolute value.

2. Now we insert the new value $W_0^{(1)} = W_0^{(0)} + \Delta W$ into (5.30), where the increase ΔW must be smaller than the distance between two consecutive eigenvalues. Since, again, we don't know the eigenvalues and their spacing yet, determining a correct step ΔW requires an educated guess and some trial and error. We integrate the system, and determine $\psi_0^{(1)}(\xi)$. If $\psi_0^{(1)}(\xi_{\max})$ has the same sign as $\psi_0^{(0)}(\xi_{\max})$ we iterate the procedure, with $W_0^{(i+1)} = W_0^{(i)} + \Delta W$, until we find $\psi_0^{(i+1)}(\xi_{\max})\,\psi_0^{(i)}(\xi_{\max}) < 0$.

3. When $\psi_0^{(i+1)}(\xi_{\max})\,\psi_0^{(i)}(\xi_{\max}) < 0$, i.e., when $\psi_0^{(i+1)}(\xi_{\max})$ and $\psi_0^{(i)}(\xi_{\max})$ have opposite sign, the interval $(W_0^{(i)}, W_0^{(i+11)})$ contains the correct ground-state eigenvalue W_0, which can be determined with the required accuracy, for instance, by the bisection method. This will lead to W_0 and $\psi_0(\xi)$.

4. Once W_0 has been determined, we determine the first-excited eigenvalue W_1 and eigenfunction $\psi_1(\xi)$ starting from the initial value $W_1^{(0)} = W_0 + \Delta W$, and proceeding as in points 1-3. Successive bound eigenstates are determined analogously, always starting with $W_{i+1}^{(0)} = W_i + \Delta W$. Note that the finite square well always has at least one bound state (the ground state), and its number of bound states is finite.

Here follows a possible Python code for determining the bound states of a square well with half-width $\xi_0 = 10$.

Listing 5.2 FiniteWell.py

```
1  #!/usr/bin/env python3
2  #
3  import numpy as np
4  from scipy.integrate import odeint,simps
5  import matplotlib.pyplot as plt
6  #
```

Lines 1-5 are the usual headers.

```
7  xi0=10.0
8  nPointsWell=100
9  nPointsPlot=3*nPointsWell
10 nPoints=5*nPointsWell
11 scale=0.2
12 xiMaxPlot=(xi0*nPointsPlot)/nPointsWell
13 xiMax=(xi0*nPoints)/nPointsWell
14 EigvStep=0.05
```

```
15  DeltaXi=xi0/nPointsWell
16  tolerance=1.0e-12;
17  #
18  xi=np.linspace(0,xiMax,nPoints)
19  #
```

Line 7 defines the square-well half-width `xi0` (ξ_0). Lines 8-10 are the numbers for the sampling points for the wavefunctions from 0 to the right border of the potential well (`nPointsWell`), from 0 to the right end of the plot (`nPointsPlot`), and the total number of points used for the calculations (`nPoints`). Variable `xiMaxPlot` is the highest plotted ξ value, while `xiMax` is the highest ξ value used for calculations. Variable `EigvStep` is the increase step ΔW, `DeltaXi` is the spacing between consecutive points, and `tolerance` is the required accuracy on the eigenvalues W_n. Line 18 builds the ξ array consisting of `nPoints` evenly spaced values from 0 to $\xi_{\max}$ (the points at which the functions must be evaluated).

```
20  def dfdxi(y,xi,params):
21    psi,dpsidxi=y      #     unpack y
22    E,xi0=params       #     unpack parameters
23    if xi<xi0:
24      derivs=[dpsidxi,-E*psi]
25    else:
26      derivs=[dpsidxi,(1-E)*psi]
27    return derivs
28  #
```

Lines 20-28 define the function `dfdxi(y,xi,params)`, which returns the derivatives of ψ and of $\chi = \mathrm{d}\psi/\mathrm{d}\xi$. Array `y` contains the values of ψ and $\mathrm{d}\psi/\mathrm{d}\xi$ at the start point of each integration step, which are unpacked at Line 21. The array `xi` contains the points at which the functions ψ and $\mathrm{d}\psi/\mathrm{d}\xi$ must be evaluated. The array `params` contains the trial eigenvalue $W_n^{(i)}$, unpacked as `E`, and the half-width of the square well ξ_0, unpacked as `xi0`. Lines 23-26 evaluate the derivatives, which are stored into the array `derivs`. The derivative of ψ always equals $\chi = \mathrm{d}\psi/\mathrm{d}\xi$, while we have (Lines 23-26)

$$\frac{\mathrm{d}\chi}{\mathrm{d}\xi} = \frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} = \begin{cases} -W_n^{(i)}\psi & \text{if} \quad \xi < \xi_0 \, , \\ \left(1 - W_n^{(i)}\right)\psi & \text{if} \quad \xi > \xi_0 \, . \end{cases} \tag{5.34}$$

Line 27 returns the derivatives to the calling function.

```
29  def SymmWell(params,xi,iEv,EigvStart,EigvStep,tolerance,dfdxi,psi):
30    # ........................................................ initialize
31    eigv1=EigvStart
32    params[0]=eigv1
33    if iEv%2==0:
34      y=[1.0,0.0]
35    else:
36      y=[0.0,1.0]
37    psoln=odeint(dfdxi,y,xi,args=(params,))
38    PsiEnd1=psoln[-1,0]
39    # ............................................... search for interval
40    while True:
41      eigv2=eigv1+EigvStep
42      if eigv2>1.0:
43        return -1
```

```
44          params[0]=eigv2
45          psoln=odeint(dfdxi,y,xi,args=(params,))
46          PsiEnd2=psoln[-1,0]
47          if (PsiEnd1*PsiEnd2)<0.0:
48              break
49          PsiEnd1=PsiEnd2
50          eigv1=eigv2
51      # ..................................... logarithmic search for eigenvalue
52      while True:
53          eigvmid=(eigv1+eigv2)/2.0
54          if abs(eigv1-eigv2)<tolerance:
55              break
56          params[0]=eigvmid
57          psoln=odeint(dfdxi,y,xi,args=(params,))
58          PsiEndMid=psoln[-1,0]
59          if (PsiEndMid*PsiEnd1)>0 :
60              PsiEnd1=PsiEndMid
61              eigv1=eigvmid
62          else:
63              PsiEnd2=PsiEndMid
64              eigv2=eigvmid
65      # ................................................. list wave function
66      del psi[:]
67      for i in range(len(xi)):
68          psi.append(psoln[i,0])
69      # ..................................................................
70      return eigvmid
71  #
```

Lines 29-70 define the function `SymmWell(params, xi, iEv, EigvStart, EigvStep, tolerance, dfdxi, psi)`, which returns the eigenvalue W_n, stored in `eigvmid`, and the corresponding discretized eigenfunction ψ_n, stored in the list `psi`. The arguments `params`, `xi`, `EigvStep`, `tolerance` and `dfdxi` (the function starting at Line 20) have been discussed above. Variable `iEv` is the index n labeling both W_n and ψ_n, needed because $\psi_n(\xi)$ is even if `iEv` is even, odd if `iEv` is odd. Variable `Eigvstart` is the start trial value $W_n^{(0)}$, while `EigvStep` is ΔW, the step used for the search, `psi` is the address of an array where the discretization of ψ_n will be stored.

The lower limit for the eigenvalue search is `eigv1` (corresponding to $W_n^{(0)}$), which is initially set equal to `EigvStart` at Line 31. Line 32 stores `eigv1` into `params(0)`, for passing it to function `dfdxi()`. Lines 33-36 set the values of $\psi(0)$ and $\chi(0)$ according to (5.31). Line 37 calls the library function `scipy.integrate.odeint()`, discussed in Section 5.3, which integrates a system of ordinary differential equations. Line 39 copies the value of $\psi_n^{(0)}(\xi_{\max})$ into `PsiEnd1`.The loop 40-50 searches for an interval containing the eigenvalue W_n. Line 41 assigns the value $W_n^{(i+1)} = W_n^{(i)} + \Delta W$ to `eigv2`. If $W_n^{(i+1)} > 1$ we are above the well depth ($E > V_0$), and Lines 42-43 break the search, forcing the function to return an impossible negative eigenvalue. Lines 44-46 call `odeint()` again, and evaluate $\psi_n^{(i+1)}(\xi_{\max})$, stored in `PsiEnd2`.

The loop stops if $\psi_n^{(i+1)}(\xi_{\max})\,\psi_n^{(i)}(\xi_{\max}) < 0$, otherwise `PsiEnd2` and `eiv2` are copied into `PsiEnd1` and `eiv1`, and the procedure is iterated. The loop 52-64 evaluates W_n with the required accuracy. Line 53 assigns the arithmetic mean of the upper and lower bounds of the interval to `eigvmid`. If the interval width is smaller than `tolerance` the loop is terminated at Line 55. Otherwise `eigvmid` is stored in `params[0]`, `odeint()` is called at Line 57, and the corresponding value of $\psi_n(\xi_{\max})$ is stored into `PsiEndMid`. In Lines 59-64 if `PsiEndMid` and `PsiEnd1` have the same sign, `PsiEndMid` replaces `PsiEnd1`, otherwise `PsiEndMid` repalces `PsiEnd1`, in any case the interval width is halved. At Lines 66-68 list `psi` is cleared, then it is filled with the discretized eigenfunction. At Line 70 `SymmWell()` returns the eigenvalue to the calling function. Here end the function definitions, and the main program starts at Line 73.

```
72  # ..................................................  ......................
73  x=np.linspace(-xiMaxPlot,xiMaxPlot,(2*nPointsPlot)+1)
74  # ............................................................ draw grid
75  plt.grid(True)
76  # ......................................................................
77  eigv=[]
78  EigvStart=0.0;
79  i=0
```

Line 73 stores the ξ interval to be plotted into list `x`. Line 75 asks for a grid in the plot, Line 77 creates an empty list for storing the eigenvalues, Line 78 assigns the lower end of the search interval of the first eigenvalue, `EigvStart`. Line 79 assigns the index of the ground state, $i = 0$, the eigenfunction will be symmetric.

```
80  while True:
81    params=[EigvStart,xi0]
82    psi=[]
83    eigv.append(SymmWell(params,xi,i,EigvStart,EigvStep,tolerance,dfdxi,psi))
84    if eigv[i]>0:
85      print(i,eigv[i])
86    else:
87      break
88    # ...................................... truncate diverging tail of psi
89    while len(psi)>5:
90      if abs(psi[-2])>abs(psi[-1]):
91        break
92      psi.pop()
93    # ........................................................ normalize psi
94    NormFact=np.sqrt(2.0*simps(np.square(psi),dx=DeltaXi,even='first'))
95    # ............................................ truncate to plot length
96    del psi[(nPointsPlot+1):]
97    if len(psi)<(nPointsPlot+1):
98      while len(psi)<(nPointsPlot+1):
99        psi.append(0.0)
100   normpsi=[i*(scale/NormFact) for i in psi]
101   psineg=list(reversed(normpsi))
102   if i%2==1: # ......................... odd functions are antisymmetric
103     for k in range(len(psineg)):
104       psineg[k]=-psineg[k]
105   # ...................................................... form whole psi
106   psineg.pop()
107   psi=psineg+normpsi
108   #——————————————————————————————————————————
109   EnerShift=eigv[i]
110   psi=[x+EnerShift for x in psi]
111   plt.plot([-xiMaxPlot,xiMaxPlot],[EnerShift,EnerShift],'black')
112   plt.plot(x,psi)
113   # .................................................... next eigenvalue
```

```
114     EigvStart=eigv[i]+EigvStep
115     i+=1
```

The loop 80-115 searches for the eigenvalues and eigenfunctions of our problem. Line 81 assigns the values of `params` needed by `dfdxi()`, Line 83 calls `SymmWell()` and appends the new energy eigenvalue to `eigv`. The loop is interrupted if `eigv[i]<0`, meaning that we have reached the top of the well. If a new eigenvalue has been found the loop 89-93 truncates the list `psil` where the calculated $\psi(\xi)$ starts to increase because of the round-off error on the eigenvalue. Line 94 evaluates the normalizing constant

$$k = \sqrt{2\int_0^\infty |\psi_n(\xi)|^2 \mathrm{d}\xi}, \tag{5.35}$$

such that $\Psi_n(\xi) = \psi_n(\xi)/k$ is a normalized wavefunction. Actually the upper integration limit is obviously not infinity, but the last point of the list `psi`. Line 96 deletes the list points above the plot limit. If `psi` was already too short, it is zero-padded at Lines 97-99. Line 100 evaluates the normalized wavefunction Ψ_n, times a scale factor needed for the plot. Lines 101-107 build the complete wavefunction, inserting the values corresponding to $\xi < 0$. The function is even if `i` is even, odd if `i` is odd. Line 106 pops the last value of `psineg`, otherwise the value $\psi_n(0)$ would appear twice in the complete list built at Line 107. Lines 109-113 plot the wavefunction, shifted upwards by the energy eigenvalue. Line 111 plots a straight horizontal Line corresponding to the eigenvalue.

Line 114 assigns the lower limit for the search of the next eigenvalue, and Line 115 increases the eigenstate index.

```
116  # ...................................................... plot square well
117  plt.plot([-xiMaxPlot,-xi0],[1.0,1.0],color='black')
118  plt.plot([-xi0,-xi0],[1.0,0.0],color='black')
119  plt.plot([xi0,xi0],[0.0,1.0],color='black')
120  plt.plot([xi0,xiMaxPlot],[1.0,1.0],color='black')
121  plt.ylim(0.0,1.1)
122  plt.ylabel(r'Energy/$V_0$',fontsize=18)
123  plt.xlabel(r'$x\,\frac{\sqrt{2mV_0}}{\hbar}$',fontsize=24)
124  plt.tight_layout()
```

Lines 117-124 plot the shape of the square potential well and write the horizontal and vertical axes labels.

```
125  # ------------------------------------------------------------------------
126  plt.savefig('SquareWell00.eps', format='eps', dpi=1000)
127  plt.show() # show the plot
```

Line 126 saves the plot in encapsulate PostScript format (.eps), and Line 127 shows the plot on the computer monitor. The result is shown in Fig. 5.5. The horizontal black lines correspond to the energy eigenvalues divided by V_0, namely

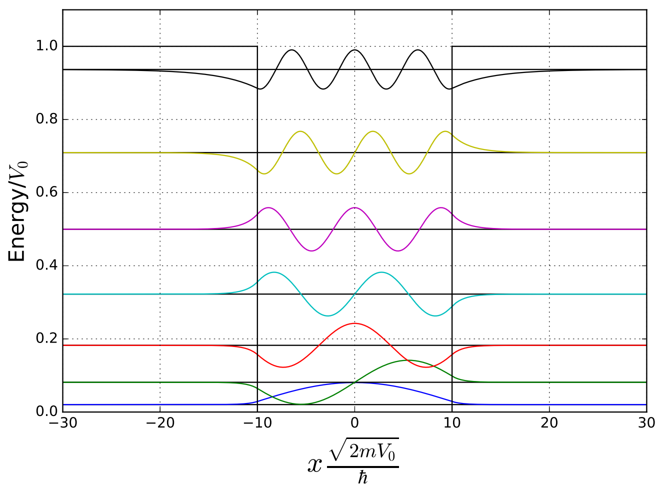


Figure 5.5 The seven bound eigenstates of a finite potential well of half-width $x_0 = 10\hbar/\sqrt{2mV_0}$, i.e., $\xi_0 = 10$. The ground state is always bound, whatever the width of the well. The number of excited bound eigenstates increases with increasing ξ_0.

W_0	0.020379039559702515
W_1	0.08135854295251191
W_2	0.18242255589320847
W_3	0.32253401889174704
W_4	0.4996922434624138
W_5	0.7095036776365305
W_6	0.9368079801646677

(5.36)

these values are printed on the computer monitor by Line 85. As we know from quantum mechanics, a finite square well always has at least one bound state (the ground state). The number of bound excited states depends on the depth and on the width of the well. In our case, $\xi_0 = x_0\sqrt{2mV_0}/\hbar = 10$, we have seven bound states, six excited states plus the ground state. Eigenstates of higher energy are not bound, but free. The number of bound states increases with increasing ξ_0, i.e., with increasing x_0 at constant V_0, with increasing V_0 at constant x_0, or with both x_0 and V_0 increasing.

5.5.3 The Harmonic Oscillator

Contrary to the square well, the quantum harmonic oscillator has an exact analytical solution. All eigenstates are bound, with energy eigenvalues $E_n = (n + 1/2)\hbar\omega$, and Hermite polynomials as eigenfunctions. Here, however, we shall solve the problem by numerical integration combined with the shooting method, and compare our results to the analytical solutions.

The potential energy for the harmonic oscillator is $V(x) = m\omega^2x^2/2$, where m is the mass of the "oscillating" particle, and $\omega = \sqrt{k/m}$, k being the Hooke constant. The corresponding Schrödinger equation is thus

$$\left(\frac{m\omega^2}{2}x^2 - \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\psi_n(x) = E_n\psi_n(x)\ . \tag{5.37}$$

Equation (5.37) can be rewritten in the following form, suitable for ODE numeric integration

$$\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_n(x)}{\mathrm{d}x^2} = \left(\frac{m\omega^2}{2}x^2 - E_n\right)\psi_n(x)\ . \tag{5.38}$$

In order to write (5.38) in terms of dimensionless quantities, we introduce the new variable

$$\xi = \frac{x}{\alpha}, \qquad \text{so that} \qquad x = \alpha\xi\ , \tag{5.39}$$

where α is a quantity with the dimensions of a length, to be chosen later. We obtain

$$\frac{\hbar^2}{2m\alpha^2}\frac{\mathrm{d}^2\psi_n(\xi)}{\mathrm{d}\xi^2} = \frac{m\alpha^2\omega^2}{2}\left(\xi^2 - \frac{2}{m\alpha^2\omega^2}E_n\right)\psi_n(\xi)\ . \tag{5.40}$$

We divide both sides by $m\alpha^2\omega^2/2$,

$$\frac{\hbar^2}{m^2\omega^2\alpha^4}\frac{\mathrm{d}^2\psi_n(\xi)}{\mathrm{d}\xi^2} = \left(\xi^2 - \frac{2}{m\alpha^2\omega^2}E_n\right)\psi_n(\xi)\ . \tag{5.41}$$

and we choose α as

$$\alpha = \sqrt{\frac{\hbar}{\omega m}}\ , \tag{5.42}$$

which has the dimensions of a length, as required. The equation reduces to

$$\frac{\mathrm{d}^2\psi_n(\xi)}{\mathrm{d}\xi^2} = \left(\xi^2 - \frac{2}{\hbar\omega}E_n\right)\psi_n(x)\ . \tag{5.43}$$

If we further define the quantity

$$W_n = \frac{E_n}{\hbar\omega}\ , \tag{5.44}$$

which is the nth energy eigenvalue measured in units of $\hbar\omega$, our final equation involves only dimensionless quantities, and is written

$$\frac{\mathrm{d}^2\psi_n(\xi)}{\mathrm{d}\xi^2} = \left(\xi^2 - 2W_n\right)\psi_n(x)\ . \tag{5.45}$$

Equation (5.45) is equivalent to the following system of two first-order ordinary differential equations (ODE)

$$\begin{aligned}\frac{\mathrm{d}\psi_n}{\mathrm{d}\xi_n} &= \chi_n\ ,\\ \frac{\mathrm{d}\chi_n}{\mathrm{d}\xi} &= \left(\xi^2 - 2W_n\right)\psi_n(x)\ .\end{aligned} \tag{5.46}$$

As in the case of the finite square well, if the correct eigenvalues W_n, and the corresponding appropriate initial values $\psi_n(0)$ and $\chi_n(0)$ are introduced into (5.46), numerical integrations lead to the correctly discretized $\psi_n(\xi)$ and $\chi_n(\xi) = \mathrm{d}\psi_n(\xi)/\mathrm{d}\xi$ functions. Again, the potential energy is an even function of x (and of ξ), implying that the eigenfunctions $\psi_n(\xi)$ are either even, thus with $\chi_n(0) = \mathrm{d}\psi_n(0)/\mathrm{d}\xi = 0$, or odd, with $\psi_n(0) = 0$. The eigenfunction corresponding to the ground state, $\psi_0(\xi)$, is even. Thus we assume again the initial conditions (5.31), and, again, we determine the eigenvalues and eigenfunctions by the shooting method. The harmonic oscillator has infinite eigenvalues, in the following we shall confine ourselves to the lowest seven states, $n = 0, 1, 2, \ldots, 6$.

Listing 5.3 QuantOscill.py

```python
#!/usr/bin/env python3
#
import numpy as np
from scipy.integrate import odeint,simps
import matplotlib.pyplot as plt
plt.rc('text', usetex=True)
#
nPoints=500
nPointsPlot=200
```

```
10 xiMax=10.0
11 xiMaxPlot=(xiMax*nPointsPlot)/nPoints
12 DeltaXi=xiMax/float(nPoints)
13 scale=4.0
14 nEigen=7
15 EigvStep=0.005
16 tolerance=1.0e-12;
17 #
```

Variable `nPoints` is the number of points used for calculations, `nPointsPlot` is the number of points displayed in the plot, `xiMax` is the maximum ξ values used for calculations, where it is assumed that $\psi_n(\xi)$ is practically zero for the evaluated functions (up to $n = 6$), `xiMaxPlot` is the maximum *xi* value displayed in the plot. `DeltaXi` is the ξ spacing between two consecutive points, needed for evaluating the integral of $|\psi|^2$ used for normalizing ψ. Quantity `nEigen` is the number of evaluated eigenstates, 6 plus the ground state in our case: since the bound eigenstates of the present problem are infinite, we must set a limit somewhere!

```
18 xi=np.linspace(0,xiMax,nPoints)
19 #
20 def dfdxi(y,xi,params):
21   psi,dpsidt=y      #    unpack y
22   E,=params         #    unpack parameters
23   derivs=[dpsidt,(xi*xi-2.0*E)*psi]
24   return derivs
25 #
```

Analogous to the square well. Here the tentative eigenvalue `E` is the only parameter needed by the function `dfdxi()`, Line 23 evaluates the derivative $d\chi/d\xi$ according to (5.46).

```
26 def SymmWell(params,xi,iEv,EigvStart,EigvStep,tolerance,dfdxi,psi):
27   # ........................................................ initialize
28   eigv1=EigvStart
29   params[0]=eigv1
30   if iEv%2==0:
31     y=[1.0,0.0]
32   else:
33     y=[0.0,1.0]
34   psoln=odeint(dfdxi,y,xi,args=(params,))
35   PsiEnd1=psoln[-1,0]
36   # ................................................ search for interval
37   while True:
38     eigv2=eigv1+EigvStep
39     params[0]=eigv2
40     psoln=odeint(dfdxi,y,xi,args=(params,))
41     PsiEnd2=psoln[-1,0]
42     if (PsiEnd1*PsiEnd2)<0.0:
43       break
44     PsiEnd1=PsiEnd2
45     eigv1=eigv2
46   # .................................... logarithmic search for eigenvalue
47   while True:
48     eigvmid=(eigv1+eigv2)/2.0
49     params[0]=eigvmid
50     if abs(eigv1-eigv2)<tolerance:
51       break
```

```
    psoln=odeint(dfdxi,y,xi,args=(params,))
    PsiEndMid=psoln[-1,0]
    if (PsiEndMid*PsiEnd1)>0 :
      PsiEnd1=PsiEndMid
      eigv1=eigvmid
    else:
      PsiEnd2=PsiEndMid
      eigv2=eigvmid
  # ................................................... list wave function
  del psi[:]
  for i in range(len(xi)):
    psi.append(psoln[i,0])
  # ......................................................................
  return eigvmid
#
```

Analogous to the corresponding code for the finite square well.

```
# ............................................ evaluate and draw potential
x = np.linspace(-xiMaxPlot,xiMaxPlot,(2*nPointsPlot)+1)
y = 0.5*x**2 # potential.
plt.plot(x,y) # x^2
# ............................................................. draw grid
plt.grid(True)
# ......................................................................
```

These lines draw the harmonic potential on the plot. The potential is

$$V(x) = \frac{1}{2}\,\omega^2 m\,x^2 \quad\Rightarrow\quad V(\xi) = \frac{1}{2}\,\hbar\omega\,\xi^2 \quad\Rightarrow\quad V(\xi) = \frac{1}{2}\,\xi^2\,, \tag{5.47}$$

the last formula being in units of $\hbar\omega$. The rest is analogous to the code for the finite square well.

```
eigv=[]
EigvStart=0.0;
i=0
```

Analogous to the finite square well.

```
while i<nEigen:
  params=[EigvStart]
  psi=[]
  eigv.append(SymmWell(params,xi,i,EigvStart,EigvStep,tolerance,dfdxi,psi))
  print(i,eigv[i])
  # ..................................... truncate diverging tail of psi
  while len(psi)>5:
    if abs(psi[-2])>abs(psi[-1]):
      break
    psi.pop()
  # ........................................................ normalize psi
  NormFact=np.sqrt(2.0*simps(np.square(psi),even='first'))
  # ........................................... truncate to plot length
  del psi[(nPointsPlot+1):]
  if len(psi)<(nPointsPlot+1):
    while len(psi)<(nPointsPlot+1):
      psi.append(0.0)
  normpsi=[i*(scale/NormFact) for i in psi]
```

```
95      psineg=list(reversed(normpsi))
96      if i%2==1:  # ........................... odd functions are antisymmetric
97        for k in range(len(psineg)):
98          psineg[k]=-psineg[k]
99      # ...................................................... form whole psi
100     psineg.pop()
101     psi=psineg+normpsi
102     #----------------------------------------------
103     EnerShift=eigv[i]
104     psi=[x+EnerShift for x in psi]
105     plt.plot([-xiMaxPlot,xiMaxPlot],[EnerShift,EnerShift],'black')
106     plt.plot(x,psi)
107     # ..................................................... next eigenvalue
108     EigvStart=eigv[i]+EigvStep
109     i+=1
```

Lines 77-109 constitute the main loop of the program, analogous to the main loop of the square well. The only important difference is that the number of bound eigenstates of the harmonic oscillator is infinite, thus Line 77 sets the number of required eigenstates.

```
110   # ..........................................................................
111   plt.ylabel('$W=E/(\hbar\omega)$',fontsize=18)
112   plt.xlabel('$\\displaystyle\\xi=\\sqrt{\\frac{\\omega_m}{\\hbar}}\\,x$',fontsize=24)
113   plt.tight_layout()
114   # ..........................................................................
115   plt.savefig('QuantOscill00.eps', format='eps', dpi=1000)
116   plt.show() # show the plot
```

The numerically evaluated eigenvalues are, in units of $\hbar\omega$

$$\begin{array}{ll} W_0 & 0.4999999798237699 \\ W_1 & 1.4999999905895576 \\ W_2 & 2.500000022660503 \\ W_3 & 3.4999999952432175 \\ W_4 & 4.500000038020879 \\ W_5 & 5.499999974849539 \\ W_6 & 6.500000020207548 \, , \end{array} \tag{5.48}$$

they approximate within some 10^{-8} the analytically calculated values

$$W_n = n + \frac{1}{2} \tag{5.49}$$

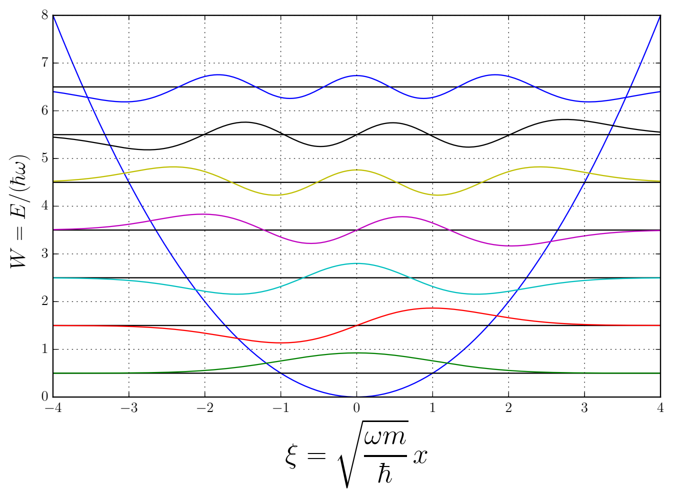


Figure 5.6 The ground state and the first six excited eigenstates of the quantum harmonic oscillator, as obtained by numerical integration.

The version of the shooting method discussed in the last sections of this chapter can be adapted to any symmetric one-dimensional attractive potential. Notable cases are the ammonia inversion potential and the oxetane ring-puckering potential in molecular physics.

Chapter 6

Tkinter Graphics

6.1 Tkinter

A *graphical user interface* (GUI) is a user interface that allows users to interact with a computer by clicking the mouse on graphical icons representing, for instance, buttons or menus, rather than by typing commands at the command line. As with all other computer graphical tools, for long time a problem with GUIs has been the lack of cross-platform compatibility, i.e., the impossibility to use the same GUI on different operating systems, notably Linux, macOS and Windows.

Tcl (suggested pronunciation: "tickle") is a high-level programming language designed for being very simple but powerful. The most popular Tcl extension is the *Tk* toolkit, first announced in 1991, which provides a graphical user interface library for a variety of operating systems, thus achieving a wide cross-platform compatibility. The popular combination of Tcl with the Tk extension is referred to as Tcl/Tk, and enables building a GUI natively in Tcl. Tcl/Tk is included in the standard Python installation in the form of *Tkinter*, standing for "Tk interface". Tkinter, which we are going to consider in this chapter, is Python's de facto standard GUI. Tkinter is included with the standard Linux, Microsoft Windows and macOS installations of Python.

There are several popular GUI library alternatives available, such as wxPython, PyQt (PySide), Pygame, Pyglet, and PyGTK, which, however, we are not going to consider here.

We shall still use the command line for preparing our Tkinter based scripts, but, once our scripts are running, we interact with the program execution through the Tkinter GUI. Further, what is perhaps more important, Tkinter provides more freedom than Pyplot both in drawing figures and in animation on the computer monitor. In the present chapter we shall discuss the basics of Tkinter graphics, while Tkinter animation will be considered in Chapter 7.

6.2 The Root Window and Tkinter Color Management

We start by describing how Tkinter manages the colors we use for graphics. Tkinter represents colors with strings. There are two ways to specify colors in Tkinter:

1. You can use locally predefined standard color names. The list is platform dependent, and you can inquire on the internet what is available for your particular platform. However, the color strings `'white'`, `'black'`, `'red'`', `'green'`, `'blue'`, `'cyan'`, `'yellow'`, and `'magenta'` are always available. This is enough for most applications.

2. You can define your own colors by using strings specifying the intensities of the three primary colors *red*, *green* and *blue* in hexadecimal digits, according to the RGB additive color model. The intensity of each primary color is represented by one ore two hexadecimal digits, according to the color depth. The relative intensity of each primary color is 0 – f (decimal 0 – 15) if a single hexadecimal digit is used, 00 – ff (decimal 0 – 255) if two digits are used. The full color string comprises a hash symbol (#) followed either by three or six hexadecimal digits. For example, in the 6-hexadecimal-digits representation, ”#ffffff” corresponds to white (maximum intensity, 255, or ff in hexadecimal, for all three primary colors), ”#000000” to black (minimum intensity, 0, for all primary colors), ”#ff0000” to pure bright red, ”#010000” to the darkest possible red, ”#00ff00” to pure bright green, ”#0000ff” to pure bright blue, and ”#00ffff” to bright cyan (green plus blue, both at maximum intensity).

Here follows a simple script that you can use to test the correspondence between strings and colors on your computer monitor, we can call it *checkcolor.py*. You can use it by typing, for instance
`$>checkcolor.py e0cc0f`
which asks for the relative color intensities (in decimal), red=224, green=204, blue=15.

Listing 6.1 checkcolor.py

```
1  #!/usr/bin/env python3
2  from tkinter import Tk,Canvas
3  from sys import argv
4  #
5  script,col=argv
6  colstring="#"+col
7  root=Tk()
8  root.title('Check Color')
9  canvas=Canvas(root,width=200,height=200,background=colstring)
10 canvas.grid(row=0,column=0)
11 #
12 root.mainloop()
```

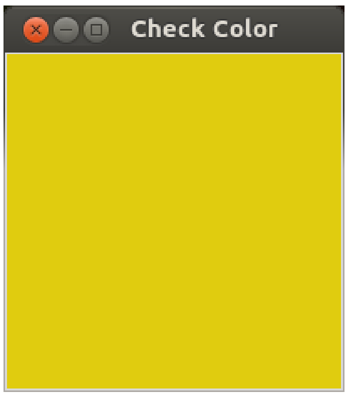


Figure 6.1

Functions `Tk()` and `Canvas()` are imported from Tkinter at Line 2, while the list `argv` is imported from the `sys` library at Line 3. As we already know, list `argv` comprises what we typed on the the command line, so `checkcolor.py` is copied into `script`, and `e0cc0f` is copied into `col` at Line 5. Thus, string `colstring` at Line 6 becomes `#e00cc0f` in our case. Line 7 creates the root window (which is always needed when using Tkinter graphics, it is the only window we shall use in this program), and Line 8 writes the title *Check Color* in the frame of the root window, as shown in Fig. 6.1. Line 9 creates a *canvas*, the surface where we can draw and paint, 200 pixel wide and 200 pixel high in the root window: Tkinter measures lengths in *pixels* (abbreviated as px). The background color of the canvas is set to the color coded in `colstring`. In Line 10 we are introduced to the Tkinter `grid()` geometry manager. Just think of the root window as divided into contiguous rectangular surfaces organized in rows and columns. Rows and columns are numbered from zero upwards. Since here the canvas is the only widget present in the root window, it is located at row=0, column=0. Note that writing, for instance, `canvas.grid(15,27)` would not alter the output, since empty rows and columns are simply ignored by Tkinter. However, Line 10 *must* be in the script, otherwise Python does not know where

to locate the canvas. Just see what happens if you cancel it out. We shall see the importance of the grid geometry manager in Section 7.3, Listing 7.3. Line 12 starts the execution of the program, and the root window frame and the colored canvas are displayed. The only way to close the program is to click the mouse on the `x` in the small red circle at the upper left of the frame. Later we shall learn more "refined" ways to exit programs. You can experiment all possible color encodings. The result is shown in Fig. 6.1. Also note that, if you type
`$>checkcolor.py`
on the terminal command line, without the color code, Python will complain that something is missing in the command line.

As a further example of the use of the color codes, Listing 6.2 draws an approximate rainbow

Listing 6.2 Rainbow.py

```
1  #!/usr/bin/env python3
2  from tkinter import Tk,Canvas
3  #
4  root=Tk()
5  root.title('Rainbow')
6  canvas=Canvas(root,width=800,height=150,background="#ffffff")
7  canvas.grid(row=0,column=0)
8  #
```

The code above is analogous to the code of Lines 1-10 of Listing 6.1, only, the list `sys.argv` is not needed here. Line 6 creates a canvas 800 pixels wide and 150 pixels high belonging to the root window, and the background color is set to white.

```
9  for i in range(0,800):
10     ColString="#"
11     if i<256:
12       r=255;g=i;b=0;
13     elif i<512:
14       r=511-i;g=255;b=i-256;
15     else:
16       r=0;g=767-i;b=255;
17       if i>672:
18         r=(i-672)*2
19       if g<0:
20         g=0
21 #
22     ColString=ColString+format(r,'02x')+format(g,'02x')+format(b,'02x')
23     line=[i,0,i,150]
24     canvas.create_line(line,fill=ColString)
25 #
26 root.mainloop()
```

The loop 9-24 paints 800 vertical lines, numbered by the index `i`, each line one-pixel wide, in the canvas. Each line will have a different color, according to its index `i`. The integer variables `r`, `g` and `b` represent the intensities of the primary colors red, green and blue. Line 10 creates a one-character string containing only the initial hash symbol `#`. For $0 \leq i < 256$ quantity `r` is assigned the maximum value 255 (maximum red intensity), `b` is always 0, while `g` gradually increases from 0 to 255. For $256 \leq i < 512$ the value of `r` decreases from 255 to 0, `g` has always its maximum value 255 (maximum green intensity), and `b` increases from 0 to 255. For $i \geq 512$ the value of `r` is always 0, `g` decreases from 255 to 0, and `b` has always its maximum value 255. For $672 < i < 800$ we have `g` = 0, `b` = 255, while `r` increases from 2 to 127, in order to reproduce violet. The color vision in the human eye is due to the presence of three types of photoreceptor cells in the retina, called *cones*. The three types of cones have different response curves to the light frequency. The first type responds the most to light of long wavelengths, peaking at about 560 nm, corresponding to red. The second type responds the most to light of medium-wavelength, peaking at 530 nm, corresponding to green. The third type responds the most to short-wavelength light, peaking at 420 nm, corresponding to blue. However, the red-sensible cones are slightly excited also by the higher end of the visible radiation, where photons are more energetic. This is why some red is needed to simulate our visual perception of violet. The method `.create_line()` used at Line 24 is discussed in Section 6.3. The output of script 6.2 is shown in Fig. 6.2.

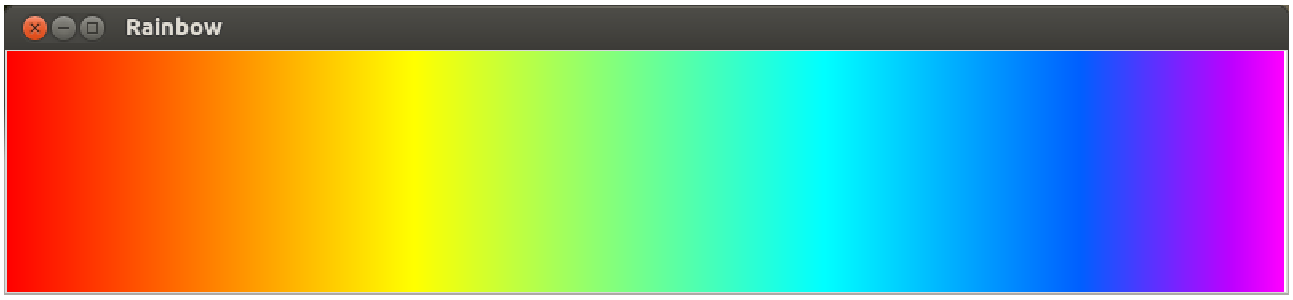


Figure 6.2 The “rainbow” output of Listing 6.2.

6.3 Drawing Geometric Shapes on the Canvas

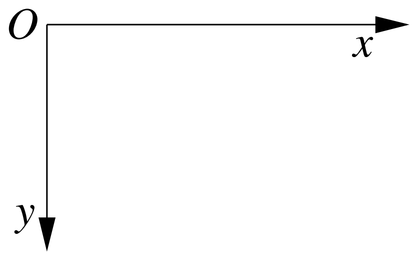


Figure 6.3 The x and y axis on the Tkinter canvas.

Tkinter has its `.create` methods for drawing geometrical shapes and writing text on the canvas. Geometric shapes and text are positioned on the canvas using the coordinate system shown in Fig. 6.3. As usual when dealing with displays on a computer monitor, the coordinate origin is located at the upper left corner of the window, and the y axis is directed downwards. Both the x and the y coordinates are measured in pixels.

We have already met the method `.create_line()` at Line 24 of Listing 6.2, where it was used to draw vertical lines of different colors. Listing 6.3 illustrates the use of the further methods `.create_rectangle()`, `.create_polygon()`, `.create_oval()`, `.create_arc()` and `.create_text()`. All these methods have both mandatory and optional arguments. See Appendix D fot a more complete discussion

Listing 6.3 GeomShapes.py

```
#!/usr/bin/env python3
from tkinter import Tk,Canvas,ARC,CHORD,PIESLICE
from numpy import cos,sin,pi
#
cw=600
ch=500
```

```
7   root=Tk()
8   root.title('Geometric Shapes')
9   canvas=Canvas(root, width=cw, height=ch, background="#ffffff")
10  canvas.grid(row=0,column=0)
```

Variables `cw` and `ch` are the canvas width and height, respectively. Lines 7-10 create the root window, and create and locate the canvas.

```
11  # ........................................................ rectangle
12  canvas.create_rectangle(40,10,150,100, fill='#00ff00')
13  canvas.create_text(95,120,text='This is a rectangle',\
14     font=('Helvetica','14'))
```

The method `.create_rectangle()` at Line 12 creates a rectangle with opposite vertices ($x_1 = 40\,\text{px}, y_1 = 10\,\text{px}$) and ($x_2 = 150\,\text{px}, y_2 = 100\,\text{px}$), using light green, '#00ff00', as fill color. The mandatory arguments of this method are the four x_1, y_1, x_2 and y_2 coordinates. Here we are using the optional argument `fill='#00ff00'`, specifying the fill color. If you omit this argument, the default color is *transparent*, equivalent to `fill=''`. Another optional argument is `outline`, determining the color of the border. The default is `outline='black'`.

At Lines 13-14 the method `.create_text()` writes a text on the canvas at a position determined by its two mandatory arguments, x and y. The text to be written is specified by the optional argument `text='This is a rectangle'`. By default, the text is printed centered around the (x, y) position. Different positioning with respect to (x, y) is possible via the optional argument `anchor`, the default is `anchor=CENTER`. The optional argument `font` is a tuple comprising two strings, specifying the font, here `'Helvetica'`, and the font size, here `'14'`.

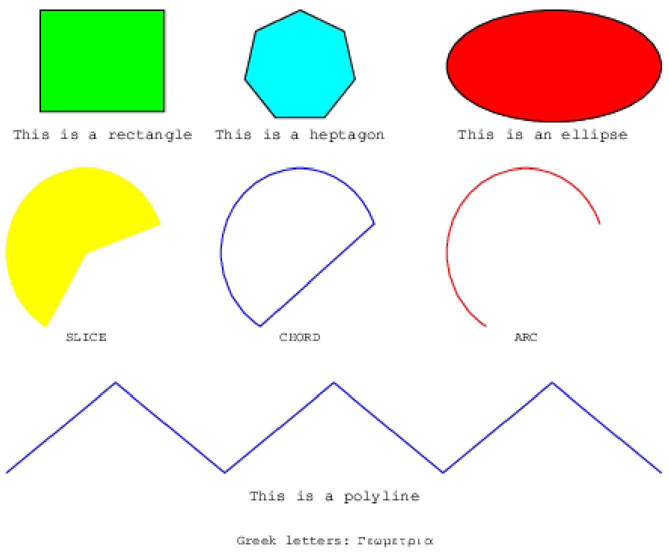


Figure 6.4 Drawing geometrical shapes and writing text on the canvas.

```
15  # ........................................................ heptagon
16  Ox=270
17  Oy=60
18  r=50.0
19  Np=7
20  poly=[]
21  i=0
22  alpha=2.0*pi/Np
23  while i<Np:
24     poly.append(Ox+r*sin(i*alpha))
25     poly.append(Oy-r*cos(i*alpha))
26     i+=1
27  canvas.create_polygon(poly, fill='#00ffff', outline='#000000')
28  canvas.create_text(270,120,text='This is a heptagon',\
29      font=('Helvetica','14'))
```

Here we create a regular polygon, i.e., a closed polyline of n line segments of equal length and n vertices, with $n = 7$ (a heptagon) in the present case. Our heptagon is centered at $O_x = 270$ px, $O_y = 60$ px, and inscribed in a circle of radius $r = 50$ px. Line 20 creates the empty list `poly`, that will contain the vertices of the heptagon. Variable `alpha` defined at line 22 is the central angle, and the loop 23-26 fills the list of the vertex coordinates. Method `.create_polygon()` at Line 27 creates a *polygon* whose vertices are specified by the (x, y) coordinates contained in the list `poly`, the mandatory argument. The optional argument `fill='#00ffff'` specifies that the color of the polygon surface is bright cyan, while the other optional argument `outline='#000000'` specifies that the border is black.

```
30  # ...................................................... ellipse
31  canvas.create_oval(400,10,590,109,fill='red')
32  canvas.create_text(485,120,text='This␣is␣an␣ellipse',\
33      font=('Helvetica','14'))
```

Method `create_oval()` draws an ellipse inscribed in a rectangle of opposite vertices (400, 10) and (590, 109). The fill color is `'red'`, the default color, `'black'`, is used for the border since the `outline` option is not specified.

```
34  # .......................................................... arc
35  canvas.create_arc(10,150,150,300,start=20,extent=220,fill='#ffff00',\
36      outline='#ffff00',style=PIESLICE)
37  canvas.create_text(80,300,text='SLICE',font=('Helvetica','12'))
38  canvas.create_arc(200,150,340,300,start=20,extent=220,fill='',\
39      outline='#0000ff',style=CHORD)
40  canvas.create_text(270,300,text='CHORD',font=('Helvetica','12'))
41  canvas.create_arc(400,150,540,300,start=20,extent=220,outline='#ff0000'\
42      ,style=ARC)
43  canvas.create_text(470,300,text='ARC',font=('Helvetica','12'))
```

Method `create_arc()` is called with different options. Option `start` is the start angle, in degrees, of the arc. The angle is measured from the $+x$ direction, counterclockwise. Option `extent` is the angular width of the arc, again in degrees. Option `style=PIESLICE` draws a *slice* of a pie chart, `style=CHORD` draws a chord connecting the endpoints of the arc, and `style=ARC` simply draws the arc. Constants `ARC`, `CHORD` and `PIESLICE` are defined in the TKinter library and imported at Line 2.

```
44  # ......................................................... line
45  line=[]
46  i=0
47  dx=(cw-20)/6
48  dy=40
49  while i<7:
50      line.append(10+i*dx)
51      line.append(380+dy)
52      dy=-dy
53      i+=1
54  canvas.create_line(line, fill='blue')
55  canvas.create_text(300,440,text='This␣is␣a␣polyline',\
56      font=('Helvetica','14'))
```

Method `create_line()` at Line 54 draws a polyline comprising an arbitrary number n of line segments, obviously including the single segment as special case, and $n+1$ vertices. The mandatory argument `line` is a list comprising the coordinates of the polyline vertices in the form $[x_0, y_0, x_1, y_1, \dots, x_n, y_n]$. The optional argument `fill` specifies the line color. List `line` is created at lines 45-53.

```
57  # ................................................ Greek letters
58  canvas.create_text(300,480,text=\
59     'Greek letters: \
60  \u0393\u03B5\u03c9\u03BC\u03B5\u03C4\u03C1\u03B9\u03B1',\
61     font=('Helvetica','12'))
62  #
63  root.mainloop()
```

The `create_text()` command at lines 58-61, split into four lines because of page size, shows the use of Greek letters. Unfortunately it is not (yet?) possible to insert LaTeX text into Tkinter, as we did under Matplotlib. The only way out is using the UTF-8 encoded Greek characters, listed in Table E.2 of Appendix E.

6.4 Plotting a Function with Tkinter

6.4.1 Plotting a Hyperbola

Plotting a function with Tkinter is slightly less easy than with Matplotlib, but still straightforward. Plotting relies on the method `canvas.create_line()`, which draws a polyline. If the line segments of the polyline are sufficiently short, the polyline is indistinguishable from a smooth curve: remember that, in any case, you cannot have a resolution better than 1 px on the computer monitor.

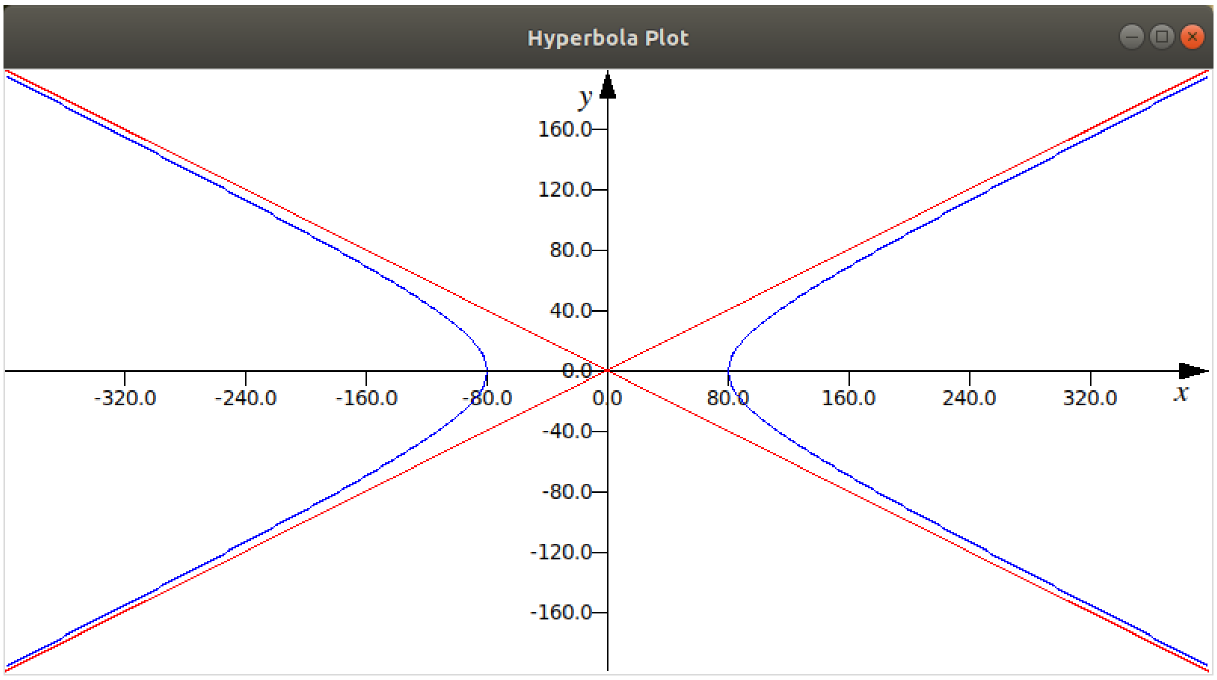


Figure 6.5 Plotting a hyperbola under Tkinter.

As an example, Listing 6.4 draws a hyperbola of equation

$$\frac{x^2}{a^2} - \frac{y^2}{b^2} = 1 \; , \tag{6.1}$$

with a=80 and b=40, on the canvas. The pixel is used as unit of length.

Listing 6.4 HyperbolaPlot.py

```
 1 #!/usr/bin/env python3
 2 from tkinter import Tk,Canvas,E,LAST,N
 3 import numpy as np
 4 #
 5 cw=800
 6 ch=400
 7 Ox=cw/2
 8 Oy=ch/2
 9 # ................................... create root window and canvas
10 root=Tk()
11 root.title('Hyperbola Plot')
12 canvas=Canvas(root, width=cw, height=ch, background="#ffffff")
13 canvas.grid(row=0,column=0)
```

In addition to the functions `Tk()` and `Canvas()`, we import also the Tkinter constants `E`, `LAST` and `N`. The canvas size is 800×400 pixels, `Ox` and `Oy` are the coordinates of the origin of our *xy* reference frame relative to the canvas reference.

```
14 # ........................................................... axes
15 canvas.create_line(0,Oy,cw-1,Oy, fill='black',arrow=LAST,
16                    arrowshape=(20,20,5))
17 canvas.create_line(Ox,ch-1,Ox,0, fill='black',arrow=LAST,
18                    arrowshape=(20,20,5))
19 canvas.create_text(cw-20,Oy+11,text='x',font=('Times','16',
20                                              'italic'))
21 canvas.create_text(Ox-15,15,text='y',font=('Times','16',
22                                              'italic'))
```

Lines 15-16 and 17-18 draw the *x* and *y* axes on the canvas, respectively. The two axes have arrows at their terminal endpoints (`arrow=LAST`), the shape of the arrows is specified by the `arrowshape` optional parameter, see Appendix D. Lines 19-20 and 21-22 write the symbols *x* and *y* at the axes ends.

```
23 # ....................................................... x-ticks
24 dx=80
25 i=1
26 x=0
27 while x<cw-dx:
28   x=i*dx
29   canvas.create_line(x,Oy,x,Oy+10)
30   canvas.create_text(x,Oy+10,text=str(x-Ox),anchor=N)
31   i+=1
32 # ....................................................... y-ticks
33 dy=40
34 i=1
35 y=0
36 while y<ch-dy:
```

```
37      y=i*dy
38      txt=str(y-Oy)
39      canvas.create_text(Ox-10,ch-y,text=str(y-Oy),anchor=E)
40      i+=1
```

Lines 24-40 draw the ticks along the *x* and *y* axes, respectively. The *x* ticks are spaced by 80 px, the *y* ticks by 40 px. The arguments of the method `.create_text()` are discussed in Appendix D.

```
41  # ..................................................... asymptotes
42  canvas.create_line(0,0,cw-1,ch-1,fill='red')
43  canvas.create_line(0,ch-1,cw-1,0,fill='red')
```

Lines 42-43 draw the hyperbola asymptotes, the two red diagonals in Fig. 6.5.

```
44  # .............................. make lists of hyperbola coordinates
45  a=80.0
46  b=40.0
47  y=-ch/2
48  hyp1=[]
49  hyp2=[]
50  while y<ch/2:
51      x=(a/b)*np.sqrt(y*y+b*b)
52      hyp1.append(Ox+x)
53      hyp1.append(Oy-y)
54      hyp2.append(Ox-x)
55      hyp2.append(Oy-y)
56      y+=2
```

The equation of our hyperbola is (6.1). The parameters *a* and *b* are defined at lines 45 and 46, all values are in pixels. Line 47 sets the initial value of *y* as `-ch/2`, at the bottom of the canvas in our *xy* reference frame. Lines 48 and 49 create the two empty lists `hyp1` and `hyp2` that will contain the coordinate samplings for the right and left branch of the hyperbola, respectively. Loop 50-56 fills `hyp1` and `hyp2` by evaluating *x* as a function of *y*. It is convenient evaluate *x* as a function of *y*, rather than *y* a function of *x*, because *x*(*y*) is a double-valued function, while *y*(*x*) is a four-valued function. The value of *y* is increased by 2 px at every step. You are invited to experiment the results of changing the *y* step increase at Line 56.

```
57  # ................................................. draw hyperbola
58  canvas.create_line(hyp1,fill='blue')
59  canvas.create_line(hyp2,fill='blue')
60  # ..................................................................
61  root.mainloop()
```

Lines 58 and 59 draw the two hyperbola branches.

6.4.2 Saving an Image of the Canvas

As we saw in Section 3.3, Listing 3.5, the package `matplotlib.pyplot` can save its plots to figures through the method `.savefig()`. Matplotlib can save a figure in the formats *.png*, *.pdf*, *.ps*, *.eps* and *.svg*. Obviously, also the images that we draw on the Tkinter canvas can be saved to figures. For this we have the method `.postscript()`, which saves figures **only** in *Encapsulated PostScript*. This, however, is not a relevant limitation: there are many available programs that can convert image files between different figure formats. The author's (personal) choice is the use of the ImageMagick®

package, available for Linux, Windows and macOS, among others. Once ImageMagick® is installed, and you want to convert an Encapsulated PostScript file naned, say, `myfigure.eps` to any other format, say *.jpg*, you simply type

```
convert -density 300 myfigure.eps myfigure.jpg
```

Thus, for instance, the last lines of Listing 6.4 must be changed to

```
60  # ..............................................................
61  canvas.update()
62  canvas.postscript(file='hyperb.eps',colormode='color')
63  root.mainloop()
```

Line 61 updates the canvas, so that the figure can be copied from it. We shall see in Chapter 7 that the method `.update()` is essential in Tkinter animation for refreshing the canvas at each new animation frame. Method `.postscript()` at Line 62 creates the Encapsulated PostScript file `hyperb.eps`. The optional argument `colormode` can have the values `'color'` for color output, `'gray'` for grayscale and `'mono'` for black and white. Since `.postscript()` is a *canvas* mode, only the canvas, not the window frame, is reproduced in the figure file.

Chapter 7

Tkinter Animation

7.1 Introduction

Tkinter animation is based on the same principle of all computer animations, as well as cinematography and TV: successive images (frames) are shown on the monitor at a given frame rate (24 frames per second in the case of 35 mm sound films), giving the illusion of motion to the human eye. This task is performed by a loop, often an infinite loop, which, at each cycle,

1. cleans the canvas, removing the preceding frame (from the canvas, not from the monitor!);
2. draws the new frame on the canvas, while the preceding frame is still displayed on the monitor;
3. copies the new frame from the canvas to the monitor;
4. waits an appropriate delay time in order to keep pace with the required frame rate;
5. returns to point 1.

In choosing the frame rate for an *interactive* animation, we must keep in mind that the computer must have the time to perform all calculations needed to draw the new frame, and actually redraw the picture, in the interval between two consecutive pictures. When the calculations involved are too complex, and/or drawing the pictures requires too much time, the animation will be slower than the requested frame rate. In this case, an alternative is asking our program to store all the single frames in a file, which we shall watch as a movie *after* running the program. This, however, will prevent interactivity.

As a simple example, the following code shows a ball (actually, a red circle) moving on the canvas and bouncing at the canvas borders.

Listing 7.1 FramedBall.py

```
1  #!/usr/bin/env python3
2  from tkinter import Tk,Canvas,ALL
3  # ........................................ open Tkinter root window
4  root=Tk()
5  root.title("Framed ball")
```

Line 4 creates the root window of our program, and Line 5 writes the title of the root window.

```
 6 # ........................................ canvas width and height
 7 cw=800
 8 ch=640
 9 # ...................................... add canvas to root window
10 canvas=Canvas(root,width=cw,height=ch,background='white')
11 canvas.grid(row=0,column=0)
12 # ................................................... variables
13 delay=20 #milliseconds
14 rad=20
15 color="red"
16 x=rad
17 y=ch-rad
18 vx=4.0
19 vy=-5.0
```

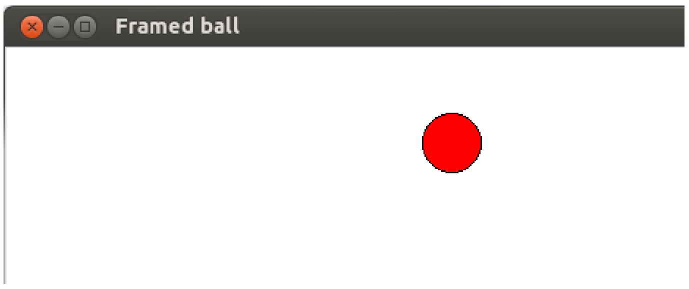


Figure 7.1 Ball bouncing at the canvas borders.

Quantities `cw` and `ch` are the width and height of the canvas in pixels, respectively. Line 10 creates the canvas of the required width and height. It also specifies that the canvas belongs to the root window, and that the background color is white. Line 13 sets a delay period of 20 ms, thus, the time interval between two successive frames of our *movie* will be 20 ms *plus* the time needed to calculate and draw a single frame. Lines 14-19 define the variables describing the ball: the radius in px, `rad` and the color `color`, set to red. Lines 17 and 18 assign the initial x and y coordinates of the ball center: the initial x position equals the radius, while the initial y position equals the canvas height minus the radius. Thus, the ball is located at the lower left corner of the canvas: as usual in computer graphics, the $x = 0$ axis is the canvas left border, while the $y = 0$ axis is the canvas *upper* border, the y axis being directed downwards. Lines 18 and 19 assign the initial x and y components of the ball velocity, `vx` and `vy`, respectively. Actually, `vx` and `vy` are the x and y displacements of the ball at each cycle (each animation step). In other words, we are measuring the ball velocity in "pixels/cycle". Note that a negative y velocity is directed upwards on the monitor.

```
20 # .................................................. main loop
21 while True:
22   # ........................................ draw ball on canvas
23   canvas.delete(ALL)
24   canvas.create_oval(x-rad,y-rad,x+rad,y+rad,fill=color)
25   canvas.update()
26   # .................... is the ball bouncing on the canvas borders?
27   if (x+rad)>=cw:
28     vx=-abs(vx)
29   elif (y+rad)>=ch:
30     vy=-abs(vy)
31   elif x<=rad:
32     vx=abs(vx)
33   elif y<=rad:
34     vy=abs(vy)
35   # ....................... update position and velocity components
```

```
36     x+=vx
37     y+=vy
38     # ............................................. wait delay time
39     canvas.after(delay)
```

Lines 21-39 constitute the program's main loop (the *animation loop*). At each cycle, Line 23 clears the canvas, i.e., the preceding frame. constant `ALL` is imported from Tkinter at Line 2. Line 24 draws the ball in the canvas: an ellipse inscribed in a rectangle (actually, a square, so that the ellipse is actually a circle) of opposite corners `(x-rad,y-rad)` and `(x+rad,y+rad)`, and filled with the ball color. The circle is thus centered at (x,y). The drawing on the canvas is actually done at Line 25 by the command `canvas.update()`. Lines 27-34 produce the bouncing effect: if the distance between the ball center and one of the canvas borders is equal to or smaller than `rad`, the x or y velocity component is reversed, according to the case. Note that here we are using the function `abs()`, which returns the absolute value of the argument as an integer if the argument is integer, as a float if the argument is a float. Function `math.fabs()` returns the absolute value always as a float, even if the argument is an integer. Lines 36 and 37 update the ball position for the next "movie frame". Line 39 forces the program execution to wait the required delay time between two successive frames. The program is exited by clicking on the red `x` at the upper left corner of the root window. This usually causes the computer to report an error, that you can ignore. When you close the window, your program still tries to do the next iteration, and you get an error message because the canvas no longer exists.

7.2 Adding Uniform Acceleration

Adding a uniform acceleration is very simple: we need to add only two lines to Listing 7.1, and change one line, as discussed in the comments to Listing 7.2. This listing draws a bouncing ball in the presence of gravity (and absence of friction!)

Listing 7.2 GravityBall.py

```
1  #!/usr/bin/env python3
2  from tkinter import Tk,Canvas,ALL
3  # ...................................... open Tkinter root window
4  root=Tk()
5  root.title("Gravity␣ball")
6  # ...................................... canvas width and height
7  cw=800
8  ch=400
9  # ...................................... add canvas to root window
10 canvas=Canvas(root,width=cw,height=ch,background='white')
11 canvas.grid(row=0,column=1)
12 # ...................................................... variables
13 delay=20 #milliseconds
14 rad=20
15 color="red"
16 x=rad
17 y=ch-rad
18 vx=4.0
19 vy=-7.5
20 ay=0.1
```

Line 20 is the first added line: it assigns the value 0.1 to the variable `ay`, the *y* (and only nonzero) component of the ball acceleration. The acceleration is measured in “pixels/cycle^2”, and, being positive, is directed downwards on the computer monitor, simulating gravity.

```
21 # ................................................... main loop
22 while True:
23   # ...................................... draw ball on canvas
24   canvas.delete(ALL)
25   canvas.create_oval(x-rad,y-rad,x+rad,y+rad, fill=color)
26   canvas.update()
27   # .................... is the ball bouncing on the canvas borders?
28   if (x+rad)>=cw:
29     vx=-abs(vx)
30   elif (y+rad)>=ch:
31     vy=-abs(vy)
32   elif x<=rad:
33     vx=abs(vx)
34   elif y<=rad:
35     vy=abs(vy)
36   # ........................ update position and velocity components
37   x+=vx
38   y+=vy+0.5*ay
39   vy+=ay
40   # ............................................. wait delay time
41   canvas.after(delay)
```

Line 38 is the line we had to change. The *y* motion is occurring with uniform acceleration, thus, the *y* displacement of the ball in a time interval Δt is $\Delta y = v_y\,\Delta t + 0.5\,a_y\,\Delta t^2$. Here we are using the loop *cycle* as time unit, thus $\Delta t = \Delta t^2 = 1$. Line 39 is the last added line, it updates the vertical component of velocity for the next “movie frame”.

7.3 Adding Interactive Buttons

Up to now, we could stop and exit our programs only by clicking the mouse on the `x` in the small red circle at the upper left of the window frame. When we do this for listings 7.1 and 7.2, an error is reported on the terminal because we interrupted the execution of an infinite loop. Another possibility would be to replace the loop command “`while True:`” in the code with, for instance, the command “`for i in range(5000):`”, this would stop the program after 5000 cycles. A more refined way is adding *interactive buttons*, which allow us to control the program during its execution. Here follows a listing, where only the additions to, and changes from, Listing 7.2 are commented.

Listing 7.3 ButtonBall.py

```
#!/usr/bin/env python3
from tkinter import Tk,Button,Canvas,Frame,ALL,W
# .............................................. Global variables
RunAll=True
RunMotion=False
```

Two further functions, `Button()` and `Frame()`, and one further constant, `W`, are imported from Tkinter. Two global variables, `RunAll`, initially set to `True`, and `RunMotion`, initially set to `False`, are added. The program will run as long as `RunAll` is true, the ball will move when

`RunMotion` is true, and be in “standby” when `RunMotion` is false. According to Line 5, the ball will stand still at the beginning of the program execution. These two variables are *global*: they are common to the main program and to the functions called by clicking the mouse on the control buttons.

```
 6  # ............................................... Start/Stop motion
 7  def StartStop():
 8     global RunMotion
 9     RunMotion=not RunMotion
10     if RunMotion:
11        StartButton[”text”]=”Stop”
12     else:
13        StartButton[”text”]=”Restart”
```

Here we define the function `StartStop()`, called by pressing the Start/Stop button, see comments to Lines 30-33 below. This function switches the value of the global variable `RunMotion` from `True` to `False` and vice versa, and changes the label on the Start/Stop button accordingly. If the ball is moving, pressing the button will stop it, and put it in motion if it is in stand-by. The variable `RunMotion` is declared as *global*: it is shared by the main program and `StartStop()`. Failing to declare `RunMotion` as global would cause an error message: Python would interpret the variable as local to `StartStop()`, and complain that Line 9 is using a variable *before* it is assigned a value.

```
14  # ................................................... Exit program
15  def StopAll():
16     global RunAll
17     RunAll=False
```

Here we define the function `StopAll()`, called by pressing the Close button. This function assigns the value `False` to the global variable `RunAll`, causing the program execution to stop.

```
18  # ............................................ Create root window
19  root=Tk()
20  root.title(”Button␣ball”)
21  # ....................................... Add canvas to root window
22  cw=800
23  ch=400
24  canvas=Canvas(root, width=cw, height=ch, background='white')
25  canvas.grid(row=1,column=0)
26  # ...................................... Add toolbar to root window
27  toolbar=Frame(root)
28  toolbar.grid(row=0,column=0,sticky=W)
```

Line 25 locates the canvas at row 1 instead of row 0 as in the previous scripts, because row 0 will be occupied by a horizontal toolbar, containing the control buttons. Line 27 creates the toolbar as a *frame* belonging to the root window, and Line 28 locates it at row 0, column 0, just above the canvas. The option `sticky=W` aligns the buttons at the *left* (*West* in a geographical map) of the toolbar. The other possibility would be `sticky=E` for aligning the buttons at the right. Values `N` and `S` have no effect in a single-row toolbar. Omitting the `sticky` option would center the buttons in the toolbar. Constants `W`, `E`, `N` and `S` are defined by Tkinter.

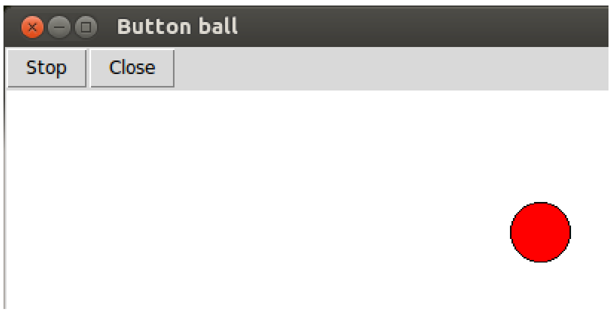


Figure 7.2 Control buttons on the *toolbar* of the root window

```
29 # ............................................... Toolbar buttons
30 StartButton=Button(toolbar ,text=”Start”,command=StartStop)
31 StartButton.grid(row=0,column=0)
32 CloseButton=Button(toolbar , text=”Close”, command=StopAll)
33 CloseButton.grid(row=0,column=1)
```

Line 30 creates the Start/Stop button, belonging to the toolbar, see Fig. 7.2. The initial text on the button is “Start”, because initially the ball is in stand-by. The command associated to the button is the function `StartStop()`, defined at Lines 7-13. Line 31 locates the button at row 0 (the only row) and column 0 of the toolbar. Lines 32-33 create and locate the Close button, which stops the program execution by calling function `StopAll()`.

```
34 # ..................................................... Variables
35 delay=20 #milliseconds
36 rad=20
37 color=”red”
38 x=rad
39 y=ch-rad
40 vx=4.0
41 vy=-7.5
42 ay=0.1
43 # ..................................................... Main loop
44 while RunAll:
45   # ........................................ Draw ball on canvas
46   canvas.delete(ALL)
47   canvas.create_oval(x-rad ,y-rad ,x+rad ,y+rad , fill=color)
48   canvas.update()
49   # ................................. Bouncing on the canvas borders
50   if RunMotion:
51     if (x+rad)>=cw:
52       vx=-abs(vx)
53     elif (y+rad)>=ch:
54       vy=-abs(vy)
55     elif x<=rad:
56       vx=abs(vx)
57     elif y<=rad:
58       vy=abs(vy)
59     # ................................. Update position and velocity
60     x+=vx
61     y+=vy+0.5*ay
62     vy+=ay
63   # ---------------.......................--------- Wait delay time
64   canvas.after(delay)
65   #------------------------
66 root.destroy()
```

The loop 44-64 iterates as long as `RunAll` is true. When the loop is interrupted, the root window is destroyed at Line 66. During the loop execution, the position of the ball is updated by Lines 49-62 if `RunMotion` is true, otherwise the ball stands still. Now, each time you click the mouse on the Start/stop button of Fig. 7.2 the ball stops if it was moving, and vice versa. If you click on the Close button the program terminates without error messages.

7.4 Numerical Parameters, Entries, Labels and Mouse Dragging

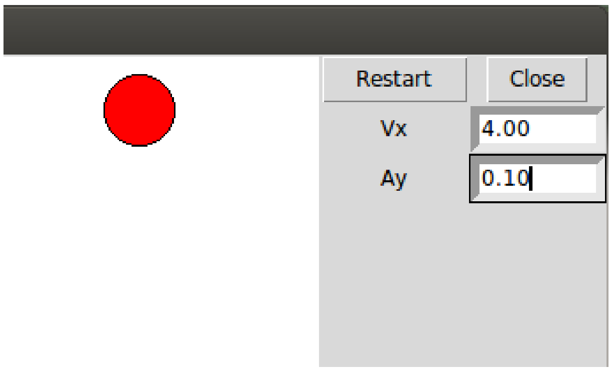


Figure 7.3 Control buttons, *labels* and *entries* on the toolbar.

It is often interesting to observe how the program behavior changes if some numerical parameters are changed. A possibility is changing the lines of the listing where the variables are assigned, for instance Line 40 of Listing 7.3 for the initial horizontal velocity `vx`, or Line 42 for the vertical acceleration `ay`. In this case one must rerun the program.

But it is also possible to change the parameter values interactively, during the program execution. For this, we need to introduce appropriate *labels* and *entries* in the toolbar, as shown in Fig. 7.3. After clicking the mouse on the entry widget, the user can enter a new value by typing it on the keyboard. Then, the program can read the new text on the entry and perform the required conversions. The label widget is a standard Tkinter widget used to display a text or image on the screen. Here we shall use it to specify the name of the parameter displayed in the nearby entry.

Further, it is possible to change the initial conditions by dragging the objects on the canvas by means of the mouse. Listing 7.4 follows, as usual only the changes from Listing 7.3 are commented.

Listing 7.4 MouseEntryBall.py

```
1  #!/usr/bin/env python3
2  from tkinter import *
3  # ............................................ Global variables
4  RunAll=True
5  RunMotion=GetData=Grabbed=False
6  # ............................................ Start/Stop motion
7  def StartStop():
8     global RunMotion
9     RunMotion=not RunMotion
10    if RunMotion:
11       StartButton[”text”]=”Stop”
12    else:
13       StartButton[”text”]=”Restart”
14 # ............................................... Exit program
15 def StopAll():
16    global RunAll
17    RunAll=False
18 # ............................................... Read entries
19 def ReadData(*arg):
20    global GetData
21    GetData=True
```

From this listing on, we are importing *everything* from Tkinter at Line 2, in spite of this being discouraged at the end of Section 1.8. From the author's experience, importing everything from the Tkinter package (and from Tkinter only!) never led to variable conflicts. You are simply advised to be careful.

The new global variables `GetData` and `Grabbed`, both initially set to *False*, are added at Line 5. When the motion is in standby, if `Getdata` is *True* the program will read new values from the entries, if `Grabbed` is *True* the mouse cursor will grab the ball and move it on the canvas. The value of `GetData` is turned to `True` by the new function `ReadData()`, defined at Lines 18-21.

```
22 # ......................................................... Grab ball ****
23 def GrabBall(event):
24   global Grabbed,rad,RunMotion,x,y
25   if not RunMotion:
26     Grabbed=((x-event.x)**2+(y-event.y)**2)<rad**2
27 # ...................................................... Release ball ****
28 def ReleaseBall(event):
29   global Grabbed
30   Grabbed=False
31 # ......................................................... Drag ball ***
32 def DragBall(event):
33   global Grabbed,x,y
34   if Grabbed:
35     x,y=event.x,event.y
```

All three functions above have a single argument, `event`. Python *events* can come from various sources, here we are interested in keyboard key presses and mouse operations by the user.

If the ball is in standby (`RunMotion` is *False*), function `GrabBall()` checks if the distance of the mouse pointer, located on the canvas at `(event.x,event.y)`, from the ball center, located at `(x,y)`, is smaller than the ball radius, `rad`. In this case the ball is grabbed by the mouse cursor by setting `Grabbed` equal to *True*. Pressing the mouse left button is the *event* that activates function `GrabBall()`, see Line 46 below.

The event calling function `ReleasBall()`, defined at lines 27-30, is releasing the left mouse button, see Line 48 below. The function releases (frees) the grabbed ball.

Function `DragBall()`, defined at lines 31-35, copies the mouse-cursor coordinates `(event.x, event.y)` into the ball-center coordinates `(x,y)`, thus forcing the ball to follow the mouse-cursor movements on the canvas. The event activating this function, provided that the the global variable `Grabbed` is *True*, is the motion of the mouse cursor over the canvas, see Line 47 below.

```
36 # .............................................. Create root window
37 root=Tk()
38 root.title("Entry␣ball")
39 root.bind('<Return>',ReadData)
40 # ......................................... Add canvas to root window
41 cw=800
42 ch=400
43 canvas=Canvas(root, width=cw, height=ch, background='white')
44 canvas.grid(row=0,column=0)
45 # ...................................................... Mouse button ***
46 canvas.bind('<Button-1>',GrabBall)
47 canvas.bind('<B1-Motion>',DragBall)
48 canvas.bind('<ButtonRelease-1>',ReleaseBall)
```

Line 39 binds the *Return* key of the keyboard to the function `ReadData()`: whenever the *Return* key is pressed, `ReadData()` is called, and `GetData` is set to *True*. See Appendix F.

Line 46 binds the event "pressing the left mouse button" to the function `GrabBall()`, defined at lines 23-26, provided that the mouse cursor is inside the canvas. In Tkinter notation, event `<Button-1>` corresponds to pressing the left mouse button, `<Button-2>` to pressing the middle mouse button, and `<Button-3>` to pressing the right button. Codes `<Button-4>` `<Button-5>` refer to the events of turning the mouse wheel forward and backward. Again, see Appendix F.

Line 47 binds the event “moving the mouse while the left button is pressed” to the function `DragBall()`. Codes `<B2-motion>` and `<B3-motion>` refer to mouse motion while the middle, or right, button is pressed, respectively.

Line 48 binds the event “releasing the left mouse button” to the function `<ButtonRelease-1>`. Thus, pressing the left mouse button when the mouse cursor is on the ball (closer to the ball center than the ball radius) will grab the ball. Moving the mouse keeping the left button pressed will drag the ball over the canvas, and releasing the left mouse button will free the ball.

```
49  # ..................................... Add toolbar to root window
50  toolbar=Frame(root)
51  toolbar.grid(row=0,column=1,sticky=N)
52  # ................................................... Toolbar buttons
53  StartButton=Button(toolbar,text=”Start”,command=StartStop,width=7)
54  StartButton.grid(row=0,column=0)
55  CloseButton=Button(toolbar, text=”Close”, command=StopAll)
56  CloseButton.grid(row=0,column=1)
```

The Start button and the Close button are located in *subcolumns* 0 and 1 of the toolbar, respectively. In this program we use a vertical toolbar, located in column 1, at the right of the canvas (located in column 0), see Fig. 7.3.

```
57  # ..................................... Toolbar labels and entries
58  LabVx=Label(toolbar,text=”Vx”)
59  LabVx.grid(row=1,column=0)
60  EntryVx=Entry(toolbar,bd=5,width=8)
61  EntryVx.grid(row=1,column=1)
62  LabAccel=Label(toolbar,text=”Ay”)
63  LabAccel.grid(row=2,column=0)
64  EntryAccel=Entry(toolbar,bd=5,width=8)
65  EntryAccel.grid(row=2,column=1)
```

Lines 58 and 59 create the label `Vx` and locate it in subrow 1, column 0 of the toolbar: subrow 0 is occupied by the buttons. Lines 60 and 61 create the entry where we can type new values for the horizontal velocity component, and locate it at the right of the label, at subrow 1 and subcolumn 1 of the toolbar. Line 60 also specifies that the border of the entry is 5 pixels (`bd=5`), and that the entry will show a maximum of 8 characters (`width=8`). Lines 62-65 create the label and the entry for the vertical acceleration `ay`.

```
66  # ......................................................... Variables
67  delay=20 #milliseconds
68  rad=20
69  color=”red”
70  x=rad
71  y=ch-rad
72  vx=4.0
73  vy=-7.5
74  ay=0.1
75  # ............................... Write variable values into entries
76  EntryVx.insert(0,'{:.2f}'.format(vx))
77  EntryAccel.insert(0,'{:.2f}'.format(ay))
78  # ......................................................... Main loop
79  while RunAll:
80    # ......................................... Draw ball on canvas
```

```
81      canvas.delete(ALL)
82      canvas.create_oval(x-rad,y-rad,x+rad,y+rad, fill=color)
83      canvas.update()
84      # ............................................ Ball is moving
85      if RunMotion:
86          # ........................................... Bouncing
87          if (x+rad)>=cw:
88              vx=-abs(vx)
89          elif (y+rad)>=ch:
90              vy=-abs(vy)
91          elif x<=rad:
92              vx=abs(vx)
93          elif y<=rad:
94              vy=abs(vy)
95          # ............................ Update position and velocity
96          x+=vx
97          y+=vy+0.5*ay
98          vy+=ay
99      # .............................................. Read entries
100     elif GetData:
101         try:
102             vx=float(EntryVx.get())
103         except ValueError:
104             pass
105         try:
106             ay=float(EntryAccel.get())
107         except ValuError:
108             pass
109         EntryVx.delete(0,'end')
110         EntryVx.insert(0,'{:.2f}'.format(vx))
111         EntryAccel.delete(0,'end')
112         EntryAccel.insert(0,'{:.2f}'.format(ay))
113         GetData=False
114     # ............................................. Wait delay time
115     canvas.after(delay)
116     #-----------------------
117 root.destroy()
```

Lines 100-113 are effective when the ball is in standby (when `RunMotion` is *False*) and `GetData` is *True*. Line 102 reads what is typed in the entry `EntryVx` and converts it to a float value, assigned to the variable `vx`. The reason for the `try` statement at Line 101 is that you might have typed some characters that are not numbers in the entry. In this case the function `float()` could not convert the value and would report an *exception* (in Python, errors detected during execution are called *exceptions*). Lines 101-104 tell the code to try if it is possible to convert the entry string into a float value, if the conversion is successful, the value is assigned to `vx`. If a `ValueError` exception is raised, i.e., conversion was not possible, Line 104 tells the program to do nothing: `vx` preserves its old value. Lines 105-108 check if the string typed into the entry `EntryAccel` can be converted into a new numerical value for `ay`. Line 109 deletes the present content of the entry `EntryVx` from 0, i.e., the first character of the string, to the end of the string. Line 110 rewrites the new value formatted with two digits after the decimal point. Line 113 resets the variable `GetData` to *False*.

You can type new values for the horizontal velocity and for the vertical acceleration of the ball at any time, provided that the ball is in standby. The corresponding variables will assume the new values only after you press both the *Return* key and the *Restart* button, no matter in which order. When the ball is in standby, you can also grab it and change its position with the mouse.

7.5 Creating Video Files under Tkinter

It is often convenient to create video files from our Python animations, both for sending them to friends (or for showing them in conferences), and because animations can involve complex computations between successive frames, causing the program to run very slowly. Unfortunately Tkinter does not have any method equivalent to `.FuncAnimation()` that we met in Section 3.7. The easiest way is using one of the many available programs that record the entire computer screen or a selected part of it.

A good choice for Linux is `SimpleScreenRecorder` by Maarten Baert. It is easy to install and to use, and has the possibility to reduce the video frame rate if your animation is running too slow due to the complex computations mentioned above. Recording the screen of a Mac is easy if you are using macOS Mojave: just hit the keyboard shortcut Shift+cmd+5 and all the controls for capturing video and still images from your desktop will appear. You can record the whole screen, a section, or a specific window, then trim, save or share the resulting footage. Windows 10 offers the built-in Xbox app, featuring screen capturing tools. Launch the Xbox app, then press the Windows and G icons on the keyboard and choose 'Yes this is a game' option. If you want to change the video quality or adjust the audio settings, you can do so by opening Game DVR options menu. If you are satisfied with one of the above options, or if you have found another screen-capturing application of your taste, you can skip the rest of Section 7.5. Honestly, you are advised to do so.

Creating a video file under Tkinter is possible and absolutely not complicated. However, it is true that it can be somewhat time-consuming, but it is the computer's time, not necessarily yours! The basic idea is copying each animation frame into a picture file, then merging all the pictures into a single video file with the help of an external program. As we saw in Section 6.4.2, the method `canvas.postscript()` saves the canvas content into an Encapsulated PostScript (*eps*) file. Thus, if we want to create a video file from Script 7.4, we start by modifying Lines 78-94 as follows

Listing 7.5 EntryBall.py Modified to Create Video Files

```
75 # ................................ Write variable values into entries
76 EntryVx.insert(0,'{:.2f}'.format(vx))
77 EntryAccel.insert(0,'{:.2f}'.format(ay))
78 # ................................................. Frame counter
79 iFrame=0
80 # ..................................................... Main loop
81 while RunAll:
82   # ............................................ Draw ball on canvas
83   canvas.delete(ALL)
84   canvas.create_oval(x-rad,y-rad,x+rad,y+rad,fill=color)
85   canvas.update()
86   # ............................................... Ball is moving
87   if RunMotion:
88     # ......................................... Create video frame
89     FrameName='../VideoFrames/frame{:08d}.eps'.format(iFrame)
90     canvas.postscript(file=FrameName,colormode='color')
91     iFrame+=1
92     # .............................................. Bouncing
```

```
 93       if (x+rad)>=cw:
 94         vx=-abs(vx)
 95       elif (y+rad)>=ch:
 96         vy=-abs(vy)
 97       elif x<=rad:
 98         vx=abs(vx)
 99       elif y<=rad:
100         vy=abs(vy)
```

where we have added Line 79 and Lines 88-91. Variable `iFrame`, defined at Line 79, is an animation-frame counter. Lines 88-91 are executed only if `RunMotion` is *True* (if the ball is moving). Line 89 creates a name for the *eps* frame picture in the form `path/frameXXXXXXXX.eps`, where `XXXXXXXX` is a zero-padded integer number ranging from 0000000000 to 99999999, equal to the frame counter. Actually, in all practical cases, the highest number will be much smaller, since 10^8 is a very high number of frames. Even running at 50 frames/second, a video comprising 10^8 frames would last $10^8/50 = 2 \times 10^6$ s $\simeq$ 555.5 hours! For the path, here we are assuming that you have previously created an empty directory named `VideoFrames` parallel to your working directory, where the animation frames will be stored. Under Windows all slashes (/) in the path must be replaced by backslashes (\ ). Line 90 copies the current animation-frame canvas into the *eps* file, and Line 91 increases the frame counter.

When we stop our modified program the `VideoFrames` directory will contain all our animation frames in *eps* format. Unfortunately there is no program that can directly merge *eps* files into a video file. Thus, we must first convert our *eps* files to some other format. Here we shall convert them to *jpg* (Joint Photographic Experts Group), but also several other formats, like, for instance, *png* (Portable Network Graphics), would do the job. The program `convert` of the ImageMagick® package can do the conversion for us. Our *jpg* files can then be merged into a video file, for instance *mp4* (MPEG-4: Moving Picture Experts Group), or *avi* (Audio Video Interleave, created by Microsoft), by the program `ffmpeg`. *FFmpeg* is a free software project consisting of a vast software suite of libraries and programs for handling video, audio and other multimedia files and streams. It is available for the Linux, Windows and macOS platforms. Listing 7.6 does the whole conversion from the original *eps* files to the final video file. All you have to do is typing, for instance,

`MakeVideo.py bouncing.mp4` or `MakeVideo.py bouncing.avi`

in the `VideoFrames` directory, and the script will create a video file for you.

Listing 7.6 MakeVideo.py

```
#!/usr/bin/env python3
import time
import os
from sys import argv
# ............................................... Convert frames
movie=argv[1]
tt0=time.time()
nn=0
for InFile in os.listdir('.'):
  if InFile.endswith('.eps'):
    base=os.path.splitext(InFile)[0]
    OutFile=base+".jpg"
    command="convert -density 300 ./"+InFile+" -flatten ./"+OutFile
    os.system(command)
    nn+=1
```

```
16 ttt=time.time()
17 print(ttt-tt0,'␣seconds')
18 print((ttt-tt0)/nn,'␣seconds/frame')
19 # ..................................... Merge frames to video file
20 tt0=ttt
21 command='ffmpeg␣-r␣50␣-f␣image2␣-i␣./frame%08d.jpg␣-vcodec␣libx264'\
22   +'␣-crf␣25␣-vf␣scale=1280:-2␣-pix_fmt␣yuv420p␣'+movie
23 os.system(command)
24 ttt=time.time()
25 print(ttt-tt0,'␣seconds␣for␣FFmpeg')
```

Line 6 copies the second command-line argument, in our case `bouncing.mp4` or `bouncing.avi` according to your choice, into the string variable `movie`, see the discussion of Listing 2.1. Line 7 stores the initial time of the script execution into `tt0`, this will be needed for evaluating the computation time. Variable `nn` at Line 8 is an animation-frame counter, needed at line 18 for evaluating the conversion time per animation frame. Loop 9-15 converts our *eps* files to *jpg*. At Line 9, the method `os.listdir('.')` returns a list comprising the entries of the current directory, specified by the path `'.'`. Thus, the variable `InFile` iterates over all the directory entries. The string method `.endswith()` at Line 10 returns *True* if the string `InFile` ends with the suffix `.eps`, otherwise returns *False*. Thus, Lines 11-15 are executed only for *eps* files.

Method `os.path.splitext()` at Line 11 splits its argument, `InFile`, into a string pair (`root`, `ext`) such that `root + ext = InFile`, and `ext` is either empty or begins with a period and contains at most one period. Thus, if `InFile` is, for instance, `frame00000015.eps`, the string `root` is `frame00000015`, and `ext` is `.eps`. As a result, `base` is `frame00000015`, and the string `OutFile` is `frame00000015.jpg`. Line 13 builds the command string to be passed as argument to the method `os.system`, see Section 2.4. Line 14 calls the external command

```
convert -density 300 frameXX.eps -flatten frameXX.jpg
```

that converts the *eps* file to a *jpg* file. The `XX` in the file names stands for an 8-digit integer (the frame counter) with the appropriate number of leading zeros. The command option `-density` specifies the image resolution to store when converting a vector image, like *eps* in our case, to a *raster graphics*, also called *bitmap*, image such as *jpg*, *pnm* or *png*. The default resolution is 72 dots per inch, which is equivalent to one pixel per typographic point (1 point = 1/72 inch). A value of 300, as chosen here, will lead to satisfactory results for all practical purposes. The command option `-flatten` is needed to preserve our background color, otherwise some output formats, like *png*, might have a transparent background. Line 15 increases by one the frame counter.

Line 16 gets the time after all frames have been converted, and Lines 17-18 print the time needed for the whole conversion process, and the average time per single-image conversion, on the terminal. The time needed for converting a single image is of the order of 1 s, ranging from some 0.5 s up to some 3 s depending on the image complexity and on the computer speed. At a frame rate of 24 fps (frames per second), an animation of 10 minutes comprises 14 400 frames, whose conversion from *eps* to *jpg* thus requires a time of the order of 4 hours. But, once you have launched the conversion script, you can let your computer do the work alone overnight, if you wish. If you have a multiprocessor computer you can divide the conversion time by approximately a factor *n*, where *n* is the number of processors.

Lines 21-22 do the final job, merging the converted *jpg* frames into the output `mp4`, or *avi*, video file, by calling the external command `ffmpeg`. The external command is

```
ffmpeg -r 24 -f image2 -i ./frame\%08d.jpg -vcodec \
libx264 -crf 25 -vf scale=1280:-2 -pix\_fmt yuv420p movie
```

where `movie` is either `bouncing.mp4` or `bouncing.avi`. These are the meanings of the command options:

- `- r 24` stands for a frame rate of 24 fps, you can experiment with different values, obtaining effects from time-stretching (digital slow motion) to fast motion. An extremely low frame rate, like `-r 1/5` gives each image a duration of 5 seconds, good for a *slide show*, not for an animation. An extremely high frame rate can exceed the computer capabilities.
- `-f image2` tells *FFmpeg* that the input is a sequence of separate images, to be merged into a single video file.
- `-i ./frame%08d.png` specifies that the input files are in the current directory (`./`), and their names have the form `framexxxxxxxx.png`, where `xxxxxxxx` is a progressive 8-digit integer patched with trailing zeros.
- `-vcodec libx264` specifies the computer program used for en**cod**ing and **dec**oding the digital data stream, here `libx264`, which is free software available for Linux, Windows and macOS. Usually `libx264` is installed automatically when you install *FFmpeg*.
- `-crf 25` sets the quality/size tradeoff for constant-quality (no bitrate target) and constrained-quality (with maximum bitrate target) modes. Valid range is 0 to 63, higher numbers indicating lower quality and smaller output size. A value of 25 is a reasonable compromise, while 63 leads to a very low quality. The default value is 23.
- `-vfscale=1280:-2` is a scale filter which resizes the image to a horizontal width of 1280 pixels. You can specify both width and height by typing, for instance, `-vfscale=1280:800`, thus changing the aspect ratio. If you want to keep the aspect ratio you can type `-1` for the vertical size, `-vfscale=1280:-1`, this will calculate the height of the output image according to the aspect ratio of the input image. Some codecs require the size of width and height to be a multiple of a certain number n. You can achieve this by setting the width or height to $-n$, as in the present case.
- `-pix_fmt yuv420p` ensures compatibility with a wide range of playback programs. It is required here, for example, for the video to be playable by Windows Media Player
- `movie`, has been set equal to our second command-line argument at Line 6, i.e., either `bouncing.mp4` or `bouncing.avi`, according to your choice. It is the name of the video output file. If *mp4* or *avi* are not convenient for you, FFmpeg supports many common and some uncommon image formats, like, for instance, *gif*.

If you wish, you can change the file extensions `.jpg` at lines 12 and 21 with the extensions `.png`, `.pnm` or other. The program will run anyway, in our experiments we found that the conversion to `.jpg` was faster, but you might want to experiment a little yourself.

As stated above, in a *multiprocessor*, or *multicore*, computer, the time needed for converting the animation frames from *eps* to *jpg* can be reduced by a factor approximately equal to the number of "logical processors". This is done by letting the logical processors work in parallel as much as possible. Script 7.7 is an example of how we can do this. Assuming that you have 4 logical processors, the usage is

```
MakeVideoParallel.py 4 bouncing.mp4
```

where the number 4 can be replaced by the actual number of available processors, and the extension `.mp4` can be replaced by the extension `.avi` or whatever video format you prefer.

Listing 7.7 MakeVideoParallel.py

```
#!/usr/bin/env python3
import math
import time
import os
from sys import argv,exit
# ..................................... Is script called correctly?
if len(argv)!=3:
  print('usage:␣MakeVideoParallel.py␣NumberOfProcessors␣␣OutputFile')
  exit()
# ..................... Number of processors and name of output file
nproc=int(argv[1])
movie=argv[2]
# ............................. Form lists of input and output files
ListIn=[]
ListOut=[]
for InFile in os.listdir("."):
  if InFile.endswith(".eps"):
    ListIn.append(InFile)
    base=os.path.splitext(InFile)[0]
    OutFile=base+".jpg"
    ListOut.append(OutFile)
nn=len(ListIn)
# ......................... Convert animation frames from eps to jpg
tt0=time.time()
i=0
while i<nn:
  j=0
  command=''
  while j<nproc:
    if (i+j)<nn:
      command+="convert␣-density␣300␣./"+ListIn[i+j]+"␣-flatten␣./"\
        +ListOut[i+j]
    if j<(nproc-1) and (i+j)<(nn-1):
      command+="|"
    j+=1
  os.system(command)
  i+=nproc
ttt=time.time()
print(ttt-tt0,'␣seconds')
print((ttt-tt0)/nn,'␣seconds/image')
# .................................. Merge jpg files into video file
tt0=ttt
command='ffmpeg␣-r␣24␣-f␣image2␣-i␣./frame%08d.jpg␣-vcodec␣libx264'\
  +'␣-crf␣25␣-vf␣scale=1280:-2␣-pix_fmt␣yuv420p␣'+movie
os.system(command)
ttt=time.time()
print(ttt-tt0,'seconds␣for␣FFmpeg')
```

Lines 7-9 check if the number of entered command-line arguments is correct, they must be 3: i) `MakeVideoParallel.py`, ii) the number of processors, iii) the name of the output video file. If this is not the case the script warns you and exits. Line 11 copies the number of processors to be used into the integer variable `nproc`, Line 12 copies the name of the output video file into the string variable `movie`.

Lines 14-22 form the lists of the names of the input *eps* files, `ListIn`, and of the output *jpg* files, `ListOut`. The integer variable `nn` is the number of animation frames to be converted.

Lines 24-40 perform the format conversion. They build composit command strings of the type

```
convert -density 300 ./ frame00000000.eps -flatten frame0000000.jpg |
convert -density 300 ./ frame00000001.eps -flatten frame0000001.jpg |
...
```

where the vertical bars " | " are used to join separate commands into a single command string, to be passed as argument to the method `os.system()`. Thus, Line 36 launches the joined commands simultaneously, and they can be simultaneously executed by different processors, if available. The rest of the script is analogous to Listing 7.6.

7.6 Animation and Ordinary Differential Equations

7.6.1 Euler's Method

A motion occurring with uniform acceleration is just a special case. In the general case the force acting on a body will be some function of both the body position and velocity, and, because of Newton's second law, we must deal with differential equations. In most cases the differential equations describing the motion have no analytical solution, and we must use the numerical methods discussed in Chapter 5. As a first simple example, simple because the acceleration is actually constant, we shall apply Euler's method, presented in Section 5.2, to the program of our Listing 7.4. As usual, we shall comment only the changes to the original listing.

Listing 7.8 GravityEuler.py

```python
#!/usr/bin/env python3
from tkinter import *
# ............................................ Global variables
RunAll=True
RunMotion=GetData=False
# ............................................ Start/Stop motion
def StartStop():
   global RunMotion
   RunMotion=not RunMotion
   if RunMotion:
      StartButton["text"]="Stop"
   else:
      StartButton["text"]="Restart"
# ................................................. Exit program
def StopAll():
   global RunAll
   RunAll=False
# ................................................. Read entries
def ReadData(*arg):
```

```
20      global GetData
21      GetData=True
22  # ........................................................ Variables
23  delay=20 #milliseconds
24  rad=20
25  color=”red”
26  x=rad
27  y=rad
28  vx=4.0
29  vy=7.5
30  ay=-0.2
31  mass=10
32  ener=mass*(0.5*(vx**2+vy**2)-ay*y)
```

Two new variables are added: the mass of the ball, set equal to 10 in arbitrary units, and the energy of the ball, evaluated at Line 32 as the sum of the potential and kinetic energies.

```
33  # ............................................ Create root window
34  root=Tk()
35  root.title(”Gravity␣Euler”)
36  root.bind('<Return>',ReadData)
37  # ...................................... Add canvas to root window
38  cw=800
39  ch=400
40  canvas=Canvas(root, width=cw, height=ch, background='white')
41  canvas.grid(row=0,column=0)
42  # ..................................... Add toolbar to root window
43  toolbar=Frame(root)
44  toolbar.grid(row=0,column=1,sticky=N)
45  # ................................................ Toolbar buttons
46  nr=0
47  StartButton=Button(toolbar,text=”Start”,command=StartStop,width=7)
48  StartButton.grid(row=nr,column=0)
49  CloseButton=Button(toolbar, text=”Close”, command=StopAll)
50  CloseButton.grid(row=nr,column=1)
51  nr+=1
52  # ..................................... Toolbar labels and entries
53  LabVx=Label(toolbar,text=”Vx”)
54  LabVx.grid(row=nr,column=0)
55  EntryVx=Entry(toolbar,bd=5,width=8)
56  EntryVx.grid(row=nr,column=1)
57  nr+=1
58  LabAccel=Label(toolbar,text=”Ay”)
59  LabAccel.grid(row=nr,column=0)
60  EntryAccel=Entry(toolbar,bd=5,width=8)
61  EntryAccel.grid(row=nr,column=1)
62  nr+=1
63  # .................................................. Energy label
64  EnerLab0=Label(toolbar,text='Energy:',font=(”Helvetica”,11))
65  EnerLab0.grid(row=nr,column=0)
66  EnerLab=Label(toolbar,text='{:8.3f}'.format(ener),font=(”Helvetica”,11))
67  EnerLab.grid(row=nr,column=1,sticky=W)
68  nr+=1
69  # ........................... Write variable values into entries
70  EntryVx.insert(0,'{:.2f}'.format(vx))
```

```
71 EntryAccel.insert(0,'{:.2f}'.format(ay))
```

Two new labels are added to the toolbar at lines 63-67. Label `EnerLab0`, defined at Lines 64-65. simply contains the word “Energy”, while Label `EnerLab`, defined at Lines 66-67 contains the value of the total energy of the bouncing ball. Its value will be updated every ten iterations of the main animation loop.

```
72 # ........................................................ Main loop
73 count=0
74 while RunAll:
75   # ............................................ Draw ball on canvas
76   canvas.delete(ALL)
77   canvas.create_oval(x-rad,ch-(y+rad),x+rad,ch-(y-rad),fill=color)
78   canvas.update()
79   # ................................................. Ball is moving
80   if RunMotion:
81     # ................................................... Bouncing
82     if (x+rad)>=cw:
83       vx=-abs(vx)
84     elif (y+rad)>=ch:
85       vy=-abs(vy)
86     elif x<=rad:
87       vx=abs(vx)
88     elif y<=rad:
89       vy=abs(vy)
90     # ................ Update position and velocity, Euler algorithm
91     x+=vx
92     y+=vy
93     vy+=ay
```

A new variable `count`, initialized to zero, is defined at line 73. Lines 74-116 constitute the main animation loop of the program. The Euler method is a first-order method, with velocity and position updated at each iteration at Lines 91-93. The x component of velocity is constant between consecutive bouncings at the left and right borders of the canvas. The differential equation for the y motion is

$$m\,\frac{\mathrm{d}^2y}{\mathrm{d}t^2} = ma_y\,, \tag{7.1}$$

which, according to Section 5.1, can be rewritten as the system of two first-order differential equations

$$\begin{aligned}\frac{\mathrm{d}y}{\mathrm{d}t} &= v_y\\ \frac{\mathrm{d}v_y}{\mathrm{d}t} &= a_y\,,\end{aligned} \tag{7.2}$$

which Euler’s method solves by the recursive formulas (5.5)

$$y_{i+1} = y_i + v_i\,\Delta t\,, \quad v_{y,i+1} = v_{y,i} + a_y\,\Delta t\,, \tag{7.3}$$

corresponding to Lines 92 and 93, since we have $\Delta t = 1$ in our units.

```
94   # ..................................................... Read entries
95   elif GetData:
96     try:
 97            vx=float(EntryVx.get())
 98        except ValueError:
 99            pass
100        try:
101            ay=float(EntryAccel.get())
102        except ValuError:
103            pass
104        EntryVx.delete(0,'end')
105        EntryVx.insert(0,'{:.2f}'.format(vx))
106        EntryAccel.delete(0,'end')
107        EntryAccel.insert(0,'{:.2f}'.format(ay))
108        GetData=False
109    # ............................................... Write energy
110    count+=1
111    if count >=10:
112        count=0
113        ener=mass*(0.5*(vx**2+vy**2)-ay*y)
114        EnerLab['text']='{:8.3f}'.format(ener)
115    # ............................................... Wait delay time
116    canvas.after(delay)
117    #-------------------------
118 root.destroy()
```

The variable `count` is incremented at Line 110. Every ten lines the total energy of the bouncing ball is evaluated at line 113 and displayed on the toolbar label.

Euler integration is a first-order method, and its limits are apparent if we run Script 7.8 for a few minutes: the ball jumps slowly become higher and higher, implying that energy is not conserved. This is seen also by looking at the value displayed by the energy label in the toolbar. The reason is simple: the first of (7.3) assumes a constant velocity during the execution of each step (obviously, the velocity is different from step to step), equal to the initial velocity of the step. But, in reality, the velocity decreases during the step because a_y is negative. Thus, independently of the ball going upwards or downwards, the calculated position at the end of each step is slightly higher than the correct position, leading to a slow increase in the calculated energy. Since a_y is constant, all errors have the same sign and there is no hope of random cancellation.

7.6.2 The Leapfrog Method

In contrast to Euler integration, leapfrog integration is a second-order method, yet it requires the same number of function evaluations per step. Unlike Euler integration, it is stable for oscillatory motion, as long as the time-step Δt is constant and $\Delta t \leqslant \omega/2$, ω being the angular frequency of the oscillation. In leapfrog integration, the equations for updating position and velocity are

$$\begin{aligned} x_i &= x_{i-1} + v_{i-\frac{1}{2}}\,\Delta t\ , \\ a_i &= F(x_i)\ , \\ v_{i+\frac{1}{2}} &= v_{i-\frac{1}{2}} + a_i \Delta t\ , \end{aligned} \tag{7.4}$$

with positions and accelerations evaluated at "integer times" $i\,\Delta t$, and velocities evaluated at "half-integer" times $\left(i+\frac{1}{2}\right)\Delta t$. The advantage of the method is that, at each step, the position is still updated assuming a constant velocity, but the velocity is calculated at the middle of the step rather than at one of the end points. Equations (7.4) can be re-arranged to the “kick-drift-kick” form

$$\begin{aligned} v_{i+\frac{1}{2}} &= v_i + a_i \frac{\Delta t}{2} \, , \\ x_{i+1} &= x_i + v_{i+\frac{1}{2}} \, \Delta t \, , \\ v_{i+1} &= v_{i+\frac{1}{2}} + a_{i+1} \frac{\Delta t}{2} \, , \end{aligned} \tag{7.5}$$

used in Script 7.9, where Euler integration of Listing 7.8 is replaced by leapfrog integration. Note that leapfrog integration cannot be applied in the presence of a velocity-dependent acceleration.

Listing 7.9 GravityFrog.py

```
#!/usr/bin/env python3
from tkinter import *
# ............................................... Global variables
RunAll=True
RunMotion=GetData=False
# .............................................. Start/Stop motion
def StartStop():
   global RunMotion
   RunMotion=not RunMotion
   if RunMotion:
      StartButton["text"]="Stop"
   else:
      StartButton["text"]="Restart"
# ................................................... Exit program
def StopAll():
   global RunAll
   RunAll=False
# ................................................... Read entries
def ReadData(*arg):
   global GetData
   GetData=True
# ...................................................... Variables
delay=20 #milliseconds
rad=20
color="red"
x=rad
y=rad
vx=4.0
vy=7.5
ay=-0.1
mass=10
ener=mass*(0.5*(vx**2+vy**2)-ay*y)
# ............................................ Create root window
root=Tk()
root.title('Gravity Leapfrog')
root.bind('<Return>',ReadData)
# ...................................... Add canvas to root window
cw=800
ch=400
canvas=Canvas(root, width=cw, height=ch, background='white')
canvas.grid(row=0,column=0)
```

```
42 # ......................................... Add toolbar to root window
43 toolbar=Frame(root)
44 toolbar.grid(row=0,column=1,sticky=N)
45 # ............................................... Toolbar buttons
46 nr=0
47 StartButton=Button(toolbar,text="Start",command=StartStop,width=7)
48 StartButton.grid(row=nr,column=0)
49 CloseButton=Button(toolbar, text="Close", command=StopAll)
50 CloseButton.grid(row=nr,column=1)
51 nr+=1
52 # ........................................ Toolbar labels and entries
53 LabVx=Label(toolbar,text="Vx")
54 LabVx.grid(row=nr,column=0)
55 EntryVx=Entry(toolbar,bd=5,width=8)
56 EntryVx.grid(row=nr,column=1)
57 nr+=1
58 LabAccel=Label(toolbar,text="Ay")
59 LabAccel.grid(row=nr,column=0)
60 EntryAccel=Entry(toolbar,bd=5,width=8)
61 EntryAccel.grid(row=nr,column=1)
62 nr+=1
63 # .................................................... Energy label
64 EnerLab0=Label(toolbar,text='Energy: ',font=("Helvetica",11))
65 EnerLab0.grid(row=nr,column=0)
66 EnerLab=Label(toolbar,text='{:8.3f}'.format(ener),font=("Helvetica",11))
67 EnerLab.grid(row=nr,column=1,sticky=W)
68 # ................................ Write variable values into entries
69 EntryVx.insert(0,'{:.2f}'.format(vx))
70 EntryAccel.insert(0,'{:.2f}'.format(ay))
71 # ....................................................... Main loop
72 iter=0
73 while RunAll:
74   # ............................................ Draw ball on canvas
75   canvas.delete(ALL)
76   canvas.create_oval(x-rad,ch-(y+rad),x+rad,ch-(y-rad),fill=color)
77   canvas.update()
78   # .................................................. Ball is moving
79   if RunMotion:
80     # ................................................... Bouncing
81     if (x+rad)>=cw:
82       vx=-abs(vx)
83     elif (y+rad)>=ch:
84       vy=-abs(vy)
85     elif x<=rad:
86       vx=abs(vx)
87     elif y<=rad:
88       vy=abs(vy)
89     # ............. Update position and velocity, leapfrog algorithm
90     x+=vx
91     vy+=0.5*ay
92     y+=vy
93     vy+=0.5*ay
```

Lines 91-93 code equations (7.5) for the present case: constant acceleration and $\Delta t = 1$.

```
    # ................................................. Read entries
    elif GetData:
      try:
        vx=float(EntryVx.get())
      except ValueError:
        pass
      try:
        ay=float(EntryAccel.get())
      except ValuError:
        pass
      EntryVx.delete(0,'end')
      EntryVx.insert(0,'{:.2f}'.format(vx))
      EntryAccel.delete(0,'end')
      EntryAccel.insert(0,'{:.2f}'.format(ay))
      GetData=False
    # ................................................. Write energy
    iter+=1
    if iter >=10:
      iter=0
      ener=mass*(0.5*(vx**2+vy**2)-ay*y)
      EnerLab['text']='{:8.3f}'.format(ener)
    # ............................................... Wait delay time
    canvas.after(delay)
    #------------------------
  root.destroy()
```

Running Listing 7.9 shows that now energy is conserved.

7.6.3 The *odeint* integration

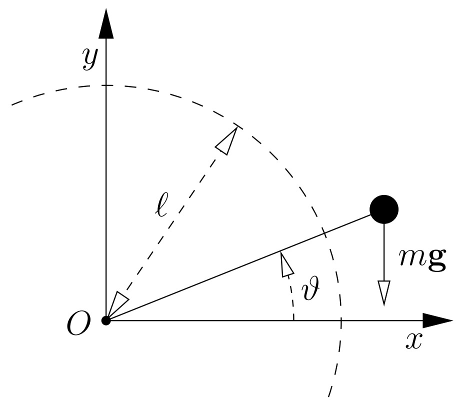


Figure 7.4

As a relatively simple example, we consider the elastic-string pendulum of Fig. 7.4, where a bob of mass m is bound to the pivot O by a massless rubber string of rest length ℓ in the presence of standard gravity acceleration $\boldsymbol{g}$. We restrict ourselves to a motion occurring in a vertical plane. Differently from the case of Section 5.4, here the position of the bob cannot be specified by a single coordinate, as the angle ϑ. Thus we shall use the Cartesian coordinates of Fig. 7.4, whose origin O is located on the pivot, while the y axis is antiparallel to the gravity acceleration $\boldsymbol{g}$. The bob of the pendulum is subject to the gravitational force $-m\boldsymbol{g}$. Further, if the distance $\sqrt{x^2+y^2}$ of the bob from the pivot is greater than ℓ, i.e., if the bob is located outside of the dashed circle of the figure, the string exerts an elastic force

$$\boldsymbol{f}_{\text{el}} = -k\left(\sqrt{x^2+y^2}-\ell\right)(\hat{\boldsymbol{x}}\cos\vartheta + \hat{\boldsymbol{y}}\sin\vartheta)\ , \quad \text{where} \quad \vartheta = \arctan\left(\frac{y}{x}\right)\ , \tag{7.6}$$

where k is the Hooke constant of the rubber band, and $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$ are the unit vectors along the x and y axes, respectively. Obviously, the rubber band exerts no force if $\sqrt{x^2+y^2} < \ell$ (bob inside the dashed circle). Further, we assume the presence of a frictional force proportional to the bob velocity

$$\boldsymbol{f}_{\text{fr}} = -\eta\boldsymbol{v}\ , \tag{7.7}$$

through a given constant coefficient η. As in Section 5.4, we shall solve the differential equations by the function `odeint()`. Our two-dimensional problem requires the integration of the following system of four first-order differential equations

$$\begin{aligned}
\frac{\mathrm{d}x}{\mathrm{d}t} &= v_x \,, \\
\frac{\mathrm{d}v_x}{\mathrm{d}t} &= \begin{cases} -\eta v_x & \text{if} \quad \sqrt{x^2+y^2} < \ell \,, \\ -k\left(\sqrt{x^2+y^2}-\ell\right)\cos\vartheta - \eta v_x & \text{if} \quad \sqrt{x^2+y^2} > \ell \,, \end{cases} \\
\frac{\mathrm{d}y}{\mathrm{d}t} &= v_y \,, \\
\frac{\mathrm{d}v_y}{\mathrm{d}t} &= \begin{cases} -g - \eta v_y & \text{if} \quad \sqrt{x^2+y^2} < \ell \,, \\ -g - k\left(\sqrt{x^2+y^2}-\ell\right)\sin\vartheta - \eta v_y & \text{if} \quad \sqrt{x^2+y^2} > \ell \,. \end{cases}
\end{aligned} \tag{7.8}$$

In section Section 5.4 we called `odeint()` only once, obtaining the discretization of the whole motion. Here we need to call `odeint()` before drawing each animation frame, in order to obtain an animation “in real time”. Thus, while the array `t` of Listing 5.1 comprised the 101 time points at which we wanted to evaluate the bob positions, here it will comprise only two time points: the starting and the final point of the interval between two consecutive frames, arbitrarily chosen as $t_0 = 0$ and $t_1 = 0.01$ s. The listing follows.

Listing 7.10 BentBandPendulum.py

```
 1 #!/usr/bin/env python3
 2 from tkinter import *
 3 import numpy as np
 4 import time
 5 from scipy.integrate import odeint
 6 # ........................................... interaction functions
 7 def StartStop():# ....... start/stop pendulum motion
 8   global RunIter
 9   RunIter=not RunIter
10   if RunIter:
11     StartButton['text']='Stop'
12   else:
13     StartButton['text']='Restart'
14 def ReadData(*args):# ................. read entries
15   global GetData
16   GetData=True
17 def StopAll():# ...................... exit program
18   global RunAll
19   RunAll=False
20 # ............................................. Global variables
21 RunAll=True
22 GetData=RunIter=False
```

Lines 7-19 define the three functions `StartStop()`, `ReadData()` and `StopAll()`, already encountered in the preceding listings. The program runs as long as the global variable `Runall` is *True*. The pendulum moves if the global variable `RunIter` is *True*, otherwise it is in stand-by. New data are read from the entries in the toolbar if `ReadData` is *True*.

```
# ............................................. Canvas data
ButtWidth=9
cw=800
ch=640
Ox=cw/2
Oy=ch/2
```

Variable `ButtWidth` is the maximum number of characters that can be written on a toolbar button, while `cw` and `ch` are the canvas width and height in pixels, respectively. Variables `Ox` and `Oy` are the x and y cooordinates of the pendulum pivot on the canvas, in pixels.

```
# ........................................ Physical parameters
g=9.8            # m/s^2
L=4.0            # m
m=5.0            # kg
Hooke=500.0      # N/m
eta=0.0          # kg/s
dt=0.01          # s
```

These are the physical quantities determining the pendulum motion, in SI units. Quantity `g` is the gravitational acceleration at the Earth's surface, in ms^{-2}, `L` is the rest length of the elastic band, in meters, `m` is the bob mass, in kg, `Hooke` is the Hooke constant of the elastic band, in N/m, `eta` is the proportionality factor η between drag force and velocity, in Ns/m=kg/s. As default we assume absence of friction, or $\eta = 0$. You can experiment interactively on how different values of η affect the motion while running the program. Finally, `dt` is the time step Δt used in the numerical integration of our differential equations.

```
# ...........................................................
prad=3           # pivot radius
rad=12           # bob radius
bColor='red'     # bob color
```

This are parameters used for drawing the pendulum: `prad` is the pivot radius and `rad` the bob radius, in pixel, `bColor` is the bob color.

```
# ..........................................................
scale=50.0       # pixels/m
tau=20           # milliseconds
```

Quantity `scale` is the ratio S, expressed in px/m, of a length on the computer monitor, in px, to the corresponding real length in m. Thus the rest length of our rubber band, 4 m, corresponds to 200 pixels. Quantity `tau` is the required time interval τ between two consecutive animation frames. Tkinter requires τ to be an integer number of milliseconds.

```
# ................................. Initial position and velocity
xx=1.1*L
vx=0.0
yy=0.0
vy=0.0
# ................................. variable and parameter vectors
y=[xx,vx,yy,vy]
params=[L,Hooke,m,eta,g,Ox,Oy,scale,dt,tau]
```

Quantities `xx` and `yy` are the coordinates of the initial position of the bob, `vx` and `vy` the components of its initial velocity. List `y` comprises the initial conditions, at each animation step, for `odeint`.

```
51 # ..................................... derivatives-computing function
52 def dfdt(y,t,params):
53   xx,vx,yy,vy = y                        # unpack initial conditions
54   L,Hooke,m,eta,g,Ox,Oy,scale,dt,tau=params     # unpack parameters
55   length=np.sqrt(xx**2+yy**2)
56   stretch=length-L
57   theta=np.arctan2(yy,xx)
58   if stretch>0:
59     force=-Hooke*stretch
60   else:
61     force=0.0
62   fx=force*np.cos(theta)-eta*vx
63   fy=force*np.sin(theta)-eta*vy
64   ax=(fx/m)
65   ay=(fy/m)-g
66   derivs=[vx,ax,vy,ay]
67   return derivs
```

Function `dfdt()` returns the derivatives needed by `odeint()` for numerical integration. Lines 53 copies the values of position and velocity at the beginning of the integration step from the list `y`. Line 54 copies the values of the parameters from the list `params`. The length of the possibly stretched rubber band, $\sqrt{x^2+y^2}$, is evaluated at Line 55, and the corresponding band extension, $\sqrt{x^2+y^2}-\ell$, at Line 56. Line 57 evaluates the angle ϑ between the string and the x axis. Lines 58-63 evaluate the x and y components, f_x and f_y, of the combined force acting on the bob due to drag and Hooke's law, according to (7.8), Lines 64-65 evaluate the corresponding acceleration components, taking also gravity into account. The derivatives of the elements of the list `y` are stored into the array `derivs` at Line 66. At Line 67 the function `dfdt()` returns `derivs`.

```
68 # ............................................... Create root window
69 root=Tk()
70 root.title('Elastic-Band␣Pendulum')
71 root.bind('<Return>',ReadData)
72 # ......................................... Add canvas to root window
73 canvas=Canvas(root,width=cw,height=ch,background='#ffffff')
74 canvas.grid(row=0,column=0)
75 # ........................................ Add toolbar to root window
76 toolbar=Frame(root)
77 toolbar.grid(row=0,column=1,sticky=N)
```

Lines 69-71 create the root window `root`, write the title and bind the Return keyboard key to the function `ReadData()`. Lines 73-77 create the canvas where our animation will take place, and the toolbar where buttons and entries will be located. The toolbar is located at the right of the canvas.

```
78 # ................................................... Toolbar buttons
79 nr=0
80 StartButton=Button(toolbar,text='Start',command=StartStop,\
81   width=ButtWidth)
82 StartButton.grid(row=nr,column=0,sticky=W)
83 nr+=1
84 ExitButton=Button(toolbar, text='Exit', command=StopAll,
85                   width=ButtWidth)
86 ExitButton.grid(row=nr,column=0,sticky=W)
87 nr+=1
```

Lines 79-87 create the buttons bound to the functions `StartStop()` and `StopAll()`.

```
 88 # ............................................ Label and Entry arrays
 89 LabVar=[]
 90 EntryVar=[]
 91 VarList=['x\u2080','vx\u2080','y\u2080','vy\u2080']
 92 nVar=len(VarList)
 93 LabPar=[]
 94 EntryPar=[]
 95 ParList=['Length','Hooke','Mass','\u03B7','g','Ox','Oy',\
 96     'scale','Time␣step','\u03C4/ms']
 97 nPar=len(ParList)
```

The lists that will contain the labels and entries for the variables and parameters of the problem, `LabVar`, `EntryVar`, `LabPar`, and `EntryPar` are created as initially empty lists at lines 89, 90, 93 and 94. The lists of the variable and parameter names, `VarList` and `ParList`, to be used in the labels, are created at lines 91 and 95. For the elements of `VarList` UTF-8 encoded subscripts are used, see Table E.1 of Appendix E. The variable names are actually x_0 (the initial x position), vx_0 (the initial x velocity component), y_0 (the initial y position), and vy_0 (the initial y velocity component). The variables of the program are the components of the bob position, x and y, and of the bob velocity, v_x and v_y. The parameters are the rest length of the rubber string, ℓ, the Hooke constant of the rubber band, k, the mass of the pendulum bob, m, the friction coefficient, η (UTF-8 code `\u03B7`), the gravity acceleration, g, the coordinates of the pivot with respect to the window frame, O_x and O_y, the length scale, the time step, Δt, and the interval between two consecutive frames, τ (UTF-8 code `\u03C4`), see Fig. 7.6. Variables `nVar` and `nPar` are the numbers of variables and parameters of the problem, respectively.

```
 98 # ........................................................ Entries
 99 for i in range(nVar):
100     LabVar.append(Label(toolbar,text=str(VarList[i]),\
101         font=('Helvetica',12)))
102     LabVar[i].grid(row=nr,column=0)
103     EntryVar.append(Entry(toolbar,bd =5,width=ButtWidth))
104     EntryVar[i].grid(row=nr,column=1)
105     nr+=1
106 for i in range(nPar):
107     LabPar.append(Label(toolbar,text=str(ParList[i]),\
108         font=('Helvetica',12)))
109     LabPar[i].grid(row=nr,column=0)
110     EntryPar.append(Entry(toolbar,bd =5,width=ButtWidth))
111     EntryPar[i].grid(row=nr,column=1)
112     nr+=1
```

Loop 99-105 adds the names of the variables, listed in `VarList`, to the label list `LabVar`, and locates each label at row `nr` (incremented at Line 105), column 0 of the toolbar. Then creates the entry for each variable and locates it at the right of the corresponding label, at row `nr`, column 1. Loop 106-112 adds the names of the parameters, listed in `ParList` to the parameter-label list `LabPar`, and locates the labels and the corresponding entries in the toolbar. The labels and entries for the variables and parameters are located in the toolbar as shown in Fig. 7.6.

```
113 # ..................................................... time label
114 CycleLab0=Label(toolbar,text='Period:',font=('Helvetica',11))
115 CycleLab0.grid(row=nr,column=0)
```

```
116 CycleLab=Label(toolbar,text='␣␣␣␣␣',font=('Helvetica',11))
117 CycleLab.grid(row=nr,column=1,sticky=W)
118 nr+=1
119 # ............................................ Initialize entries
120 for i in range(len(VarList)):
121     EntryVar[i].insert(0,'{:.3f}'.format(y[i]))
122 for i in range(len(ParList)):
123     EntryPar[i].insert(0,'{:.3f}'.format(params[i]))
```

Lines 114-117 create two further labels, one, in column 0, with the name `Period:`, the other, in column 1, will be updated every ten iterations and show the value of the average time interval between two successive animation frames. Lines 120-123 write the initial variable and parameter values, formatted with three digits after the decimal point, into the corresponding entry windows.

```
124 # ..............................................................
125 t=[0.0,dt]
126 tcount=0
127 tt0=time.time()
```

Array `t` comprises the end points of the time interval between two successive computation steps of `odeint()`. An animation frame will be drawn at each step. Variable `tcount` is a counter, that will be incrased by 1 at each animation step. Function `time.time()` returns the number of seconds elapsed since the *epoch* as a float. For Unix, *epoch* is January 1st, 1970, at 0 hours. The actual value of *epoch* is usually not relevant, because only the differences between values returned by `time.time()` at different instants of the program execution are used in most programs.

```
128 # ..................................................... Main loop
129 while RunAll:
130     StartIter=time.time()
131     # ............................................. Draw pendulum
132     canvas.delete(ALL)
133     canvas.create_oval(Ox-scale*L,ch-Oy+scale*L,\
134         Ox+scale*L,ch-Oy-scale*L,outline='green',width=1)
135     canvas.create_line(0,ch-Oy,cw,ch-Oy,fill='green')
136     canvas.create_oval(Ox-prad,ch-(Oy+prad),Ox+prad,ch-(Oy-prad),\
137         fill='black')
138     lengthsq=xx**2+yy**2
139     length=np.sqrt(lengthsq)
140     if length>=L:
141         canvas.create_line(Ox,ch-Oy,Ox+scale*xx,ch-Oy-scale*yy,fill='black')
142     else:
143         alpha=np.arcsin(length/L)
144         beta=np.arctan2(yy,xx)
145         gamma=(np.pi/2.0)+beta-alpha
146         xx2=0.5*L*np.cos(gamma)
147         yy2=0.5*L*np.sin(gamma)
148         canvas.create_line(Ox,ch-Oy,Ox+scale*xx2,ch-Oy-scale*yy2,\
149             Ox+scale*xx,ch-Oy-scale*yy,fill='black')
150     canvas.create_oval(Ox+scale*xx-rad,ch-Oy-scale*yy-rad,\
151         Ox+scale*xx+rad,ch-Oy-scale*yy+rad,fill=bColor)
152     canvas.update()
```

Loop 129-202 is our animation loop. Line 129 stores in `StartIter` the initial time of the iteration (the time elapsed since *epoch*). Lines 133-134 draws a green circle of radius ℓ (the rest length of the string): the elastic force is active if the center of the bob is outside the circle, inactive if the bob is inside. Lines 135 draw a horizontal green line passing through the origin (through the pivot). Lines 136-137 draw draw a black circle in the origin, representing the pivot of the pendulum. Lines 138-139 evaluate the length of the rubber band, equal to the distance between the bob and the pivot. If the length of the rubber band is equal to, or longer than, its rest length ℓ, it is represented by a straight line drawn at Line 141. If the distance is shorter than ℓ, the rubber band is represented by a polyline comprising two line segments of equal length, starting on the pivot and ending at the center of bob, as shown in Fig. 7.5. The length of each line segment is $\ell/2$. Lines 148-149 draw the polyline. The angles α (`alpha`), β (`beta`) and γ (`gamma`), evaluated at Lines 143-145, are shown in Fig. 7.5, and are used at Lines 146 and 147 to evaluate the position (x_2, y_2) where the rubber band is bent, see Fig. 7.5. Obviously, a real rubber band would be bent in a more complicated, practically unpredictable way. Our purpose here is just to show that the distance between bob and pivot is smaller than ℓ. The bob is drawn at Lines 150-151 and the canvas is updated at Line 152.

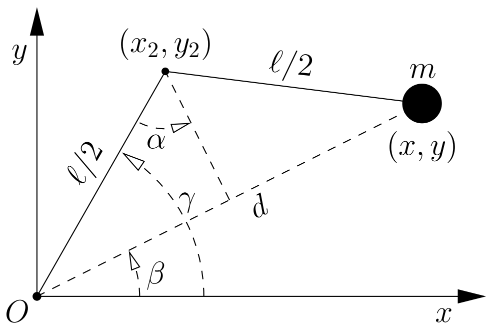


Figure 7.5 The angles α, β and γ of Listing 7.10.

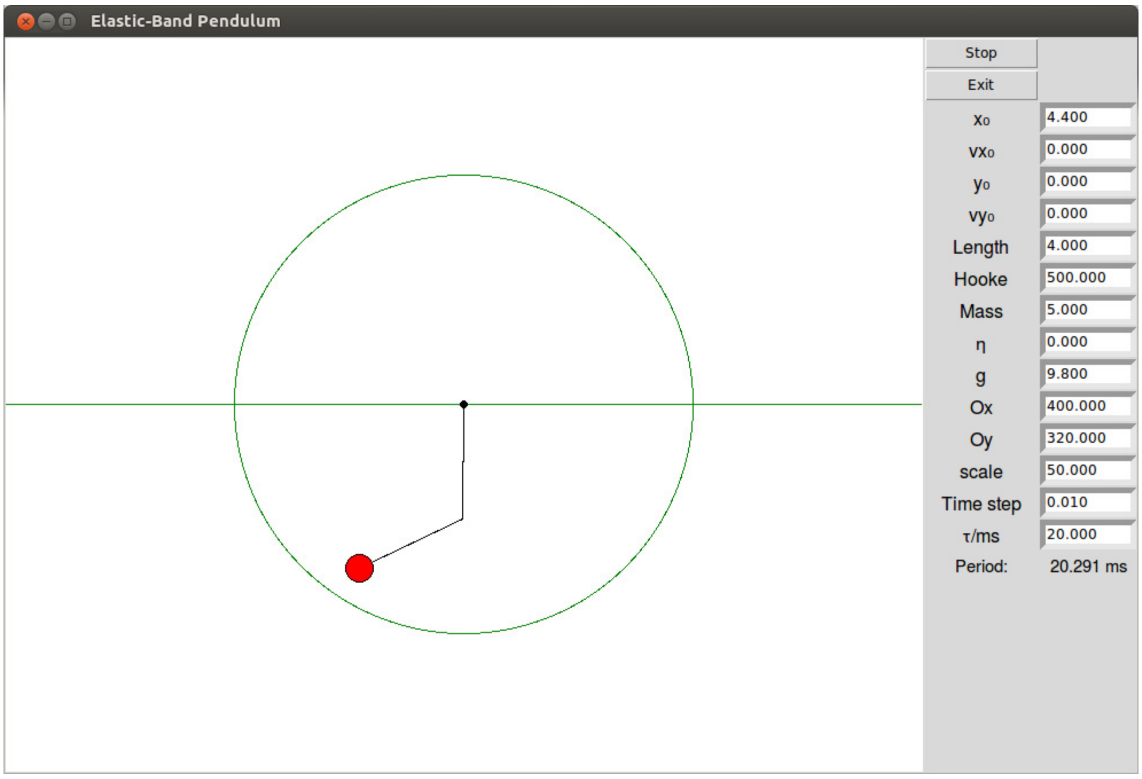
```
153    if RunIter:
154      # .......................... Velocity and position for next frame
155      psoln = odeint(dfdt,y,t,args=(params,))
156      xx=psoln[1,0]
157      vx=psoln[1,1]
158      yy=psoln[1,2]
159      vy=psoln[1,3]
160      # ............................................... Update vector
161      y=[xx,vx,yy,vy]
```

If `RunIter` is *True*, Lines 155-159 evaluate the bob position and velocity at the next step by calling `odeint()`, and the new values, x, v_x, y and v_y are stored into the list `y` at Line 161.

```
162    # .................................................... Read entries
163    elif GetData:
164      i=0
165      while i<nVar:
166        try:
167          y[i]=float(EntryVar[i].get())
168        except ValueError:
169          pass
170        i+=1
171      i=0
172      while i<nPar:
173        try:
174          params[i]=float(EntryPar[i].get())
175        except ValueError:
176          pass
177        i+=1
178      i=0
179      while i<nVar:
180        EntryVar[i].delete(0,END)
181        EntryVar[i].insert(0,'{:.3f}'.format(y[i]))
```

```
182          i+=1
183      i=0
184      while i<nPar:
185          EntryPar[i].delete(0,END)
186          EntryPar[i].insert(0,'{:.3f}'.format(params[i]))
187          i+=1
188      xx,vx,yy,vy=y
189      L,Hooke,m,eta,g,Ox,Oy,scale,dt,tau=params
190      tau=int(tau)
191      t=[0.0,dt]
192      GetData=False
```

If `RunIter` is *False* and `GetData` is *True*, Lines 163-178 read the start-values array and the parameters array from the corresponding entries in the toolbar (they may have been changed by typing new values on the keyboard). At Lines 179-187 the values are rewritten into the entries, formatted with three digits after the decimal point. Lines 188-189 copy the values from the lists. Line 190 takes care that `tau`, the required time interval between two consecutive frames, must be an integer number of milliseconds. Line 191 inserts the new value of `dt` into the list `t`. Once the new data have been read, Line 192 sets `GetData` to *False*.



x0	4.400
vx0	0.000
y0	0.000
vy0	0.000
Length	4.000
Hooke	500.000
Mass	5.000
η	0.000
g	9.800
Ox	400.000
Oy	320.000
scale	50.000
Time step	0.010
τ/ms	20.000
Period:	20.291 ms

Figure 7.6

```
193  # .............................................. cycle duration
194  tcount+=1
195  if tcount%10==0:
196      ttt=time.time()
197      elapsed=ttt-tt0
```

```
198         CycleLab['text']='%8.3f'%(elapsed*100.0)+' ms'
199         tt0=ttt
200     # ............................................................
201     ElapsIter=int((time.time()-StartIter)*1000.0)
202     canvas.after(tau-ElapsIter)
```

Line 194 increases the iteration counter. Every 10 iterations Line 198 writes the average iteration duration, in ms, into label `CycleLab` at the bottom of the toolbar.

```
203     ElapsIter=int((time.time()-StartIter)*1000.0)
204     canvas.after(tau-ElapsIter)
205     #------------------------------------------------------------
206 root.destroy()
```

Line 203 stores the time elapsed from the beginning of the current iteration, in ms, into `ElapsIter`. If `ElapsIter` is shorter than `tau` (the requested time interval between two consecutive frames), Line 204 cauases the program so wait for `tau-ElapsIter` milliseconds before starting the successive iteration. Note that if `ElapsIter` is longer than `tau` Line 204 has no effect, and the program runs slower than required.

7.7 Length and Time Scaling

Script 7.10 can be instructive about some problems involved with length and time scaling in computer animation. Obviously it is convenient to use a coherent system of units when writing the differential equations to be solved by `odeint()`. If we choose SI units, lengths will be measured in meters, masses in kilograms, times in seconds, ... These units are consistently used in function `dfdt()` defined at Lines 52-67, and passed to `odeint()` at Line 155. This is why the rest length of our rubber band is given in m at Line 31. But a length of 4 m would not fit into the computer monitor, and, in any case, the methods that draw items on the canvas expect lengths and coordinates to be given in px (pixels). The problem is handled by introducing the variable `scale`, corresponding to S, the number of px on the monitor that corresponds to a real length of 1 m. All real lengths and positions expressed in m must be converted into px by multiplying them by S before being passed to the Tkinter functions that draw on the canvas.

A pixel is the smallest single component of a digital image. This, on the computer display, corresponds to a small square of uniform color and of side p, the value of p depending on the specific display size and resolution of our computer. The display size is the physical size of the area where pictures and videos are displayed. The size of a screen is usually described by the length of its diagonal in inches. The display resolution is usually given in width×height with the units in pixels. For instance, on a display of size 22″ and resolution 1680×1050 pixels we have 96 dots per inch. Thus the side of a pixel is $p = 0.0254/96 \simeq 2.6458 \times 10^{-4}$ m.

Variable `scale` is assigned the value as $S = 50.0$ at Line 41. Thus, a real length of L, expressed in m, is represented by a line of LS px on the monitor. Since the side of a pixel is p, the ratio of a length represented on the display to the orignal real length is

$$\rho_L = \frac{LS\,p}{L} = S\,p\ . \tag{7.9}$$

Thus, the rest length of our elastic band, 4 m, corresponds to $LS = 200$ px on the canvas. With the assumed monitor size and resolution, we have $\rho_\mathrm{L} = S\,p \simeq 1.3229 \times 10^{-2}$, and if we measure the radius of the green circle of Fig. 7.6 with a ruler we find

$$r = LSp \simeq 0.0529 \text{ m} = 5.29 \text{ cm} . \tag{7.10}$$

Times are measured in seconds in our computations, and Line 35 defines Variable `dt`, corresponding to the time step Δt used for the numerical solution of our differential equations (see Chapter 5), as 0.01 s, or 10 ms. On the other hand Python requires the time interval τ between two successive animation frames to be given as an integer number of milliseconds, and variable `tau` is defined at Line 42 as 20 ms. Thus the ratio of the time observed in our animation to the real time is

$$\rho_\mathrm{t} = \frac{1000\,\Delta t}{\tau} , \tag{7.11}$$

the factor 1000 at the numerator is due to τ being expressed in milliseconds rather than in seconds. With the values of Script 7.10 we obtain $\rho_\mathrm{t} = 2$, and our animated motion is slower than the real motion by a factor 2. The ratio of the velocity of an object on the monitor to the corresponding real velocity is thus

$$\rho_\mathrm{v} = \frac{\rho_\mathrm{L}}{\rho_\mathrm{t}} = \frac{Sp\tau}{1000\,\Delta t} . \tag{7.12}$$

Again, the values of Script 7.10 lead to $\rho_\mathrm{v} \simeq 6.6145 \times 10^{-3}$. A real velocity of 1 m/s is represented by a velocity of 6.6145 mm/s on the monitor.

The time scale ρ_t can be adjusted by changing the values of Δt and/or τ. Increasing Δt, and/or decreasing τ, makes ρ_t larger, and movements on the display slower. Vice versa, ρ_t is decreased by decreasing Δt and/or increasing τ. It is important to note that the values of Δt and τ cannot be arbitrarily changed, but each of them has its own permissible range. The upper limit to Δt is set by the convergence of the finite-difference method used for the integration of the differential equations. In simple words, the values of our functions at time $t+\Delta t$ cannot be *too* different from their values at time t. The lower limit to Δt is mainly set by the computer precision, and by the animation becoming too slow. The upper limit to τ is set by the fact that a large time interval between two successive animation frames can cause the impression of a "step-wise animation". The lower limit to τ is strongly computer-dependent, being set by the computer speed. The time interval between two successive frames cannot be shorter that the time τ_calc needed to solve the differential equations and to redraw the canvas. If τ is set to a value shorter than τ_calc Line 202 simply has no effect. The reader is invited to experiment on the animation behavior when the values in the entries `Time step` and τ/`ms` are changed.

Chapter 8

Classes

8.1 The `class` Statement

Python is an *object-oriented* programming (OOP) language. While *procedure-oriented* programming (POP) languages are mainly based on variables and functions, OOP languages add, and stress, *objects*. Often objects correspond to things found in the real world. A graphics program may have objects such as “circle” or “square”, a physics program may have objects such as “electron” or “nucleus”. An object is a collection of data (variables) characterizing the object itself, and methods (functions) acting on those data. It is certainly possible to write Python programs not using objects, as we have done in the previous chapters. But objects are one of the strengths of Python. Python, as most OOP languages, is class-based: Python objects are instances of *classes*. This means that the structure and behavior of an object are defined by a *class*, a class being a blueprint of all objects of a specific type. For example, a celestial-mechanics program can define objects “Earth” and ”Jupiter” as instances of the class “planet”. A class is defined by the `class` statement, ending with a colon. Its methods are defined by using the `def` statement, just as usual functions. As usual, code blocks are defined by their indentation. Listing 8.1 should give a first idea of how a class is structured.

Listing 8.1 ClassExample.py

```
#!/usr/bin/env python3
# .............................. class particle
class particle:
  color='red'
  def __init__(self,mass,x,vx):
    self.m=mass
    self.x=x
    self.vx=vx
    self.px=mass*vx
    # ............................ move particle
  def move(self):
    self.x+=self.vx
# ..........................................
pt1=particle(10,10,3.5)
pt2=particle(20,15,-2.1)
center=(pt1.m*pt1.x+pt2.m*pt2.x)/(pt1.m+pt2.m)
print("momentum1 = {:.1f}".format(pt1.px))
print("momentum2 = {:.1f}".format(pt2.px))
```

```
19  print("center␣of␣mass␣=␣{:.3f}".format(center))
20  print('color1:',pt1.color,'␣␣color2:',pt2.color)
```

Lines 3-12 comprise the definition of a class named `particle`. This class has two *methods*, one *class variable* and four *instance variables*. Line 4 defines the class variable color, which is set equal to `'red'`. A class variable is a variable which has the same value for all class instances: all our particles will be red. Lines 5-9 define the `__init__()` method, note the leading and trailing double underscores (__) reserved by Python to the names of special methods. Method `__init__()` is a function that creates a new object belonging to the class (a new class instance) in a given *initial state*, specified by the initial values of some *instance variables*. Here method `__init__()` has four arguments, the first, `self`, is a reference to the current instance of the class. The other arguments are the mass, initial position and initial velocity of a particle moving in one dimension (along the x axis). Lines 6-8 copy the argument values of `__init__()` into instance variables of the new class instance. Instance variables are variables that are specific to the object, and may differ from one instance to the other of the same class. Instance variables are prefixed by "`self.`", like `self.m`, in the class declaration. Line 9 defines the momentum of the particle. Lines 11-12 define the `move()` method which, when called, displaces the particle position by `vx`. In an animation, a loop will iteratively call the `move()` method, each time displacing the particle. Thus, here the velocity is actually measured in pixels/cycle, as in previous scripts.

Lines 14-15 create two new "particles", i.e., two new instances of the class. The first particle is called `pt1`, with `mass` $m_1 = 10$, position $x_1 = 10$, and velocity $v_1 = 3.5$, the second is called `pt2`, with $m_2 = 20$, $x_2 = 15$, and $v_2 = -2.1$. This is how class instances are created.

Line 16 evaluates the center of mass of the two particles, `center` (x_c in mathematical notation)

$$x_c = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}\,. \tag{8.1}$$

Note the *dot notation* for accessing the instance variables relative to each particle: `pt1.m` indicates the mass of particle 1, `pt2.m` indicates the mass of particle 2. Lines 17 and 18 print the values of the momenta of particle 1 and particle 2. Line 19 prints the center of mass of the two-particle system. Line 20 prints the colors of the two particles, both red, because `color` is a class variable. This is what we see when we run the script

```
$>ClassExample.py
momentum1 = 35.0
momentum2 = -42.0
center of mass = 13.333
color1:  red color2:  red
```

8.2 A First Example: Two Colliding Balls

Script 8.2 provides a first example of the use of classes in Tkinter animation. Two balls of different size and mass, both instances of the class `ball`, move on the canvas, bouncing against the canvas borders and colliding elastically with each other. As usual, a backslash (\) at the end of a code line indicates that a long command is split over multiple lines.

Listing 8.2 ClassCollide.py

```
1  #!/usr/bin/env python3
2  from tkinter import *
3  from numpy import arctan2,cos,sin,sqrt
4  import time
5  # ............................................. Global variables
6  RunAll=True
7  GetData=RunIter=False
8  ButtWidth=9
9  # ....................................... ............ Canvas sizes
10 cw=800
11 ch=600
12 # ................................................. Start values
13 tau=20  #  milliseconds
14 m1=200
15 r1=40
16 x1=r1
17 y1=r1
18 vx1=5.0
19 vy1=5.0
20 m2=150
21 r2=30
22 x2=cw-r2
23 y2=r2
24 vx2=-5.0
25 vy2=5.0
```

Line 13 assigns the required time interval between two successive animation frames $\tau = 20$ ms. Lines 14-25 assign the mass in arbitrary units, radius, the initial x and y coordinates in px, the initial x and y velocity components in px/cycle, for two instances of the class `ball`. As usual in simple animations, positions are measured in pixels and velocities in pixels/(animation cycle).

```
26 # ..................................................... Class ball
27 class ball:
28   def __init__(self,mass,radius,x,y,vx,vy,color):
29     self.m=mass
30     self.rad=radius
31     self.x=x
32     self.y=y
33     self.vx=vx
34     self.vy=vy
35     self.col=color
36     self.image=canvas.create_oval(self.x-self.rad,ch-(self.y+\
37       self.rad),self.x+self.rad,ch-(self.y-self.rad),\
38         fill=self.col,outline=self.col)
```

Lines 27-108 define the class `ball`. The `__init__()` method is defined at lines 28-38: each instance of this class will have its own mass, radius, position and velocity on the canvas plane, and its own color. Lines 36-38 create a first image of the class instance on the canvas, whose position can later be changed by the methods `canvas.coords()` and `canvas.move()`. This is an alternative to what seen in Script 7.10: instead of clearing the whole canvas with the command `canvas.delete(All)` at Line 132, and redrawing everything, here each object will be moved separately on the canvas. As usual in physics, we shall use an upwards-directed y axis for computations. Conversion to the usual canvas coordinates for drawing is performed by writing `ch-self.y` instead of `self.y`. Variable `ch` is global and corresponds to the canvas height in px.

```
39    # ............................................... Move ball
40    def move(self):
41      self.x+=self.vx
42      self.y+=self.vy
43      canvas.coords(self.image, self.x-self.rad, ch-(self.y+self.rad),\
44        self.x+self.rad, ch-(self.y-self.rad))
```

Function `move()`, defined at Lines 40-44, moves the ball to its position in the successive animation frame. First, the x and y coordinates of its center are updated at lines 41-42, then, the position of `self.image` is updated by `canvas.coords()` at lines 43-44. The first argument of the canvas method `.coords()` is the object to be relocated, in this case `self.image`, the image of the class instance (the current ball) on the canvas. The other arguments are coordinates specifying the new position of the object. The number of coordinates depends on the object. Here they have the form x_1, y_1, x_2, y_2, describing the bounding box of the oval representing the ball.

```
45    # .................................... Bounce on canvas borders
46    def bounce(self):
47      if (self.x+self.rad)>=cw:
48        self.vx=-abs(self.vx)
49        self.x=2.0*(cw-self.rad)-self.x
50      if (self.x-self.rad)<=0:
51        self.vx=abs(self.vx)
52        self.x=2.0*self.rad-self.x
53      if (self.y+self.rad)>=ch:
54        self.vy=-abs(self.vy)
55        self.y=2.0*(ch-self.rad)-self.y
56      if (self.y-self.rad)<=0:
57        self.vy=abs(self.vy)
58        self.y=2.0*self.rad-self.y
```

Lines 46-58 define the method `bounce()`, which checks if the ball, at its current position, has reached one of the canvas borders or trespassed it. Trespassing can happen (mathematically, not physically!) because the ball moves by discrete steps. In this case the method makes the ball bounce at the canvas border. Lines 47 checks if the x position plus the ball radius is beyond the canvas right border. If so, the sign of the x velocity component is made negative at Line 48, and the x coordinate is reflected on the canvas border at Line 49. Lines 50-58 perform analogous checks and transformations at the other three canvas borders.

```
59      # ........................................ Elastic collision
60    def ElastColl(self, other):
61      X=other.x-self.x
62      Y=other.y-self.y
63      distsq=X**2+Y**2
64      R12sq=(self.rad+other.rad)**2
65      if distsq<=R12sq:
66        tc=0.0
67        # ................................. Adjust overlapping balls
68        if distsq<R12sq:
69          Xdot=other.vx-self.vx
70          Ydot=other.vy-self.vy
71          aa=Xdot**2+Ydot**2
```

```
 72             bbhalf=X*Xdot+Y*Ydot
 73             cc=X**2+Y**2-R12sq
 74             # ...................... Time elapsed since "real" collision
 75             tc=(-bbhalf-sqrt(bbhalf**2-aa*cc))/aa
 76             # ....................... Time reversal to collision instant
 77             other.x+=tc*other.vx
 78             other.y+=tc*other.vy
 79             self.x+=tc*self.vx
 80             self.y+=tc*self.vy
 81             # .......................... Distances at collision instant
 82             X=other.x-self.x
 83             Y=other.y-self.y
 84         # ................................. Collision reference frame
 85         alpha=arctan2(Y,X)
 86         csalpha=cos(alpha)
 87         snalpha=sin(alpha)
 88         SelfVelXi=self.vx*csalpha+self.vy*snalpha
 89         SelfVelEta=-self.vx*snalpha+self.vy*csalpha
 90         OtherVelXi=other.vx*csalpha+other.vy*snalpha
 91         OtherVelEta=-other.vx*snalpha+other.vy*csalpha
 92         SelfNewVelXi=((self.m-other.m)*SelfVelXi+2.0*other.m*OtherVelXi)/\
 93             (self.m+other.m)
 94         OtherNewXi=((other.m-self.m)*OtherVelXi+2.0*self.m*SelfVelXi)/\
 95             (self.m+other.m)
 96         self.vx=SelfNewVelXi*csalpha-SelfVelEta*snalpha
 97         self.vy=SelfNewVelXi*snalpha+SelfVelEta*csalpha
 98         other.vx=OtherNewXi*csalpha-OtherVelEta*snalpha
 99         other.vy=OtherNewXi*snalpha+OtherVelEta*csalpha
100         # ....................................................
101         other.x-=tc*other.vx
102         other.y-=tc*other.vy
103         self.x-=tc*self.vx
104         self.y-=tc*self.vy
```

Lines 60-104 define the method `ElastColl()`, that handles elastic collisions between the specific class instance (the specific ball, let us call it *ball* 1) and another class instance (another ball, let us call it *ball* 2). The method's second argument, `other`, refers to ball 2, thus, it must be another instance of the class `ball`. Lines 61-64 evaluate variables `X`, defined as $X = x_2 - x_1$, and `Y`, defined as $Y = y_2 - y_1$. Variable `distsq` is the square of the distance between the centers of the two balls, $X^2 + Y^2$, and `R12sq` is the square of the sum of the two radii, $(R_1 + R_2)^2$. If $X^2 + Y^2 > (R_1 + R_2)^2$ no collision occurs, and the method is exited at Line 65. Otherwise variable `tc`, corresponding to the time interval t_c elapsed from the collision instant to the time of the current animation frame (the two balls might be compenetrating because of their stepwise motions), is temporarily set to 0.

Line 68 checks if $X^2+Y^2 < (R_1+R_2)^2$, the other remaining possibility being $X^2+Y^2 = (R_1+R_2)^2$. In the latter case the two balls are tangent to each other, and we are exactly at the collision instant. Otherwise the two balls are partially overlapping as shown in Fig. 8.1. As mentioned above, the two balls cannot overlap in reality, but they can overlap in our simulation because they move by discrete steps. Lines 69-83 of our listing handle this case by performing a "time reversal" that brings the balls back in time to the collision instant, which occurred between the times of the two successive animation frames. The coordinates of ball i, where $i = 1, 2$, can be written as functions of time as

$$x_i(t) = x_i(0) + \dot{x}_i t \ , \quad y_i(t) = y_i(0) + \dot{y}_i t \ , \tag{8.2}$$

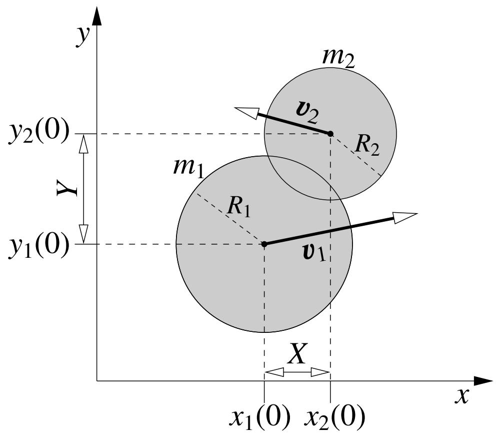


Figure 8.1

where $x_i(0)$ and $y_i(0)$ are the calculated coordinates of the overlapping balls at the current animation frame instant, that we choose as time origin, while $\dot{x}_i$ and $\dot{y}_i$ are their velocity components. Thus, for instance, $\dot{x}_1$ corresponds to the variable `self.vx`. Remember that time is measured in units of τ, the interval between between two successive frames. Accordingly, the square of the distance between the two centers, $s^2(t)$, is written, as a function of time,

$$\begin{aligned} s^2(t) &= [x_2(t) - x_1(t)]^2 + [y_2(t) - y_1(t)]^2 \\ &= \Big[(x_2(0) + \dot{x}_2 t - x_1(0) - \dot{x}_1 t)^2 + \\ &\quad (y_2(0) + \dot{y}_2 t - y_1(0) - \dot{y}_1 t)^2\Big] \\ &= \left(\dot{X}^2 + \dot{Y}^2\right) t^2 + 2\left(X\dot{X} + Y\dot{Y}\right) t + X^2 + Y^2 \ , \qquad (8.3) \end{aligned}$$

where $\dot{X} = \dot{x}_2 - \dot{x}_1$ and $\dot{Y} = \dot{y}_2 - \dot{y}_1$. In order to find the collision time t_c, such that $s^2(t_c) = (R_1 + R_2)^2$, we must solve the quadratic equation

$$\left(\dot{X}^2 + \dot{Y}^2\right) t_c^2 + 2\left(X\dot{X} + Y\dot{Y}\right) t_c + \left[X^2 + Y^2 - (R_1 + R_2)^2\right] = 0 \ . \qquad (8.4)$$

This is done at lines 69-75, where, at Line 75, we choose the negative solution `tc` because, obviously, the collision occurred before the balls overlapped. Note that we must have $|t_c| < 1$ because the collision occurred between the times of the two successive frames, separated by our time unit τ. Lines 77-80 evaluate the coordinates of the ball centers at the collision instant t_c, and Lines 82-83 the new variables $X = x_2(t_c) - x_1(t_c)$ and $Y = y_2(t_c) - y_1(t_c)$

The collision instant of two spheres of masses m_1 and m_2, radii R_1 and R_2, centers located at $[x_1(t_c), y_1(t_c)]$ and $[x_2(t_c), y_2(t_c)]$, and velocities $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$, respectively, is shown in Fig. 8.2. In a two-dimensional elastic collision between two perfectly smooth spheres, according to classical mechanics, the velocity of each sphere must be split into two perpendicular components: one tangent to the surfaces of the colliding spheres at the point of contact (along the η axis in Fig. 8.2), the other along the line joining the centers of the two spheres (along the ξ axis). Assuming that the sphere surfaces are perfectly smooth, the collision affects only the ξ velocity components, while the η components are unchanged. Denoting by $v_{1\xi}$ and $v_{2\xi}$ the ξ velocity components of the two spheres before the collision, the ξ velocity components after the collision, $w_{1\xi}$ and $w_{2\xi}$, are written

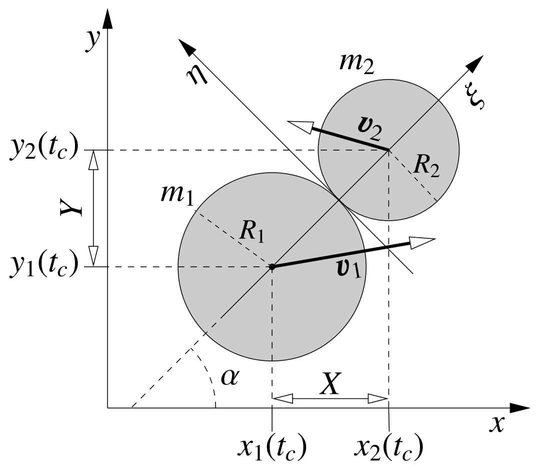


Figure 8.2

$$\begin{aligned} w_{1\xi} &= \frac{(m_1 - m_2)\, v_{1\xi} + 2\, m_2\, v_{2\xi}}{m_1 + m_2} \ , \\ w_{2\xi} &= \frac{(m_2 - m_1)\, v_{2\xi} + 2\, m_1\, v_{1\xi}}{m_1 + m_2} \ . \qquad (8.5) \end{aligned}$$

In the code, as usual, `self` refers to the specific class instance (ball 1), while argument `other`, as stated above, refers to the other ball involved in the collision, ball 2. The variables relative to ball 2 are accessed through the *dot notation*, thus, for instance, the x coordinate of its center is `other.x`. Lines 82-83 evaluate the differences between the x and y positions of the two balls, `X` and `Y`, respectively, denoted by X and Y in Fig. 8.2.

Lines 85-87 evaluate the angle α (`alpha`) between the $\xi\eta$ and xy reference frames, its cosine (`csalpha`) and sine (`snalpha`). Lines 88 and 89 evaluate the ξ and η velocity components of ball 1 before the collision, i.e., quantities $v_{1\xi}$ and $v_{1\eta}$ of (8.5), stored in `SelfXi` and `SelfEta`, respectively. Lines 90 and 91 evaluate the corresponding quantities $v_{2\xi}$ and $v_{2\eta}$ for ball 2, stored in `OtherXi` and `OtherEta`. Lines 92-93 evaluate the ξ velocity component of ball 1 after the collision, $w_{1\xi}$ stored in `SelfNewXi`, according to (8.5). Lines 94-95 store the ξ velocity component of ball 2 after the collision into `OtherNewXi`. Finally, Lines 96-99 evaluate the final velocity components of both balls in the "laboratory frame" xy, i.e., `self.vx`, `self.vy`, `other.vx`, and `other.vy`.

Lines 101-104 take into account that, since the collision took place at time $t_c < 0$, thus before the instant of the current animation frame, at $t = 0$ the two balls have moved further for a time $|t_c|$ with their new velocities.

```
105 # .............................................. Button functions
106 def ReadData(*arg):
107     global GetData
108     GetData=True
109 #
110 def StartStop():
111     global RunIter
112     RunIter=not RunIter
113     if RunIter:
114         StartButton["text"]="Stop"
115     else:
116         StartButton["text"]="Restart"
117 #
118 def StopAll():
119     global RunAll
120     RunAll=False
```

Functions `ReadData()`, `StartStop()` and `StopAll()` are the same as in Script 7.10.

```
121 # ............................................. Create root window
122 root=Tk()
123 root.title('Class␣Collide')
124 root.bind('<Return>',ReadData)
125 # ..............................................................
126 canvas=Canvas(root, width=cw, height=ch, background="#ffffff")
127 canvas.grid(row=0,column=0)
128 # ................................................ Create toolbar
129 toolbar=Frame(root)
130 toolbar.grid(row=0,column=1,  sticky=N)
```

Lines 122-124 create the root window `root`, write the title in its frame, and bind the Return keyboard key to the function `ReadData()`. Lines 126-130 create the canvas and the toolbar. The toolbar, that will contain the buttons and entries, is located at the right of the canvas

```
131 # ....................................................... Buttons
132 nr=0
133 StartButton=Button(toolbar, text="Start",command=StartStop,
134                       width=ButtWidth)
```

```
135 StartButton.grid(row=nr,column=0,sticky=W)
136 nr+=1
137 CloseButton=Button(toolbar, text="Exit", command=StopAll,
138                      width=ButtWidth)
139 CloseButton.grid(row=nr,column=0,sticky=W)
140 nr+=1
```

Lines 132-140 create the buttons bound to the functions `StartStop()` and `StopAll()`.

```
141 # .............................................. Parameter arrays
142 LabPar=[]
143 EntryPar=[]
144 ParList=['m\u2081','r\u2081','vx\u2081','vy\u2081','m\u2082','r\u2082',
145          'vx\u2082','vy\u2082','\u03C4']
146 nPar=len(ParList)
147 # ................................. Entries for new parameter values
148 for i in range (nPar):
149   LabPar.append(Label(toolbar,text=str(ParList[i]),
150                        font=("Helvetica",12)))
151   LabPar[i].grid(row=nr,column=0)
152   EntryPar.append(Entry(toolbar,bd=5,width=10))
153   EntryPar[i].grid(row=nr,column=1)
154   nr+=1
```

Lines 142-146 create the lists that will contain the labels and entries for the parameters of the problem, `LabPar` and `EntryPar`, as well as the list of the parameter names, `ParList`. For the elements of `ParList`, UTF-8 encoded subscripts are used, see Table E.1 of Appendix E. Lines 148-150 locate labels and entries on the toolbar as shown in Fig. 8.3.

```
155 # ..................................................... Time label
156 CycleLab0=Label(toolbar,text="Period:",font=("Helvetica",11))
157 CycleLab0.grid(row=nr,column=0)
158 CycleLab=Label(toolbar,text="␣␣␣␣␣",font=("Helvetica",11))
159 CycleLab.grid(row=nr,column=1,sticky=W)
160 nr+=1
```

Label `CycleLab` will show the actual duration of the time interval between two successive animation frames.

```
161 # ..................................................... Parameters
162 params=[m1,r1,vx1,vy1,m2,r2,vx2,vy2,tau]
163 for i in range(nPar):
164   buff="%.2f" % params[i]
165   EntryPar[i].delete(0,'end')
166   EntryPar[i].insert(0,buff)
```

The parameter list `params` is created, and the initial values of the parameters are written in the windows of the toolbar entries.

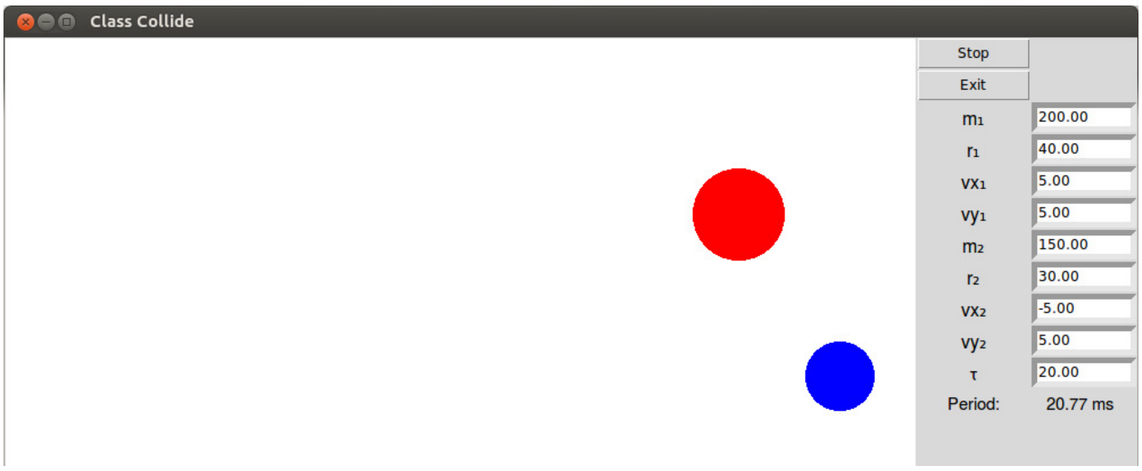
```
167 # ......................................... Create colliding balls
168 ball1=ball(m1,r1,x1,y1,vx1,vy1,"red")
169 ball2=ball(m2,r2,x2,y2,vx2,vy2,"blue")
```

The two collision partners `ball1` and `ball2` are created as instances of the class `ball`, each with its own mass, initial position and velocity, and color.

```
170 # .................................................... Time origin
```

```
171 tt0=time.time()
172 tcount=0
```

The initial time `tt0` and the counter `tcount are initialized.`



m_1 200.00
r_1 40.00
vx_1 5.00
vy_1 5.00
m_2 150.00
r_2 30.00
vx_2 -5.00
vy_2 5.00
τ 20.00
Period: 20.77 ms

Figure 8.3

```
173 # ............................................ Animation loop
174 while RunAll:
175   StartIter=time.time()
176   # ........................................... Move balls
177   if RunIter:
178     ball1.move()
179     ball1.bounce()
180     ball2.move()
181     ball2.bounce()
182     ball1.ElastColl(ball2)
```

Lines 174 -223 comprise the animation loop. Line 175 stores the start time of each iteration into `StartIter`. If `RunIter` is *True*, lines 178-182 move each ball, check if the balls are bouncing at the canvas borders and check if an elastic collisions is occurring between them. Note that the command `ball2.ElastColl(ball1)` would be equivalent to `ball1.ElastColl(ball2).`

```
183   else:
184     if GetData:
185       i=0
186       while i<nPar:
187         try:
188           params[i]=float(EntryPar[i].get())
189         except ValueError:
190           pass
191         i+=1
192       ball1.m, ball1.rad, ball1.vx, ball1.vy,\
193         ball2.m, ball2.rad, ball2.vx, ball2.vy, tau=params
194       tau=int(tau)
195       for i in range(nPar):
196         buff="%.2f" % params[i]
197         EntryPar[i].delete(0,'end')
```

```
198                 EntryPar[i].insert(0,buff)
199             ball1.x=ball1.rad-ball1.vx
200             ball1.y=ball1.rad-ball1.vy
201             ball2.x=cw-ball2.rad-ball2.vx
202             ball2.y=ball2.rad-ball2.vy
203             ball1.move()
204             ball2.move()
205             GetData=False
```

If `Runiter` is *False*, and if `GetData` is *True*, the loop 186-191 updates the list `params` reading the new values from the entries on the toolbar. The single variables are read from the `params` array at Lines 192-193. Variable `tau` is converted to an integer number of milliseconds at Line 194.

Loop 195-198 rewrites the entry windows, formatting the values with two digits after the decimal point. Lines 199-200 locate the center of ball 1 at $x = r_1 - v_{x1}$, $y = r_1 - v_{y1}$. Thus, when the method `ball1.move()` is called at Line 203, the ball center will be located at $x = r_1$, $y = r_1$. The same is done for ball 2 at Lines 201-202. Line 205 sets `GetData` to *False*, so that entries are no longer read till the Enter key is pressed again.

```
206     # ........................................... Cycle duration
207     tcount+=1
208     if tcount==10:
209         tcount=0
210         ttt=time.time()
211         elapsed=ttt-tt0
212         CycleLab['text']="%8.2f"%(elapsed*100.0)+" ms"
213         tt0=ttt
214     ElapsIter=int((time.time()-StartIter)*1000.0)
215     canvas.update()
216     canvas.after(tau-ElapsIter)
```

At Line 207 the counter `tcount` is increased by 1. When `tcount` equals 10 Line 211 determines the duration time of the last 10 loop iterations, and Line 212 prints the average duration of an iteration, in ms, in the label CycleLab at the bottom of the toolbar in Fig. 8.3.

Line 214 measures the time elapsed since the beginning of the current iteration. Line 215 updates the canvas, and Line 216 delays the next iteration till a total time τ has elapsed between two successive animation frames.

```
217     #------------------------------------------------------------
218 root.destroy()
```

8.3 A "Classical" Atom

In physics books we learn that a "classical" atom, i.e., an atom comprising a nucleus and electrons obeying the laws of classical electromagnetism, would not be stable. Such an atom would collapse because the orbiting electrons, being accelerated, would radiate energy and spiral down to the nucleus. We also learn that this is not the case because, actually, atoms obey the laws of quantum mechanics rather than the laws of classical physics. And this is the end of the story.

However, it is interesting to note that a hypothetical "classical" atom with two or more electrons, thus, any classical atom more complex than the hydrogen atom, would not be stable even disregarding radiation losses. Instinctively we might thing of a classical atom as something similar to the Solar

System, with the nucleus playing the role of the Sun and the electrons the roles of the planets. But there is a very important difference. The gravitational force between any two components of the Solar System (two planets, or a planet and the Sun) is proportional to the product of the two masses, with the mass of the Sun (1.99×10^{30} kg) being more than 1000 times larger than the mass of the most massive planet, Jupiter (1.90×10^{27} kg). This makes neglecting the interactions of the planets between themselves a reasonable start approximation. And, in any case, one ought to remember that it took to the Solar System some 4 billion years to reach the actual “stable” configuration.

On the other hand, it is true that a “classical” helium atom (our simplest example) would be a three-body system where the mass of the nucleus is much larger than the mass of each electron (by a factor of approximately 7.3×10^3), in analogy to the Solar System. But here forces are proportional to the products of the involved charges, rather than masses. Thus, the interaction between the two electrons is absolutely not negligible with respect to the nucleus-electron interactions. This makes approximations analogous to the ones used for the Solar System impossible, and an approximate analytic treatment of the problem is not feasible. Even if, obviously, a classical atom simply does not exist, it can be instructive to watch the animation generated by Script 8.3.

Listing 8.3 ClassicalAtom.py

```
 1  #!/usr/bin/env python3
 2  #
 3  from tkinter import *
 4  from scipy.integrate import odeint
 5  import numpy as np
 6  import time
 7  # ........................................... subscripts for labels
 8  sub=['\u2080','\u2081','\u2082','\u2083','\u2084','\u2085',\
 9     '\u2086','\u2087','\u2088','\u2089']
10  # ................................................ Global variables
11  RunAll=True
12  RunIter=NewBaryc=GetData=ReWrite=False
13  # ................................................. Physical values
14  q=1.602176e-19          # elementary charge/Coulomb
15  me=9.10938e-31          # electron mass/kg
16  mp=1.67262e-27          # proton mass/kg
17  ke=8.987551e9           # Coulomb's constant (N m^2/C^2)
18  r2=1.0e-10              # radius of second-electron orbit / m
19  r1=r2/3.0
20  v1=np.sqrt(ke*2.0*q**2/(me*r1)) # m/s
21  v2=np.sqrt(ke*q**2/(me*r2))     # m/s
22  dt=2.0e-19              # s
```

The list at Lines 8-9 defines numerical subscripts according to Table E.1 of Appendix E. These subscripts will be used in the the labels that appear in the toolbar, see Fig. 8.4. Lines 11-12 initialize the usual global variables needed by the toolbar buttons.

Lines 14-17 define some constants in SI units: the elementary charge q, the electron and proton masses m_e and m_p, and the Coulomb constant $k_e = 1/(4\pi\varepsilon_0)$. As initial conditions we arbitrarily assume all particles (nucleus and electrons), located on the x axis of a Cartesian reference frame, the nucleus being located at the origin. Variable `r2` is the initial distance $r_2 = x_2^0$ of the farther electron from the nucleus, arbitrarily chosen as 0.1 nm. Variable `r1` is the initial distance of the closer electron, $r_1 = -x_1^0$, from the nucleus. We arbitrarily choose $x_1^0 = -x_2^0/3$. The initial velocities of both electrons are assumed parallel to the y axis, $\boldsymbol{v}_1^0 = (0, \dot{y}_1)$ and $\boldsymbol{v}_2^0 = (0, \dot{y}_2)$. Variable `v1`, corresponding to $\dot{y}_1$, is chosen so that the closer electron would describe a circular orbit around the nucleus in the absence of electron 2. Analogously, the initial velocity of the farther electron, `-v2`, corresponding to $\dot{y}_2$, would corresponds to a circular orbit if electron 1 had collapsed onto the nucleus. Finally, `dt` is the step size dt, in seconds, used for the numerical integration of the equations of motion.

```
# ................................... Drawing and animation parameters
cycle=20              # ms
scale=3.0e12          # px/m
cw=900                # px
ch=900                # px
Ox=cw/2.0
Oy=ch/2.0
bcrad=2               # px
TrailLength=200
```

Quantity `cycle` is the *required* time interval $\Delta\tau$ between two successive animation frames. Quantity `scale` is the ratio S between a distance on the canvas, measured in px, and the corresponding real distance measured in m. Thus, a real distance of 1 m corresponds to 3×10^{12} px, a distance of 0.1 nm corresponds to 300 px on the canvas. As we shall see in the following, the value of `scale` can be interactively changed during the program execution.

As usual, `cw` and `ch` are the canvas width and height in px, respectively, while `Ox` and `Oy` are the position, in px, of the origin of our coordinate system with respect to the left upper corner of the canvas. The barycenter of the atom will be shown by a small black circle of radius 2 px (`bcrad`). In order to visualize the paths of the particles, each particle (electron or nucleus) leaves a trail on the canvas, consisting of a polyline of `TrailLength` (N_{trail} in mathematical notation) vertices, starting from the present position of the particle, as shown in Fig. 8.4.

```
# ............................................. Start/Stop function
def StartStop():
   global RunIter
   RunIter=not RunIter
   if RunIter:
      StartButton[”text”]=”Stop”
   else:
      StartButton[”text”]=”Restart”
# .................................................... Exit function
def StopAll():
   global RunAll
   RunAll=False
# ............................................... Read Data function
def ReadData(*arg):
   global GetData
   GetData=True
# ....................................................... Scale Down
def ScaleDown(*arg):
   global scale
   scale/=np.sqrt(2.0)
   ScaleLab['text']=”%10.3e”%(scale)
# ......................................................... Scale Up
def ScaleUp(*arg):
   global scale
   scale*=np.sqrt(2.0)
   ScaleLab['text']=”%10.3e”%(scale)
```

Functions `StartStop()`, `StopAll()` and `ReadData()` are the same as in Script 7.10. Function `ScaleDown()` divides `scale` by a factor $\sqrt{2}$ each tim it is called, thus reducing the lengths on the canvas. Function `ScaleUp()` muliplies `scale` by $\sqrt{2}$, thus enlarging the picture.

```
58 # ......................... Evaluate center of mass and its velocity
59 def baryc(part):
60   mtot=sum(zz.m for zz in part)
61   cx=sum(zz.x*zz.m for zz in part)/mtot
62   cy=sum(zz.y*zz.m for zz in part)/mtot
63   cvx=sum(zz.vx*zz.m for zz in part)/mtot
64   cvy=sum(zz.vy*zz.m for zz in part)/mtot
65   return [[cx,cy],[cvx,cvy]]
66 # ................................... move origin to center of mass
67 def SetBaryc():
68   global NewBaryc
69   global part
70   xcm,ycm=baryc(part)[0]
71   cvx,cvy=baryc(part)[1]
72   for zz in part:
73     zz.x-=xcm
74     zz.y-=ycm
75     zz.vx-=cvx
76     zz.vy-=cvy
77   NewBaryc=True
```

Function `baryc()` evaluates the position and velocity components of the barycenter of the system. Nucleus and electron are all instances of the class `particle` defined below, starting from Line 79. The argument `part` of `baryc()` is a list of `particle` instances, comprising the nucleus and the two electrons. Each instance has its own variables, here we are interested in mass, `m`, coordinates, `x` and `y`, and velocity components, `vx` and `vy`. Line 60 evaluates the total mass of the atom, `mtot`. Note that the `for` loop inside the argument of `sum()` runs over all the elements `zz` of the list `part`, quantity `zz.m` being the mass of each particle. Lines 61-64 evaluate the position (`cx`,`cy`) and velocity components (`cvx`,`cvy`), of the barycenter. Function `SetBaryc()` moves nucleus and electrons to their positions in the barycenter reference frame, where the origin is located on the barycenter and the total momentum is zero.

```
78 # ................................................ Class particle
79 class particle:
80   def __init__(self,mass,charge,frict,x,y,vx,vy):
81     self.m=mass
82     self.q=charge
83     self.fr=frict
84     self.x=x
85     self.y=y
86     self.trailmin=np.sqrt(self.x**2+self.y**2)*0.05
87     self.vx=vx
88     self.vy=vy
89     if self.q>0:           # nucleus
90       self.col='red'
91       self.rad=8
92     else:                  # electron
93       self.col='blue'
94       self.rad=4
```

```
95         self.image=canvas.create_oval(Ox+int(scale*self.x-self.rad),\
96           int(Oy-scale*self.y+self.rad),int(Ox+scale*self.x+self.rad),\
97             int(Oy-scale*self.y-self.rad),fill=self.col,outline=self.col)
98         self.trail=[self.x,self.y]*TrailLength
99         self.ScaledTrail=[0.0,0.0]*TrailLength
100        self.TrailImg=canvas.create_line(self.ScaledTrail,fill=self.col)
101    # ............................................ move particle
102    def move(self):
103        canvas.coords(self.image,Ox+scale*self.x-self.rad,\
104          Oy-scale*self.y+self.rad,Ox+scale*self.x+self.rad,\
105            Oy-scale*self.y-self.rad)
106    def UpdateTrail(self):
107        if abs(self.x-self.trail[-2])+abs(self.y-self.trail[-1])>self.trailmin:
108          del self.trail[:2]
109          self.trail.append(self.x)
110          self.trail.append(self.y)
111    def DrawTrail(self):
112        self.ScaledTrail[::2]=[Ox+scale*zz for zz in self.trail[::2]]
113        self.ScaledTrail[1::2]=[Oy-scale*zz for zz in self.trail[1::2]]
114        canvas.coords(self.TrailImg,self.ScaledTrail)
```

Lines 79-114 define the class `particle`. Each instance of the class has its own values for mass, charge, linear drag coefficient (`frict`), position (`x`,`y`), and velocity (`vx`,`vy`), initialized by the `__init__()` method. The instance variable `trailmin`, equal to 0.05 times the distance of the particle from the origin, is the minimum distance between two consecutive points of the trail. If the charge of the particle is positive (nucleus) the particle is represented by a red circle of radius 8 px on the canvas. If the charge is negative (electron) the particle is represented by a blue circle of radius 4 px (Lines 89-94). Lines 95-97 draw the first image of the particle on the canvas. Line 98 initializes the list `trail`, comprising `TrailLength` couples of (x, y) coordinates that will describe the trail of the particle. Line 99 initializes the list `ScaledTrail`, whose elements equal the corresponding elements of `trail` multiplied by `scale`. Line 100 generates `TrailImg`, the first image of the trail on the canvas. Both `image` and `TrailImg` will be updated at each step (frame) of our animation.

Method `move()`, at lines 102-105, moves the particle image to its new position at the next animation step. This is done through the method `canvas.coords()`, whose arguments are the image to be moved, `self.image`, and the coordinates of the new position.

Method `UpdateTrail()` checks if the present position of the particle, (`self.x`,`self.y`), differs by more than `self.trailmin` from the last couple of coordinates of the list `self.trail`. If so, the coordinates of the first (oldest) point of the polyline are removed, and the coordinates of the new position are added at the end of the list.

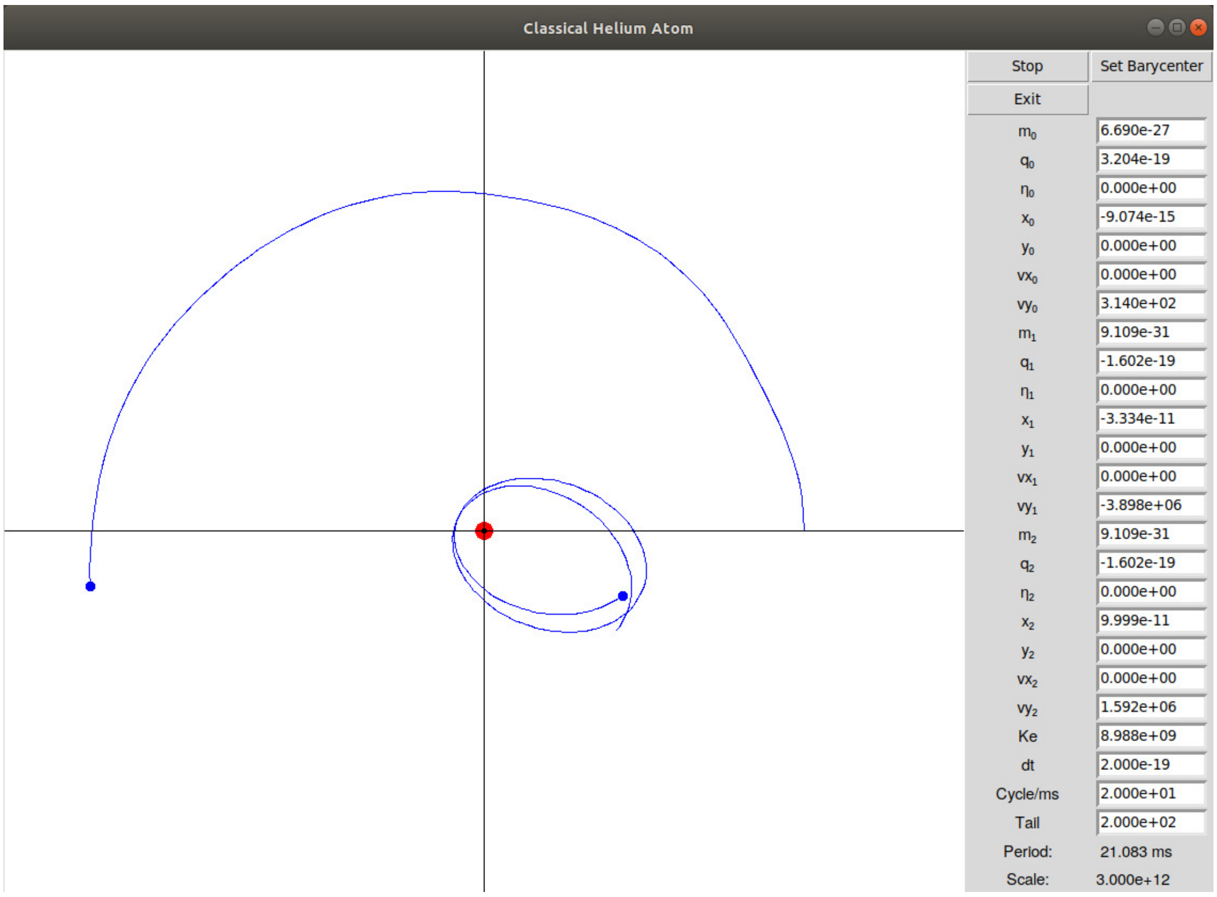
Method `DrawTrail()` evaluates the coordinates of the polyline to be drawn on the canvas. Since we use usual Cartesian coordinates for our calculations, and prefer to have the origin at the center of the canvas, we convert our coordinates by the rules

$$x_{canv} = O_x + S\,x_{Cart}\,, \quad y_{canv} = O_y - S\,y_{Cart}\,, \tag{8.6}$$

where S is the scale factor `scale`, and we take into account that the canvas y axis is directed downwards. Since x and y coordinates alternate in the list, we use *slicing* for the conversion.

```
115 # ........................................ create input vector
116 def WriteInput(bodies,val,InpV,vect):
117     nn=7*len(bodies)
```

```
118    InpV[:nn:7]=[zz.m for zz in bodies]
119    InpV[1:nn:7]=[zz.q for zz in bodies]
120    InpV[2:nn:7]=[zz.fr for zz in bodies]
121    InpV[3:nn:7]=vect[::4]=[zz.x for zz in bodies]
122    InpV[4:nn:7]=vect[1::4]=[zz.y for zz in bodies]
123    InpV[5:nn:7]=vect[2::4]=[zz.vx for zz in bodies]
124    InpV[6:nn:7]=vect[3::4]=[zz.vy for zz in bodies]
125    InpV[nn::]=val
126 # ............................................ Read Entry values
127 def ReadInput(InpV,bodies,val,vect):
128    nn=7*len(bodies)
129    for i,zz in enumerate(bodies):
130       zz.m=InpV[i*7]
131       zz.q=InpV[i*7+1]
132       zz.fr=InpV[i*7+2]
133       zz.x=vect[i*4]=InpV[i*7+3]
134       zz.y=vect[i*4+1]=InpV[i*7+4]
135       zz.vx=vect[i*4+2]=InpV[i*7+5]
136       zz.vy=vect[i*4+3]=InpV[i*7+6]
137    val[::]=InpV[nn::]
```



m_0	6.690e-27
q_0	3.204e-19
η_0	0.000e+00
x_0	-9.074e-15
y_0	0.000e+00
vx_0	0.000e+00
vy_0	3.140e+02
m_1	9.109e-31
q_1	-1.602e-19
η_1	0.000e+00
x_1	-3.334e-11
y_1	0.000e+00
vx_1	0.000e+00
vy_1	-3.898e+06
m_2	9.109e-31
q_2	-1.602e-19
η_2	0.000e+00
x_2	9.999e-11
y_2	0.000e+00
vx_2	0.000e+00
vy_2	1.592e+06
Ke	8.988e+09
dt	2.000e-19
Cycle/ms	2.000e+01
Tail	2.000e+02
Period:	21.083 ms
Scale:	3.000e+12

Figure 8.4

Lines 116-125 define the function `WriteInput()`, which copies the instance variables of the single particles into the lists `InpV` and `vect`. List `InpV` is used for interactively changing parameters during the program execution, through the toolbar entries. List `vect` is the array of initial conditions for the numerical solution of the differential equations by `odeint()`. The name `vect` is used as local variable in the `WriteInput()` and `ReadInput()` functions, in the main program the corresponding list is called `y`, see Lines 178, 179 and 275. Line 125 adds the values of the list `values`, defined at Line 175 below, at the end of `Inpv`. The first $7n$ elements of `InpV` are the instance variables of the n particles ($n = 3$ in our case, but you can easily add new electrons between Lines 172 and 173), and its last 4 elements are the elements of `values`. The two lists are thus

$$\begin{aligned}
&\texttt{InpV} = [m_0, q_0, \eta_0, x_0, y_0, \dot{x}_0, \dot{y}_0, m_1, q_1, \eta_1, x_1, y_1, \dot{x}_1, \dot{y}_1, m_2, q_2, \eta_2, x_2, y_2, \dot{x}_2, \dot{y}_2, k_\mathrm{e}, \mathrm{d}t, \Delta\tau, N_\mathrm{trail}]\ ,\\
&\texttt{vect} = [x_0, y_0, \dot{x}_0, \dot{y}_0, x_1, y_1, \dot{x}_1, \dot{y}_1, x_2, y_2, \dot{x}_2, \dot{y}_2]\ ,
\end{aligned} \tag{8.7}$$

where the numerical subscripts refer to the particles, and η_i stands for the linear drag-force coefficient on particle i. Note the use of list slicing in Lines 118-124. The elements of `InpV` appear in the entry windows of the toolbar, see Fig. 8.4.

Once we have modified some of the parameter values in the toolbar entries, function `ReadInput()`, defined at Lines 127-137, copies our new values into the class particle instances and into the `vect` and `values` lists.

```
138 # ...................................................... vect2bodies
139 def vect2bodies(vect,bodies):
140     for i,zz in enumerate(bodies):
141         zz.x=vect[4*i]
142         zz.y=vect[4*i+1]
143         zz.vx=vect[4*i+2]
144         zz.vy=vect[4*i+3]
```

Function `vect2bodies()`, defined at Lines 139-144, copies the positions and velocities of the particles from the list `vect`, see (8.7), into the particle instance variables.

```
145 # ...................................................... root window
146 root=Tk()
147 root.title('Classical␣Helium␣Atom')
148 root.bind('<Return>',ReadData)
149 root.bind('<Control-plus>',ScaleUp)
150 root.bind('<Control-minus>',ScaleDown)
151 # ........................................................... canvas
152 canvas=Canvas(root,width=cw,height=ch,background="#ffffff")
153 canvas.grid(row=0,column=0)
154 # .......................................................... toolbar
155 toolbar=Frame(root)
156 toolbar.grid(row=0,column=1, sticky=N)
```

Lines 146-150 create the root window and bind the <Return> keyboard key to the `ReadData()` function, and the <Control-plus> key combination (simultanous pressing of the <Ctrl> and <+> keys) to `ScaleUp()`, <Control-minus> to `ScaleDown()`. A canvas and a toolbar are created in the root window.

```
157 # ........................................................... buttons
158 nr=0
159 StartButton=Button(toolbar,text="Start",command=StartStop,width=11)
160 StartButton.grid(row=nr,column=0,sticky=W)
```

```
161 AdjustButton=Button(toolbar, text="Set␣Barycenter",\
162   command=SetBaryc, width=11)
163 AdjustButton.grid(row=nr, column=1, sticky=W)
164 nr+=1
165 CloseButton=Button(toolbar, text="Exit", command=StopAll, width=11)
166 CloseButton.grid(row=nr, column=0, columnspan=2, sticky=W)
167 nr+=1
```

Three buttons, bound to the functions `StartStop()`, `SetBaryc()` and `StopAll()`, respectively, are created in the toolbar, located as in Fig. 8.4.

```
168 # ............................................... Create bodies
169 part=[]
170 part.append(particle(4.0*mp,2.0*q,0.0,0.0,0.0,0.0,0.0))
171 part.append(particle(me,-q,0.0,-r1,0.0,0.0,-v1))
172 part.append(particle(me,-q,0.0,r2,0.0,0.0,v2))
173 nP=len(part)
174 # ........................................ Parameter-value list
175 values=[ke, dt, cycle, TrailLength]
176 # ............................................... input vector
177 InpV=[0]*(7*nP+len(values))
178 y=[0]*4*nP
179 WriteInput(part, values, InpV, y)
```

The nucleus, first and second electron are create at lines 170-173 as instances of the class `particle`, members of the list `part`. The nucleus, `part[0]`, has mass $4m_\mathrm{p}$ and charge $2q$, each electron, `part[1]` and `part[2]`, has mass m_e and charge $-q$. The nucleus is located in the origin with initial zero velocity, while the electrons are located at $y_1 = y_2 = 0$, $x_1 = -r_1$, $x_2 = r_2$, with initial zero x velocity components $\dot{x}_1^0 = \dot{x}_2^0 = 0$, and y velocity components $\dot{y}_1^0$ and $\dot{y}_2^0$. All values of the x position components and of the y velocity components are slightly changed if one presses the *Set Barycenter* button on the toolbar, which performs the coordinate transformation to the barycentric frame.

Line 175 generates the list `values`, comprising the Coulomb constant k_e, the numerical-integration step dt, the required time interval between two successive animation frames, and the number of vertices in the trails following the particles.

Lines 177-179 generate the lists `InpV` and `y`, and initialize them using the function `WriteInput()`.

```
180 # ................................................. Input list
181 InputStr=[]
182 for i in range(len(part)):
183   InputStr.append('m'+sub[i])
184   InputStr.append('q'+sub[i])
185   InputStr.append('\u03B7'+sub[i])  #    eta
186   InputStr.append('x'+sub[i])
187   InputStr.append('y'+sub[i])
188   InputStr.append('vx'+sub[i])
189   InputStr.append('vy'+sub[i])
190 InputStr.append('Ke')
191 InputStr.append('dt')
192 InputStr.append('Cycle/ms')
193 InputStr.append('Tail')
194 # .................................. Labels and Entries for particles
195 InputLab=[]
196 InputEntry=[]
```

```
197 for i,zz in enumerate(InputStr):
198   InputLab.append(Label(toolbar,text=zz,font=("Helvetica",11)))
199   InputLab[i].grid(row=nr,column=0)
200   InputEntry.append(Entry(toolbar,bd=3,width=12))
201   InputEntry[i].grid(row=nr,column=1)
202   InputEntry[i].insert(0,"{:.3e}".format(InpV[i]))
203   nr+=1
204 # ................................................... time label
205 CycleLab0=Label(toolbar,text="Period:",font=("Helvetica",11))
206 CycleLab0.grid(row=nr,column=0)
207 CycleLab=Label(toolbar,text="␣␣␣␣␣",font=("Helvetica",11))
208 CycleLab.grid(row=nr,column=1,sticky=W)
209 nr+=1
210 # .................................................. scale label
211 ScaleLab0=Label(toolbar,text="Scale:",font=("Helvetica",11))
212 ScaleLab0.grid(row=nr,column=0)
213 ScaleLab=Label(toolbar,text="%10.3e"%(scale),font=("Helvetica",11))
214 ScaleLab.grid(row=nr,column=1,sticky=W)
215 nr+=1
```

Lines 181-193 generate the label strings for the entries in the toolbar, as seen in the left toolbar column of Fig. 8.4, `\u03B7` is the utf-8 encoding of the Greek letter η, denoting the linear-drag constant. Lines 195-203 create the labels and entries for modifying the program parameters,located in the toolbar. Lines 205-208 create two side-by-side labels in the toolbar, one with the word *Period:*, the other reporting the actual average time interval between consecutive frames during the program execution. Lines 211-214 create two labels reporting the value of the variable `scale`.

```
216 # ..................................................... function
217 def dfdt(yInp,t,pp):
218   nn=7*(len(yInp)//4)
219   mm=np.array(pp[:nn:7])                      # masses from InpV
220   qq=pp[1:nn:7]                              # charges from InpV
221   fr=np.array(pp[2:nn:7])                     # drags from InpV
222   # ...........................................................
223   x=yInp[::4]
224   y=yInp[1::4]
225   vx=np.array(yInp[2::4])
226   vy=np.array(yInp[3::4])
227   # ......................... Coulomb contribution to force
228   distx=x-(np.tile(x,(len(x),1))).T
229   disty=y-(np.tile(y,(len(y),1))).T
230   alpha=np.arctan2(disty,distx)
231   r2=np.square(distx)+np.square(disty)
232   np.fill_diagonal(r2,1.0)
233   q2=-ke*(np.tile(qq,(len(qq),1)).T*qq)
234   ff=np.divide(q2,r2)
235   np.fill_diagonal(ff,0.0)
236   fx=ff*np.cos(alpha)
237   fy=ff*np.sin(alpha)
238   # .................... Accelerations, including linear drags
239   ax=(fx.sum(axis=1)-(vx*fr))/mm
240   ay=(fy.sum(axis=1)-(vy*fr))/mm
241   # ..................................... Build output list
242   derivs=[0]*len(yInp)
```

```
243     derivs[::4]=vx
244     derivs[1::4]=vy
245     derivs[2::4]=ax
246     derivs[3::4]=ay
247     # ........................................................
248     return derivs
```

Lines 217-247 define the function `dfdt()`, called by `odeint()` at line 274. Argument `yInp` is the list $[x_0, y_0, \dot{x}_0, \dot{y}_0, x_1, y_1, \dot{x}_1, \dot{y}_1, \ldots]$ containing the positions and velocities of the particles at the beginning of each iteration step. Argument `t` is the list $[0, \mathrm{d}t]$ defined at line 249, comprising the time points at which positions and velocities must be evaluated by `odeint()`. Here the two elements of `t` simply determine the time length of the integration step. The function call at line 274 will pass the list `InpV`, containing all program parameters, as argument `pp`. Function `dfdt()` returns the list of the derivatives of the elements of `yInp`, namely $[\dot{x}_0, \dot{y}_0, \ddot{x}_0, \ddot{y}_0, \dot{x}_1, \dot{y}_1, \ddot{x}_1, \ddot{y}_1, \ldots]$.

Line 218 evaluates `nn`, the number of `pp` elements referring to the particles (the last four elements of `pp` being the elements of `values`). The number of particles N_p equals the length of `yInp` divided by 4, since each particle has its own x and y components of position and velocity. Thus `nn` equals N_p multiplies by 7, since each particle has its own mass, charge and linear-drag coefficients, plus the x and y components of its initial position and initial velocity. Lines 219-221 create the lists `mm`, `qq` and `fr`, comprising the particle masses, charges, and linear-drag coefficients, respectively. These lists are obtained by appropriately slicing List `pp`, as discussed in Section 1.13. Lines 223-226 obtain the four lists of positions and velocities at the beginning of the integration step by slicing the list `yInp`.

Lines 228-237 evaluate the Coulomb forces acting on particles. Lines 228 and 229 evaluate the matrices of the x and y components of the interparticle distances. According to the array operations discussed in Section 1.17, we have

$$\texttt{distx} = \begin{pmatrix} 0 & x_1 - x_0 & x_2 - x_0 \\ x_0 - x_1 & 0 & x_2 - x_1 \\ x_0 - x_2 & x_1 - x_2 & 0 \end{pmatrix}, \qquad \texttt{disty} = \begin{pmatrix} 0 & y_1 - y_0 & y_2 - y_0 \\ y_0 - y_1 & 0 & y_2 - y_1 \\ y_0 - y_2 & y_1 - y_2 & 0 \end{pmatrix}. \tag{8.8}$$

Note that here the Python matrix-manipulation routines perform some unnecessary calculations because of the skew-symmetry of both matrices. Actually the evaluation of a single triangular submatrix, excluding the diagonal elements, would be sufficient for each matrix. However the available Python matrix-manipulation routines are pre-compiled and optimized, thus they run much faster than user-written nested loops evaluating the triangular submatrices only. The i, j elements of the upper triangular submatrix of matrix `alpha`, evaluated at Line 230, are thus the α_{ij} angles shown in Fig. 8.5. The i, j elements of the lower triangular submatrix of `alpha` equal $\alpha_{ji} + \pi$, therefore $\sin\alpha_{ij} = -\sin\alpha_{ji}$ and $\cos\alpha_{ij} = -\cos\alpha_{ji}$. Again here and in the following, Python matrix-manipulation routines perform some unnecessary, but fast, calculations. On the diagonal, where both arguments of function `numpy.arctan2()` are zero, the function can return either zero or π, but this is irrelevant for our purposes, since we don't need the diagonal elements of `alpha`. Line 231 creates the matrix `r2` whose elements r_{ij}^2 are the squares of the distances between particle i and particle j. Line 232 arbitrarily fills the diagonal of `r2` with ones, in order to

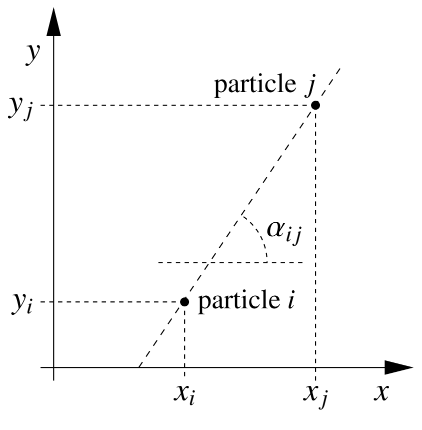


Figure 8.5

avoid divisions by zero on the matrix diagonal at Line 234, since $r_{ii}^2 = 0$. The resulting “artificial” diagonal elements are not used in the subsequent calculations. Line 233 creates the matrix `q2`, with elements $(\texttt{q2})_{ij} = -k_e q_i q_j$. Line 234 obtains the matrix `ff` by Hadamard (element by element) matrix division. The off-diagonal elements of `ff` are thus

$$-k_e \frac{q_i q_j}{r_{ij}^2} \tag{8.9}$$

corresponding to the magnitudes the Coulomb forces between the particle pairs *i*, *j*, with a plus sign if the force is attractive, and a negative sign if the force is repulsive. The diagonal elements of `ff` are zeroed by Line 235. Lines 236 and 237 form the matrices of the *x* and *y* components of the inter-particle forces. Thus, the sum of the elements of row *i* of `fx` (`fy`) is the *x* (*y*) component of the total Coulomb force acting on particle *i*. These sums of the row elements are performed at Lines 239-240, where also the contribution of the linear-drag force is added, and the total force components are divided by the particle masses in order to obtain the lists `ax` and `ay` of the particle acceleration components.

Lines 242-246 build the list `derivs` comprising the derivatives of the elements of `yInp`, which function `dfdt()` returns at Line 248, the last line of the `dfdt()` definition code.

```
249 # ........................................ numerical time interval
250 t=[0.0,dt]
251 tt0=time.time()
252 tcount=0
253 # ............................................ draw coordinate axes
254 canvas.create_line(0,Oy,cw,Oy,fill="black")
255 canvas.create_line(Ox,0,Ox,ch,fill="black")
256 # ................................. Create barycenter image on canvas
257 bc=canvas.create_oval(Ox-bcrad,Oy-bcrad,Ox+bcrad,Oy+bcrad,fill="black")
```

Line 250 builds the list `t` of the time points at which `odeint()` evaluates the solutions of the differential equations at each animation step. Line 251 stores in variable `tt0` the seconds elapsed since the *epoch*. Line 252 sets the iteration counter `tcount` to zero. Lines 254 and 255 draw the *x* and *y* axes on the canvas, and Line 257 draws a first image of the system barycenter.

```
258 # ...........................................................
259 while RunAll:
260   StartIter=time.time()
261   # .................................................. draw bodies
262   for zz in part:
263     zz.move()
264     zz.UpdateTrail()
265     zz.DrawTrail()
266   # ............................................... center of mass
267   cx,cy=baryc(part)[0]
268   cx*=scale
269   cy*=scale
270   canvas.coords(bc,Ox+cx-bcrad,Oy-cy-bcrad,Ox+cx+bcrad,Oy-cy+bcrad)
271   canvas.update()
```

Lines 259-315 comprise our main animation loop. Line 260 stores the seconds elapsed from *epoch* to each iteration start in `StartIter`. Loop 262-265 moves all particles to there new positions, and updates the particle trails. Lines 267-270 evaluate the new position of the barycenter and draw its image on the canvas. Line 271 updates the canvas.

```
272   # ........................................................ motion
273   if RunIter:
274     # ................................................ next step
275     psoln = odeint(dfdt,y,t,args=(InpV,))
276     y=psoln[1,:]
277     vect2bodies(y,part)
```

If `RunIter` is *True* lines 275-277 call `odeint()` to solve the differential equations for the particle motions and update the list `y`, comprising the particle positions and velocities at the next step. Line 277 copies the new positions and velocities stored in `y` into the class particle instances, so that the class methods `move()`, `UpdateTrail()` and `DrawTrail` can update the animation frame at the next iteration step.

```
278   # ..............................................................
279   else:
280     if NewBaryc:
281       ReWrite=True
282       WriteInput(part,values,InpV,y)
283       NewBaryc=False
284     elif GetData:
285       for i,zz in enumerate(InputEntry):
286         try:
287           InpV[i]=float(zz.get())
288         except ValueError:
289           pass
290       ReWrite=True
291       GetData=False
```

Lines 280-304 are executed only if `RunIter` is *False*. If `NewBaryc` is *True*, i.e., if the toolbar button <Set Barycenter> has been pressed, thus calling function `SetBaryc()`, variable `ReWrite` is set to *True*, and lists `InpV` and `y` are updated with the new initial positions and velocities in the barycenter reference frame. Eventually, `NewBaryc` is set to *False*.

If `GetData` is *True*, i.e., if the <Return> key has been pressed, Loop 285-289 rereads all values in the toolbar entries and updates list `InpV`. Variable `ReWrite` is set to *True* and `GetData` to *False*.

```
292     if ReWrite:
293       ReadInput(InpV,part,values,y)
294       for zz,yy in zip(InputEntry,InpV):
295         zz.delete(0,'end')
296         zz.insert(0,"{:.3e}".format(yy))
297       dt=values[1]
298       t=[0.0,dt]
299       cycle=int(values[2])
300       TrailLength=int(values[3])
301       for zz in part:
302         zz.trail=[zz.x,zz.y]*TrailLength
303         zz.ScaledTrail=[0.0,0.0]*TrailLength
304       ReWrite=False
```

If `ReWrite` is *True*, i.e., if either `NewBaryc` or `GetData` was *True*, the values stored in List `InpV` are copied into the class-particle instances, and into the lists `values` and `y`. Loop 294-296 rewrites the values in the toolbar entry-windows formatted with 3 digits after the decimal point. Lines 297-298 update variable `dt` and List `t`. Lines 299-300 update the integer values of `cycle` (in ms) and `TrailLength`. Loop 301-303 reinitializes the particle trails with the new lengths. Eventually, `ReWrite` is set to *False*.

```
305      # ................................................ cycle duration
306      tcount+=1
307      if tcount==10:
308        tcount=0
309        ttt=time.time()
310        elapsed=ttt-tt0
311        CycleLab['text']="%8.3f"%(elapsed*100.0)+" ms"
312        tt0=ttt
313      ElapsIter=int((time.time()-StartIter)*1000.0)
314      canvas.after(cycle-ElapsIter)
```

Line 306 increases the iteration counter `tcount`. Lines 307-312 are executed every 10 iterations. Variable `elapsed` is the number of seconds elapsed during the last 10 iterations, which, multiplied by 100, gives the average duration of each iteration in ms. The value is written in the last-but-one label at the bottom of the toolbar. Variable `tt0` is reinitialized.

Variable `ElapsIter` at Line 313 is the time elapsed since the start of the present iteration, in ms. Line 314 delays the start of the next iteration till `cycle` ms have elapsed since the beginning of the present iteration. If `ElapsIter>cycle`, the argument of `canvas.after()` is negative, and Line 314 is simply ignored.

```
315  #-----------------------------------------------------------------------
316  root.destroy()
```

It is interesting to experiment on this script, using the entry labels in the toolbar to change the initial parameter values, and observe how the behavior of our "classical atom" is modified. If the initial positions and velocities of the electrons are modified, in most cases the behavior becomes unstable, and, eventually, "autoionization" may result. Changing the sign of the velocity of either electron is sufficient to observe such instabilities.

A further possibility is adding new electrons between Lines 173 and 174, with arbitrary initial positions and velocities.

A "C-style" `dfdt()` Alternative Function

Function `dfdt()`, defined at Lines 217-248, can be replaced by the following code, where the nested loops at Lines 230-246 avoid the unnecessary calculation of the whole skew-symmetric matrices. This code can be easier to read for the C-minded programmer, but executes more slowly.

Listing 8.4 C-style

```
217  # ...................................................... function
218  def dfdt(yInp,t,pp):
219    nn=7*(len(yInp)//4)
220    mm=pp[:nn:7]                          # masses from InpV
221    qq=pp[1:nn:7]                         # charges from InpV
222    fr=pp[2:nn:7]                         # drags from InpV
223    # .........................................................
224    x=yInp[::4]
225    y=yInp[1::4]
226    vx=yInp[2::4]
227    vy=yInp[3::4]
```

```python
Fx=list(-array(vx)*array(fr))    # drag contribution to force x
Fy=list(-array(vy)*array(fr))    # drag contribution to force y
# .......................... Coulomb contribution to force
i=1
while i<nP:
  j=0
  while j<i:
    deltax=x[i]-x[j]
    deltay=y[i]-y[j]
    r2=deltax**2+deltay**2
    alpha=arctan2(deltay,deltax)
    ff=-ke*qq[i]*qq[j]/r2
    fx=ff*cos(alpha)
    fy=ff*sin(alpha)
    Fx[i]-=fx
    Fx[j]+=fx
    Fy[i]-=fy
    Fy[j]+=fy
    j+=1
  i+=1
# ..........................................................
derivs=[0]*len(yInp)
derivs[::4]=vx
derivs[1::4]=vy
derivs[2::4]=list(array(Fx)/array(mm))
derivs[3::4]=list(array(Fy)/array(mm))
# ........................................................
return derivs
```

Appendix A

Relevant Mathematical Functions

The `math` module comprises real, and a few integer, functions of real variables. The `cmath` module comprises complex functions of complex variables. Many functions, notably the power, logarithmic, trigonometric, ... functions have the same name in the two modules. But it is important to realize that functions of the same name belonging to different modules lead to formally different results. For instance

```
>>> from math import cos
>>> cos(0)
1.0
>>> from cmath import cos
>>> cos(0)
(1 -0j)
```

the output of the complex functions specifies that the real part of $\cos 0$ is 1, while its imaginary part is 0 (here, actually, -0). The imaginary unit, denoted by i in mathematical formulas, is coded as `j` in Python.

All `math` functions are available also in the `numpy` module, the important difference being that the `numpy` functions accept also lists or arrays as arguments. For instance:

```
>>> import numpy as np
>>> np.cos(np.pi/4)
0.7071067811865476
>>> np.cos([0,np.pi/4,np.pi/3])
array([1.        , 0.70710678, 0.5       ])
```

A.1 The `math` Module

The `math` module provides access to the mathematical functions defined by the C standard. These functions cannot be used with complex numbers as arguments and cannot return complex values: use the functions of the same name from the `cmath` module if you require support for complex numbers.

In the following we list the functions provided by this module. Except when explicitly noted otherwise, all return values are floats. Symbol *NaN*, standing for *Not a Number*, is a numeric data type value representing an undefined or unrepresentable value, especially in floating-point calculations, for instance, 0/0.

A.1.1 Number-Theoretic and Representation Functions

- `math.ceil(x)` Returns the smallest *integer* greater than or equal to `x`, $\lceil x \rceil$.
- `math.copysign(x,y)` Returns `x` with the sign of `y`.
- `math.fabs(x)` Returns $|x|$, the absolute value of `x`.
- `math.factorial(x)` Returns $x!$, the factorial of x.
- `math.floor(x)` Returns $\lfloor x \rfloor$, the largest *integer* less than or equal to `x`.
- `math.fmod(x,y)` Returns $x \bmod y$, the remainder when `x` is divided by `y`. In other words: the *dividend* x and the *divisor* y are assumed real, the *quotient* is assumed integer, and the function returns the *remainder*.
- `math.frexp(x)` Returns the mantissa and exponent of `x` as the pair `(m,y)`, where `m` is a float $0.5 \le m < 1$, `y` is an integer, and $x = m \times 2^y$.
- `math.fsum(iterable)` Returns an accurate floating point sum of values in the list `iterable`, avoiding the loss of precision due to multiple roundings in the intermediate partial sums:

```
>>> sum([.1,.1,.1,.1,.1,.1,.1,.1,.1,.1])
0.9999999999999999
>>> math.fsum([.1,.1,.1,.1,.1,.1,.1,.1,.1,.1])
1.0
```

- `math.isfinite(x)` Returns *True* if `x` is neither an infinity nor a *NaN* (Not a Number).
- `math.isinf(x)` Returns *True* if `x` is a positive or negative infinity.
- `math.isnan(x)` Returns *True* if `x` is a *NaN*.
- `math.ldexp(x,y)` Returns $x \times 2^y$. This is essentially the inverse of function `frexp()`.
- `math.modf(x)` Returns the fractional and integer parts of `x` as the pair `(f,n)`, where $x = n + f$, $0 \le f < 1$, and n is an *integer*.
- `math.trunc(x)` Returns the truncated integer value of `x`. Note that `trunc()` returns a *float*, while `floor()` returns an *integer*.

A.1.2 Power and Logarithmic Functions

- `math.exp(x)` Returns e^x.
- `math.expm1(x)` Returns $e^x - 1$.
- `math.log(x[,base])` Returns the logarithm of x to the specified base (defaults to e).

```
>>> print(math.log(10),math.log(10,10))
2.302585092994046 1.0
```

- `math.log1p(x)` Returns $\ln(1 + x)$, the natural logarithm of $(1 + x)$.
- `math.log2(x)` Returns $\log_2 x$, equivalent to `math.log(x,2)`.
- `math.log10(x)` Returns $\mathrm{Log} x = \log_{10} x$, equivalent to `math.log(x,10)`.
- `math.pow(x,y)` Returns x^y.
- `math.sqrt(x)` Returns $\sqrt{x}$.

A.1.3 Trigonometric Functions

- `math.acos(x)` Returns $\arccos x$.
- `math.asin(x)` Returns $\arcsin x$.
- `math.atan(x)` Returns $\arctan x$.
- `math.atan2(y,x)` Returns $\arctan(y/x)$, in radians. The result is between $-\pi$ and π. Since the signs of both arguments are known, `atan2()` computes the correct quadrant.
- `math.cos(x)` Returns $\cos x$.
- `math.hypot(x,y)` Returns the Euclidean norm, $\sqrt{x^2 + y^2}$.
- `math.sin(x)` Returns $\sin x$.
- `math.tan(x)` Returns $\tan x$.

A.1.4 Angular Conversion

- `math.degrees(x)` Converts angle `x` from radians to degrees.
- `math.radians(x)` Converts angle `x` from degrees to radians.

A.1.5 Hyperbolic Functions

- `math.acosh(x)` Returns $\operatorname{arcosh} x$.
- `math.asinh(x)` Returns $\operatorname{arsinh} x$.
- `math.atanh(x)` Returns $\operatorname{artanh} x$.
- `math.cosh(x)` Returns $\cosh x$.
- `math.sinh(x)` Returns $\sinh x$.
- `math.tanh(x)` Returns $\tanh x$.

Note that the prefix “arc” in the trigonometric functions is the abbreviation for *arcus*, while the prefix “ar” in the hyperbolic functions stands for *area*.

A.1.6 Special functions

- `math.erf(x)` Returns the error function

$$\operatorname{erf}(x) = \frac{1}{\sqrt{\pi}} \int_{-x}^{x} \mathrm{e}^{-t^2}\, \mathrm{d}t = \frac{2}{\sqrt{\pi}} \int_{0}^{x} \mathrm{e}^{-t^2}\, \mathrm{d}t \tag{A.1}$$

- `math.erfc(x)` Returns the complementary error function $1 - \operatorname{erf}(x)$

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} \mathrm{e}^{-t^2}\, \mathrm{d}t \tag{A.2}$$

- `math.gamma(x)` Returns $\Gamma(x)$, the Gamma function.
- `math.lgamma(x)` Returns $\ln\left(|\Gamma(x)|\right)$, the natural logarithm of the absolute value of the Gamma function at `x`.

A.1.7 Constants

- `math.pi` Mathematical constant, the ratio of circumference of a circle to its diameter, π = 3.14159...
- `math.e` Mathematical constant, base of the natural logarithms, e = 2.71828...

A.2 The `cmath` Module

A complex number is written as `x+yj`, where `x` is the real part, `y` the imaginary part, and `j` the coding of the imaginary unit i.

```
z=5.5+3.2j
>>> print(z)
(5.5+3.2j)
>>> print(z.real)
5.5
>>> print(z.imag)
3.2
```

A.2.1 Conversions to and from Polar coordinates

- `cmath.polar(z)` Returns the representation of `z` in polar coordinates, i.e., `(r,phi)` where `r` is the modulus of `z` and `phi` is the phase of `z`, thus $z = r\,e^{i\varphi}$. Function polar(z) is equivalent to `(abs(z), phase(z))`.
- `cmath.rect(r,phi)` Returns the complex number `z` with polar coordinates `r` and `phi`.

A.2.2 Power and Logarithmic Functions

- `cmath.exp(z)` Returns e^z.
- `cmath.log(z[,base])` Returns the logarithm of `z` to the given base. If the base is not specified, returns the natural logarithm of `z`. There is one branch cut, from 0 along the negative real axis to $-\infty$, continuous from above.
- `cmath.log10(z)` Returns $\operatorname{Log} z = \log_{10} z$. This has the same branch cut as `cmath.log()`.
- `cmath.sqrt(z)` Returns $\sqrt{z}$. This has the same branch cut as `cmath.log()`.

A.2.3 Trigonometric Functions

- `cmath.acos(z)` Returns $\arccos z$x. There are two branch cuts: one extends right from 1 along the real axis to ∞, continuous from below. The other extends left from -1 along the real axis to $-\infty$, continuous from above.
- `cmath.asin(z)` Returns $\arcsin z$. This has the same branch cuts as `cmath.acos()`.

- `cmath.atan(z)` Returns $\arctan z$. There are two branch cuts: One extends from `1j` along the imaginary axis to ∞j, continuous from the right. The other extends from -1j along the imaginary axis to $-\infty j$, continuous from the left.
- `cmath.cos(z)` Returns $\cos z$.
- `cmath.sin(z)` Return the $\sin z$.
- `cmath.tan(z)` Return the $\tan z$.

A.2.4 Hyperbolic Functions

- `cmath.acosh(z)` Returns $\operatorname{arcosh} z$. There is one branch cut, extending left from 1 along the real axis to $-\infty$, continuous from above.
- `cmath.asinh(z)` Returns $\operatorname{arsinh} z$. There are two branch cuts: One extends from 1j along the imaginary axis to ∞j, continuous from the right. The other extends from -1j along the imaginary axis to $-\infty j$, continuous from the left.
- `cmath.atanh(z)` Returns $\operatorname{artanh} z$. There are two branch cuts: One extends from 1 along the real axis to ∞, continuous from below. The other extends from -1 along the real axis to $-\infty$, continuous from above.
- `cmath.cosh(z)` Returns $\cosh z$.
- `cmath.sinh(z)` Returns $\sinh z$.
- `cmath.tanh(x)` Returns $\tanh z$.

A.2.5 Classification Functions

- `cmath.isinf(z)` Returns *True* if the real or the imaginary part of `z` is $+\infty$ or $-\infty$.
- `cmath.isnan(z)` Returns *True* if the real or the imaginary part of `z` is not a number (*NaN*).

A.2.6 Constants

- `cmath.pi` A complex number whose real part is π, and whose imaginary part is 0.
- `cmath.e` A complex number whose real part is e, and whose imaginary part is 0.

Appendix B

Building Your Own Library

B.1 Writing a Module

As a program gets longer, it is convenient to split it into several files for easier maintenance. You might also want to use one, or more, of your functions in several separate programs without copying their definitions into each program. You can do this by putting the definitions of the functions that you plan to use often into a file, which Python calls a *module*. Definitions from a module can then be imported into other modules, into a script, or into interactive mode with the usual `import` command.

Thus, a module is a file containing Python definitions and statements. The file name is the module name with the suffix `.py` appended. Within a module, the module's name (as a string) is available as the value of the global variable `__name__`. For instance, you can use your favorite text editor to create the file of Listing B.1, comprising two function definitions. If you call the file `mymath.py`, the module name will be `mymath`.

Listing B.1 mymath.py

```python
import math
# ....................................................... factorize
def factorize(n):
   sqnf=int(math.ceil(math.sqrt(float(n))))
   factors = []
   while n%2==0:
      factors.append(2)
      n=n//2
   i=3
   while i<=sqnf:
      while n%i==0:
         factors.append(i)
         n=n//i
         sqnf=int(math.ceil(math.sqrt(float(n))))
      i+=2
   if n!=1:
      factors.append(n)
   return factors
# ......................................................... FiboSeq
def FiboSeq(n):    # return Fibonacci sequence up to n
   result = []
   a,b = 0, 1
```

```
23     while b < n:
24       result.append(b)
25       a, b = b, a+b
26     return result
```

Line 1 imports the module `math`, needed by the function `factorize()`. Python modules can import one another, here our module imports one of Python built-in modules. Lines 3-18 define the function `factorize()`, the same that we already met in Script 2.2. Lines 20-21 define the simple function `FiboSeq()`, that returns the Fibonacci sequence up to *n*, the argument of the function. As you know, a Fibonacci sequence is a sequence of integers, whose first two elements are 0 and 1, and each successive element is the sum of the two elements that precede it.

If you are working in the same directory where you stored your `mymath.py` file, you can import your `mymath` module without problems. In interactive mode you can simply type

```
>>> import mymath
>>> mymath.factorize(33333333333333331)
 [31, 1499, 717324094199]
```

or, alternatively,

```
>>> from mymath import FiboSeq
>>> FiboSeq(400)
 [0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377]
```

You can also write a script accessing your module. Let us call it, for instance, `TestLib.py`,

Listing B.2 TestLib.py

```
#!/usr/bin/env python3
from mymath import factorize
fact=factorize(33333333333333331)
print(fact)
```

which runs as follows

```
$> TestLib.py
 [31, 1499, 717324094199]
```

Thus, everything is fine as long as you are working in the same directory where you stored your module. However, it is often convenient to build a separate directory where to store all your modules (all your library). Let us call this directory, for instance, `~/python/lib`, where the tilde (~) stands for your home directory, which is platform dependent, namely

- `/home/<username>/` under Linux;
- `/Users/<username>` under macOS;
- `C:\Users\<username>` under Microsoft Windows Vista.

Unfortunately, if you are working in a different directory your module is no longer automatically accessible. If you try to import it, this is how Python reacts

```
>>> import mymath
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ModuleNotFoundError: No module named 'mymath'
```

But don't panic: there are two possibilities to import the modules from your new directory to wherever you wish in your computer:

1. **Temporary access:** when you ask to import a module named, for instance, `mymath`, the interpreter first searches for a *built-in* module with that name. If not found, it then searches for a file named `mymath.py` in a list of directories contained in the built-in variable `sys.path`. Variable `sys.path` is a list of directories comprising i) the directory containing the input script (or the current directory); ii) the directories listed in the *environment variable* `PYTHONPATH`, if existent, see Section B.2; and iii) the installation-dependent default. This is how you can add your new directory to the list of `sys.path` when you are in interactive mode

   ```
   >>> import sys
   >>> sys.path.append('/home/<username>/python/lib')
   ```

   remember that the argument of `.append()` is operating-system dependent. From now on your module is accessible. But if you exit and reenter Python interactive mode the accessibility is lost, unless you change again the value of `sys.path` by retyping the two lines. If you wish to access your module from inside a Python script, these must be the first script lines:

   ```
   \#!/usr/bin/env python3
   import sys
   sys.path.append('/home/<username>/python/lib')
   ```

   The second and third lines must be added to every script that calls your module, but otherwise this "change" is permanent.

2. **Permanent access:** You can define an appropriate *environment variable*, as discussed in Section B.2. This will make your modules accessible from everywhere in your computer and forever.

B.2 The PYTHONPATH Environment Variable

Environment variables are *global system variables* accessible by all the processes running in a computer. Environment variables are used to store system-wide values such as the directories, or lists of directories, where to search for, for instance, executable programs or libraries. In other words, environment variables tell programs from what directories to read files, in what directories to write files, where to store temporary files-

The environment variable `PYTHONPATH` sets the search path for importing *your* python modules. Thus, for instance, you can store your `mymath` module, and all your other modules, in a directory called `~/python/lib`. Obviously, you can name the directory as you wish, and locate is wherever it is most convenient for you in your file system. By default, the variable `PYTHONPATH` is not defined on your computer, but you can easily add it. The procedure is not difficult, but operating-system dependent:

- Under Linux, look for the hidden file `.bashrc` in your home directory, edit it with your favorite editor and add the following two lines at the end

  ```
  PYTHONPATH=:.:~/python/lib
  export PYTHONPATH
  ```

the right-hand-side of the first line defines two fields, separated by a colon (" : "), where Python should search for your modules: the dot (" . ") stands for the current directory, `~/python/lib` is the directory where you write your modules. Under Linux and macOS, the character tilde (~) is a shorthand for `/home/<username>/`. Changes to your search path will take effect when you start a new shell.

- Under macOS, edit the file `.profile` and add the two lines

  ```
  PYTHONPATH = ${PYTHONPATH}:~/python/lib
  export PYTHONPATH
  ```

  Again, changes to your search path will take effect when you start a new shell.

- Under Windows, execute the following steps

  1. Access "System Settings" from your Control Panel.
  2. Click on the "Advanced" tab.
  3. Click on the "Environmental Variables" button on the bottom of the screen.
  4. Click the "New" button under the "System Variables" section.
  5. Type `PYTHONPATH` in the "Variable" field. Type the path for Python modules in the value field. Click "OK" when you are finished setting the `PYTHONPATH` environmental variable.

After doing this, your modules are permanently accessible from any of your directories.

Appendix C

The *integrate* Subpackage

C.1 `simps()`

The function
`simps(y,x=`*None*`,dx=1,axis=-1,even='avg')`

integrates $y(x)$ in dx using samples along the x axis and the composite Simpsons rule. If `x` is *None*, a uniform spacing equal to `dx` is assumed. An even number n of samples implies an odd number $n-1$ of subintervals. Since Simpson's rule requires an even number of subintervals, the parameter `even` controls how the extra subinterval is handled. This is how the function arguments are handlesd.

- `y` is the array of the function values to be integrated.
- `x` is the optional array of the abscissae of the `y` values. If `x` is not given, a uniform spacing equal to `dx` is assumed.
- `dx` , optional, is the spacing between the integration points along the x axis. It is only used when `x` is *None*. The default value 1.
- `axis` int, optional, forget this.
- `even` optional, can be `'avg'`,`'first'` or `last'`. Active only if the number of `y` values is even, implying an odd number of subinterval. Value `'first'` means using Simpsons rule for the first $n-2$ subintervals and the trapezoidal rule on the last subinterval, see Subsections 4.7.2 and 4.7.3. Value `'last'` means using Simpsons rule for the last $n-2$ subintervals and the trapezoidal rule on the first subinterval. Value `'avg'` means averaging the results of `'first'` and `'last'`.

C.2 `odeint()`

The function
```
odeint(func, y0, t, args=(), Dfun=None, col_deriv=0, full_output=0, ml=None,
mu=None, rtol=None, atol=None, tcrit=None, h0=0.0, hmax=0.0, hmin=0.0,
ixpr=0, mxstep=0, mxhnil=0, mxordn=12, mxords=5, printmessg=0)
```

integrates a system of ordinary differential equations using the solver *lsoda* from the FORTRAN library *odepack*. This is the argument list of the function, only the first three arguments are mandatory, and used in Listing 5.1:

- `func(y,t0,...)` is a function that computes the derivative(s) of the function(s) `y` at `t0`
- `y0` is an array comprising the initial conditions on `y`
- `t` is an array comprising the time points at which to solve for `y`. The initial value point should be the first element of the array
- `args` is an optional tuple comprising the extra arguments needed for evaluating the function.
- `Dfun` is the gradient (Jacobian) of `func`. Not needed here.
- `col_deriv` is an optional Boolean. It must be set to `True` if `Dfun` defines derivatives down columns (faster), otherwise `Dfun` should define derivatives across rows.
- `full_output` is an optional Boolean, `True` if to return a dictionary of optional outputs as the second output
- `printmessg` is an optional Boolean, `True` if the convergence message must be printed

Appendix D

Methods for Drawing and Writing on the Canvas

In this appendix we describe some relevant methods for drawing geometrical shapes and writing text on the Tkinter canvas.

- `create_arc(x0, y0, x1, y1, dash=, dashoffset=, disableddash=, disabledfill=, disabledoutline=. disabledoutlinestipple=, disabledstipple=, disabledwidth=, extent=, fill=, offset=, outline=, outlinestipple=, start=, state=, stipple=, style=, tags=, width=)`
  Draws an arc from the ellipse inscribed in the rectangle with opposite vertices (x_0, y_0) and (x_1, y_1). The arc is delimited by the angles `start` and `extent`

- `create_line(coord, activedash, activefill, activestipple, activewidth, arrow=, arrowshape=, capstyle=, dash=, dashoffset=, disableddash=, disabledfill=, disabledstipple=, disabledwidth=, joinstyle=, splinesteps=, state=, stipple=, tags=, width=)`
  Draws a polyline comprising n segments, whose vertices (x_0, y_0), (x_1, y_1), $\ldots (x_n, y_n)$ are elements of the list `coord`

- `create_oval(x0, y0, x1, y1, activedash=, activefill=, activeoutline=, activeoutlinestipple=, activestipple=, activewidth=, dash=, dashoffset=, disableddash=, disabledfill=, disabledoutline=, disabledoutlinestipple=, disabledstipple=, disabledwidth=, fill=, offset=, outline=, outlineoffset=, outlinestipple=, smooth=, splinesteps=, state=, stipple=, tags=, width=)`
  Draws an ellipse inscribed in the rectangle with opposite vertices (x_0, y_0) and (x_1, y_1).

- `create_polygon(coord, activedash=, activefill=, activeoutline=, activewidth=, dash=, dashoffset=, disableddash=, disabledfill=, disabledoutline=, disabledoutlinestipple=, disabledstipple=, disabledwidth=, fill=, joinstyle=, offset=, outline=,`

`outlineoffset=, outlinestipple=, smooth=, splinesteps=, state=, stipple=, tags=, width=)`
Draws a polygon on n sides and n vertices, the vertex coordinates (x_0, y_0), (x_1, y_1), $\ldots (x_{n-1}, y_{n-1}0)$ being the $2n$ elements of the list `coord`.

- `create_rectangle(x0, y0, x1, y1, activedash=, activefill=, activeoutline=, activeoutlinstipple=, activestipple=, activewidth=, dash=, dashoffset=, disableddash=, disabledfill=, disabledoutline=, disabledoutlinestipple=, disabledstipple=, disabledwidth=, fill=, offest=, outline=, outlineoffset=, outlinestipple=, state=, stipple=, tags=, width=)`
  Draws a rectangle with opposite vertices (x_0, y_0) and (x_1, y_1).

- `create_text(x, y, activefill=, activestipple=, anchor=, disabledfill=, disabledstipple=,fill=, font=, justify=, offest=, state=, stipple=, text=, width=)`
  Writes text at position (x, y). By default the text is centered on this position.

Meaning of the mandatory function arguments

- `coord`: A list of the form $[x_0, y_0, x_1, y_1, \ldots x_n, y_n]$ where (x_i, y_i) are the coordinates of the vertices of the polyline for `create_line()`, and of the vertices of the polygon for `create_polygon()`.

- `x, y`: Position of the text for `create_text()`.

- `x0, y0, x1, y1`: Opposite vertices of the rectangle for `create_rectangle()`. Opposite vertices for the rectangle bounding the ellipse for `create_arc()` and `create_oval()`.

Meaning of the optional function arguments

- `activedash, activefill, activeoutline, activeoutlinstipple, activestipple, activewidth`: These options specify the `dash`, `fill`, `stipple`, and `width` values to be used when the object is active, that is, when the mouse is over it.

- `anchor`: the default is `anchor=tk.CENTER`, meaning that the text is centered vertically and horizontally around the position (x, y). The other options are (tk.NW), (tk.N), (tk.NE), (tk.E), (tk.SE), (tk.S), (tk.SW), (tk.W), corresponding to the compass points.

- `arrow` The default is for the line to have no arrowheads. Use `arrow=tk.FIRST` to get an arrowhead at the (x_0, y_0) end of the line. Use `arrow=tk.LAST` to get an arrowhead at the far end. Use `arrow=tk.BOTH` for arrowheads at both ends.

- `arrowshape`: A tuple (d_1, d_2, d_3) describing the shape of the arrowheads added by the arrow option. The meaning of the three quantities d_1, d_2 and d_3 is shown in Fig. D.1. Thus, in general, the arrowhead is a quadrilateral, more specifically a *kite*, either convex or concave. It is a convex kite if $d_2 < d_1$: a *rhombus* in the special case $d_1 = 2d_2$. It is a concave kite, also called *dart*, if $d_2 > d_1$, as in the case of Fig. D.1. In the special case $d_2 = d_1$ it is an isosceles triangle of base $2d_3$, which can be considered a degenerate kite. Thus the command `canvas.create_line(0, 50, 100, 50, arrow=LAST, arrowshape=(20 ,20, 5))` creates a horizontal line from $(0, 50)$ to $(100, 50)$ with an isosceles triangle as arrowhead. The arrowhead starts at $x = 100 - 20 = 80$. The base of the triangle is $2 \times d_3 = 10$. All measures are in pixels. The default values for `arrowshape` are $d_1 = 8$, $d_2 = 10$, $d_3 = 3$.

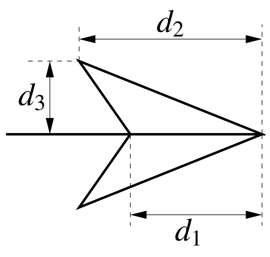


Figure D.1 Shape of the arrowhead

- `capstyle`: Specifies the shape of the ends of the line. The options are i) `tk.BUTT`: the end of the line is cut off square at a line that passes through the endpoint; ii) `tk.PROJECTING`: the end of the line is cut off square, but the cut line projects past the endpoint a distance equal to half the line's width; iii) `tk.ROUND`: the end describes a semicircle centered on the endpoint.

- `dash`: Must be a tuple of integers. The first integer specifies how many pixels should be drawn. The second integer specifies how many pixels should be skipped before starting to draw again, and so on. When all the integers in the tuple are exhausted, they are reused in the same order until the border is complete. The default is a solid line.

- `dashoffset`: If you specify a dash pattern, the default is to start the specified pattern at the beginning of the line. The `dashoffset` option allows you to specify that the start of the dash pattern occurs at a given distance after the start of the line

- `disableddash, disabledfill, disabledstipple, disabledwidth`: The `dash`, `fill`, `stipple`, and `width` values to be used when the item is in the `tk.DISABLED` state.

- `extent`: width of the arc in degrees. The arc starts at the angle given by the `start` option and extends counterclockwise for `extent` degrees.

- `fill`: the color to use in drawing the line. Default is `fill='black'`.

- `font`: if you don't like the default font, set this option to any font value. Examples:
  `font=('Helvetica', '16')` for a 16-point Helvetica regular;
  `font=('Times', '24', 'bold italic')` for a 24-point Times bold italic.

- `joinstyle`: For lines that are made up of more than one line segment, this option controls the appearance of the junction between segments. The options are i) `tk.ROUND`: the join is a circle centered on the point where the adjacent line segments meet; ii) `tk.BEVEL`: a flat facet is drawn at an angle intermediate between the angles of the adjacent lines; iii) `tk.MITER`: the edges of the adjacent line segments are continued to meet at a sharp point. The default style is `tk.ROUND`

- `justfy`: for multi-line text displays, this option controls how the lines are justified: `tk.LEFT` (the default), `tk.CENTER`, or `tk.RIGHT`.

- `offset`: the purpose of this option is to match the stippling pattern of a stippled line with those of adjacent objects.
- `outline`: the color of the border around the outside of the geometric shape, for `create_arc()`, `create_oval()`, `create_polygon()` and `create_rectangle()`. Default is black.
- `outlinestipple`: if the outline option is used, this option specifies a bitmap used to stipple the border. Default is black, and that default can be specified by setting `outlinestipple=''`.
- `smooth`: if `True`, the line is drawn as a series of parabolic splines fitting the point set. Default is `False`, which renders the line as a set of straight segments.
- `splinesteps`: if the `smooth` option is `true`, each spline is rendered as a number of straight line segments. The `splinesteps` option specifies the number of segments used to approximate each section of the line; the default is `splinesteps=12`.
- `start`: Starting angle for the slice, in degrees, measured from $+x$ direction. If omitted, you get the entire ellipse.
- `state`: normally, line items are created in state `tk.NORMAL`. Set this option to `tk.HIDDEN` to make the line invisible; set it to `tk.DISABLED` to make it unresponsive to the mouse.
- `stipple`: to draw a stippled line, set this option to a bitmap that specifies the stippling pattern, such as `stipple='gray25'`. See Section 5.7, Bitmaps for the possible values.
- `style`: the default is to draw the whole arc; use style=`tk.PIESLICE` for this style. To draw only the circular arc at the edge of the slice, use `style=tk.ARC`. To draw the circular arc and the chord (a straight line connecting the endpoints of the arc), use `style=tk.CHORD`.
- `tags`: if a single string, the line is tagged with that string. Use a tuple of strings to tag the line with multiple tags.
- `text`: the text to be displayed in the object, as a string. Use newline characters (`'\n'`) to force line breaks.
- `width`: the line's width (`create_line()`), or width of the border of the geometric shape (`create_arc()`, `creat_oval()`, `create_polygon()` and `create_rectangle()`). Default value is 1 pixel. In the case of `create_text()`, if you don't specify a width option, the text will be set inside a rectangle as long as the longest line. However, you can also set the width option to a dimension, and each line of the text will be broken into shorter lines, if necessary, or even broken within words, to fit within the specified width.

Appendix E

Unicode Characters

We advise to use LaTeXwhenever possible when subscripts, superscripts, Greek letters, ... are needed in text superposed to Python plots. However, this is not always possible, in particular when writing text on buttons and labels. Often Unicode symbols offer an acceptable alternative. UTF-8 is a variable width character encoding capable of encoding all 1 112 064 Unicode characters (they include, for instance, Greek, Hebrew, Chinese, Japanese, Korean ... characters) using one to four bytes. UTF-8 is fully backward-compatible with ASCII encoding. The following two tables give the two-byte encodings for the numerical subscripts and superscripts, and for the Greek letters.

Table E.1 UTF-8 Numerical Superscripts and Subscripts

number	0	1	2	3	4	5	6
superscript	\u2070	\u2071	\u2072	\u2073	\u2074	\u2075	\u2076
subscript	\u2080	\u2081	\u2082	\u2083	\u2084	\u2085	\u2086
number	7	8	9				
superscript	\u2077	\u2078	\u2079				
subscript	\u2087	\u2088	\u2089				

For instance, x_0 is rendered by `x\u2080`, and y^2 by `y\u2072`.

Table E.2 UTF-8 Greek Letters

Α	\u0391	Ι	\u0399	Ρ	\u03A1	α	\u03B1	ι	\u03B9	ρ	\u03C1
Β	\u0392	Κ	\u039A	Σ	\u03A2	β	\u03B2	κ	\u03BA	σ	\u03C3
Γ	\u0393	Λ	\u039B	Τ	\u03A3	γ	\u03B3	λ	\u03BB	τ	\u03C4
Δ	\u0394	Μ	\u039C	Υ	\u03A4	δ	\u03B4	μ	\u03BC	υ	\u03C5
Ε	\u0395	Ν	\u039D	Φ	\u03A5	ε	\u03B5	ν	\u03BD	φ	\u03C6
Ζ	\u0396	Ξ	\u039E	Χ	\u03A6	ζ	\u03B6	ξ	\u03BE	χ	\u03C7
Η	\u0397	Ο	\u039F	Ψ	\u03A7	η	\u03B7	ο	\u03BF	ψ	\u03C8
Θ	\u0398	Π	\u03A0	Ω	\u03A9	ϑ	\u03B8	π	\u03C0	ω	\u03C9

Each two-byte code is represented by a backslash (\) followed by a `u` and four hexadecimal digits.

Appendix F

Tkinter Events

Tkinter events can be key presses or mouse operations by the user. For each widget (root window, canvas, frame ...), it is possible to bind Python functions and methods to an event. The syntax is
`widget.bind(event, handler)`
where `widget` can be the root window itself (usually called `root` in the programs of this book) or one of its “children”, like a canvas or a frame, `event` is a keyboard or mouse event, and `handler` is a usually user-defined function. See Section 7.4 for some first examples.

A description of the mouse and keyboard events is given in the two following sections.

F.1 Mouse Events

A mouse event is generated when the mouse moves, or when a mouse button is clicked or released. The mouse events and their string codings are listed in Table F.1. The *x* and *y* canvas coordinates of where the mouse was clicked or released, or of the mouse location during the motion, are passed to the handler function through the argument as `event.x` and `event.y`. See Listing 7.4.

Table F.1 String Codings of Mouse Events

String	Event
`'<Button-`*n*`>'`	where *n* can be 1, 2, 3, 4 or 5. A mouse button is pressed over the widget. Button 1 is the leftmost button, button 2 is the middle button (where available), button 3 the rightmost button. Buttons 4 and 5 refer to turning the mouse wheel forward and backward, respectively.
`'<ButtonPress-`*n*`>'`	synonym of `'<Button-`*n*`>'`.
`'<B`*n*`-Motion>'`	The mouse is moved, with mouse button *n* being held down
`'<ButtonRelease-`*n*`>'`	Button *n* was released.
`'<Double-Button-`*n*`>'`	Button *n* was double clicked. You can use Double or Triple as prefixes.
`'<Enter>'`	The mouse pointer entered the widget (this event doesnt mean that the user pressed the `<Enter>` key!).
`'<Leave>'`	The mouse pointer left the widget.

F.2 Keyboard Events

A keyboard event occurs when a keyboard key is pressed or released. Events corresponding to pressing printable keys like, for instance, `a`, `A`, or `8` are simply represented by the strings `'<a>'`, `'<A>'` or `'<8>'`. The release of the same keys is represented by the strings `'<KeyRelease-a>'`, `'<KeyRelease-A>'`, and `'<KeyRelease-8>'`. The string `'<Key>'` binds to any key press, which key was actually pressed is passed to the handler function through the argument as `event.char`. Binding to events like pressing Ctrl plus another key, like, for instance Ctrl+a, is obtained through strings like `'<Control-a>'`. In Listing 8.3 Lines 149 and 150 bind the key combinations `'<Control-plus>'` and `'<Control-minus>'` to the handler functions `ScaleUp()` and `ScaleDown()`, respectively.

Table F.2 String Codings of Keyboard Events: Keypad and Non-Printable Keys

String	Key	String	Key
'<Alt_L>'	Left-hand Alt	'<KP_Down>'	Down arrow on the keypad
'<Alt_R>'	Right-hand Alt	'<KP_End>'	End on the keypad
'<BackSpace>'	Backspace	'<KP_Enter>'	Enter on the keypad
'<Cancel>'	Del	'<KP_Home>'	Home on the keypad
'<Caps_Lock>'	CapsLock	'<KP_Insert>'	Ins on the keypad
'<Control_L>'	Left-hand Ctrl	'<KP_Left>'	Left arrow on the keypad
'<Control_R>'	Right-hand Ctrl	'<KP_Multiply>'	$\star$ on the keypad
'<Delete>'	Del	'<KP_Next>'	PageDown on the keypad
'<Down>'	Down arrow	'<KP_Prior>'	PageUp on the keypad
'<End>'	End	'<KP_Right>'	Right arrow on the keypad
'<Escape>'	Esc	'<KP_Subtract>'	− on the keypad
'<F1>'	Function key F1	'<KP_Up>'	up arrow on the keypad
...	...	'<Next>'	PageDown
'<F12>'	Function key F12	'<Num_Lock>'	NumLock
'<Home>'	Home	'<Pause>'	Pause
'<Insert>'	Ins	'<Print>'	PrintScrn
'<Left>'	Left arrow	'<Prior>'	PageUp
'<KP_0>'	0 on the keypad	'<Return>'	Enter
...	...	'<Right>'	Right arrow
'<KP_9>'	9 on the keypad	'<Scroll_Lock>'	ScrollLock
'<KP_Add>'	+ on the keypad	'<Shift_L>'	Left-hand Shift
'<KP_Decimal>'	. on the keypad	'<Shift_R>'	Right-hand shift key
'<KP_Delete>'	Del on the keypad	'<Tab>'	Tab
'<KP_Divide>'	/ on the keypad	'<Up>'	Up arrow

Table F.2 shows the representations of the non-printable keys and of the keys of the numeric keypad, the representations of these latter always starting with `KP_`. Some printable keys are not represented by their symbols on the keyboard, but have special representations. A few of them are reported in Table F.3.

Table F.3 String Codings of Keyboard Events: Some Special Printable Keys

String	Key	String	Key	String	Key
`'<backslash>'`	\	`'<bar>'`	|	`'<quotedbl>'`	”
`'<dollar>'`	$	`'<percent>'`	%	`'<ampersand>'`	&
`'<slash>'`	/	`'<parenleft>'`	(	`'<parenright>'`	)
`'<equal>'`	=	`'<question>'`	?	`'<minus>'`	−
`'<at>'`	@	`'<asterisk>'`	$*$	`'<greater>'`	>
`'<less>'`	<	`'<comma>'`	,	`'<semicolon>'`	;
`'<period>'`	.	`'<colon>'`	:	`'<underscore>'`	_
`'<plus>'`	+	`'<minus>'`	−	`'<sterling>'`	£

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