

# Laboratory and numerical experiments in Quantum Physics

## F0047T

1. Franck–Hertz experiment
2. Atomic spectra of Hydrogen and Mercury
3. Numerical integration of the Schrödinger equation

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# 1 Objective

The objective of the lab exercise is to present a couple of experiments where there is a need for Quantum mechanics to explain the experiments. These two experiments cannot be explained within the framework of classical physics only. The lab exercise also contains a numerical calculation for the infinite potential square well with a small perturbation added to the potential.

In one experiment you will measure the spectrum of the Hydrogen atom and an other element, Mercury, as well. In the case of Hydrogen the challenge is to determine Rydbergs constant and the quantum levels only using the Bohr atom and the wave lengths you determined in the experiment. In the case of Mercury you will be asked to use the internet to backwards identify the levels you found in your experiment. Spectral analysis is an important tool in both science and industry. As an example spectral analysis is used in remote measurement of pollution and also in testing exhaust fumes for carbon monoxide using infrared spectroscopic methods.

You will also make an experiment where electrons are accelerated through a vapour consisting of Mercury (Hg) atoms. The experiment demonstrates that an atom only can absorb a specific amount of energy (the excitation energy from the ground state) in one event. The absorbed energy is emitted as a photon as the atom goes back to its ground state. The emitted photon will be in the ultraviolet regime of the spectra. The experiment you will do is called the Franck–Hertz experiment after the two physicist James Franck and Gustav Hertz. In everyday life you experience a Mercury spectra in the light from fluorescent tubes.

The last experiment is a numerical calculation that you can do on any decent computer like a PC. The system in question is a ordinary square well potential covered in the text book. After you have made a running matlab program you will add a small perturbation. You will study the relation between the shift in the perturbed energy levels compared to the unperturbed ones and how this difference relates to the symmetry of the perturbation. You will also compare the numerical results you received to results you get from a first order perturbation calculation. The numerical exercise is also training your skills in matlab programming.

Your results should be compiled into a nice lab report written in accordance to the guide lines given in ”**Lathund för rapportskrivning**”. You used these guide lines in Fysik 1, 2 and 3. Preferably you use the Latex version.

You may also use the old guide lines given in Torbjörn Löfquist’s booklet (Rapportskrivning : en introduktion) which you can find on the home page of the LTU library: <https://www.ltu.se/webbarkiv/BIB/rapport/index.html> (in Swedish).

You have by now (in your education) written a couple of lab reports and part of the lab is to exercise the skill of writing a well written lab report. A report that does not comply to the guide lines will be returned irrespective of your experimental results.

## 2 Franck–Hertz experiment

### 2.1 Experimental task

Determine the excitation energy of the first (from ground state) excited state of Mercury by means of the Franck–Hertz experiment. The key issue of the experiment is that as electrons move in a gas of Mercury they will sometimes excite a Mercury atom if their kinetic energy matches the excitation energy of the Mercury atom.

### 2.2 Equipment

The setup (see figure (1)) consists of three main parts. 3: One oven containing the experiment inside a glass tube. 2: An amplifier unit to control the experiment and process the output

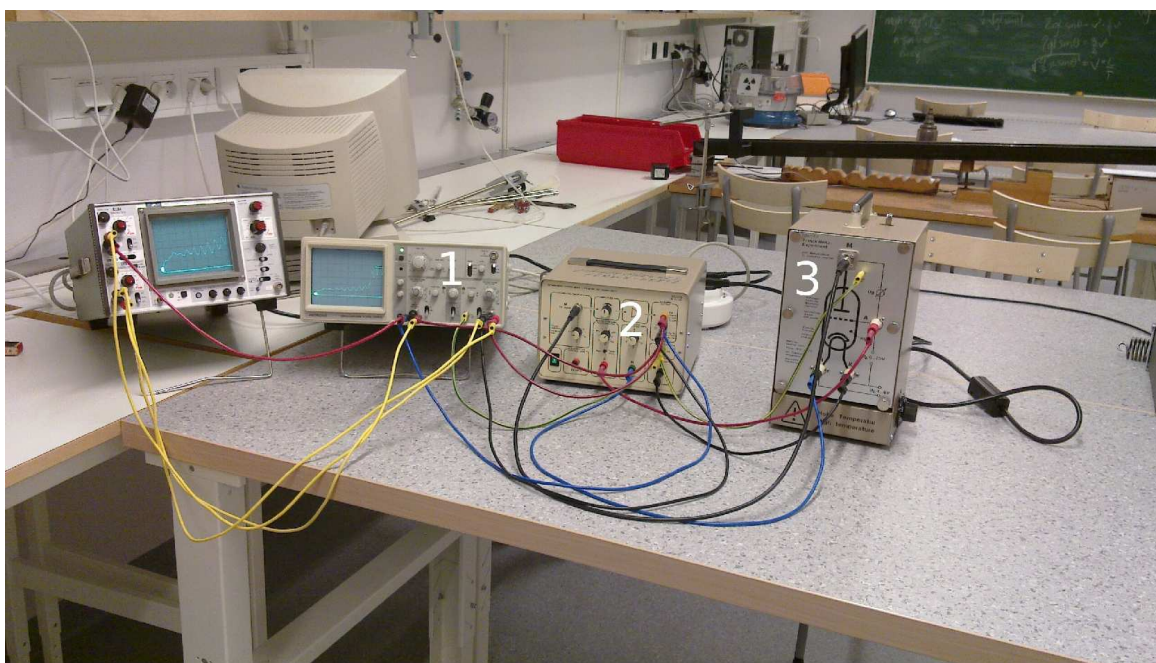


Figure 1: An overview of the setup for the Franck–Hertz experiment. From right to left you see the oven (item 3) with the Franck–Hertz tube to the left of this the specially dedicated amplifier (2) and to the left of this there is the oscilloscope (1). (In the picture there is a second oscilloscope but that is not part of the experiment.)

signal from it. 1: An oscilloscope to monitor the output signal. Inside the oven you can see an evacuated glass tube containing a small drop of Mercury. As the glass tube is heated by the heat source in the oven the glass tube will contain an amount of Mercury gas. You can control the density of the Mercury gas by adjusting the temperature of the oven. The temperature control you find on the outside of the oven. A sketch of the glass tube is shown in figure 2. In the figure you also see the important parts of the tube. Starting from left to right. The cathode (Glödkatod, negatively charged) consists of a glowing filament, marked in figure 2b by the number 1. You can control the current through the filament and as it

starts to glow it will emit electrons. The emitted electrons are accelerated towards the anode (Galleranod, positively charged) by the accelerating voltage  $U_A$ . You can control  $U_A$  on the amplifier box. The anode consists of a grating (marked in figure 2b by the number 2) and as electrons are accelerated towards it, many electrons will pass through the grating and hit the collector (Kollektor) behind it (marked in figure 2b by the number 3). Note that the distance over which the electrons are accelerated is about 1,5 cm. These electrons form the current  $I_C$  in the collector circuit. The current  $I_C$  is amplified in the amplifier unit and displayed on the oscilloscope once the experiment is up and running. You can apply an reward bias voltage (backspänning)  $U_g$  over the anode – collector system. The voltage  $U_g$  acts as a negative potential that will repel electrons as they try to reach the collector once they passed the grating anode. You can adjust the reverse bias potential in order to control the number of electrons that will reach the collector after they have passed the grating–anode.

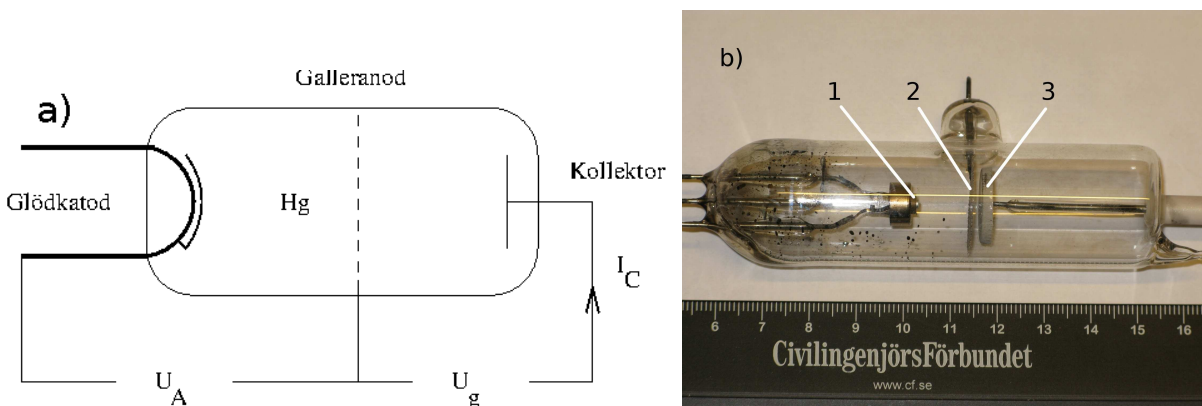


Figure 2: In a) a schematic view of the important parts of the Franck-Hertz tube. At the cathode electrons are freed from a filament (Glödkatod) as it is glowing due to a current running through it. The glowing filament emits electrons that are accelerated over the voltage  $U_A$ . Electrons that pass the grating will enter the collector circuit and will create a current  $I_C$ . By increasing the reverse bias voltage (backspänningen)  $U_g$  slower electrons that have passed the grating are prevented from reaching the collector. In b) a photo of the tube used in the experiment is shown. Indicated by numbers are 1: glowing filament, 2: grating, 3: collector. Note the size of the actual experimental area from 1 to 3. It is of just 1.5 cm length.

The current ( $I_C$ ) that will run through the collector is very small ( $10^{-10}$  A), hence the specially built amplifier. The amplifier generates an output that is proportional to the current  $I_C$  in the collector circuit. The specially built amplifier also contains circuits that generate the current for the electron source (the glowing filament denoted 'Heizung'), the accelerating potential  $U_A$  and the reverse bias potential  $U_g$ . The accelerating potential can either be set to a specific value or be run in 'ramping' mode. In ramping mode the voltage  $U_A$  increases linearly from 0V to a maximum value (of your choice) 50 times a second.

In the experiment you monitor both  $I_C$  and  $U_A$  simultaneously on an oscilloscope that is set in  $X$ - $Y$  mode.  $U_A$  is in the  $X$  channel and  $I_C$  is in the  $Y$  channel.

## 2.3 Measurement

In the experiment you will note the peculiar property that as you increase  $U_A$  the current in the collector  $I_C$  will note always increase with it. The current might even drop as you increase  $U_A$ ! You will measure the difference in  $U_A$  for adjacent maxima and minima that appear on the screen of the oscilloscope.

Check list for the experiment (read them before you actually start the experiment):

1. Before you turn any equipment on make sure to following:
  - (a) The acceleration voltage  $U_A$  in position 0 Volts.
  - (b) The knob marked "Heizung" to 0 Volts this means that the glowing filament will have no current running through it and hence no electrons will be emitted.
2. Turn on the oven at approximately 180 °C. It will take approximately 10 minutes to stabilise at this temperature.
3. Check that the electrical cables are connected properly between the amplifier and the oven containing the Franck–Hertz tube. **Note** that  $U_A$  is marked as  $U_B$  on the amplifier and that there is a division by 10 on the output of  $U_B$  to the oscilloscope.  
Next to the equipment you find a BBC–multimeter just in case you wish to assure yourself on the measurement of  $U_B$  on the oscilloscope.
4. Put the acceleration voltage  $U_A$  in position "Ramp 50 Hz" and approximately 10 V maximum voltage.
5. Connect the oscilloscope (channel X, on some scopes it might be A) so that you can see the time dependence of  $U_A$ . Note the relation between the maximum  $U_A$  according to the amplifier unit and values on the oscilloscope.
6. Turn  $U_A$  to zero and turn (knob marked "Heizung") the voltage over the glowing filament to approximately 8 Volts. If you look through the glass into the oven you can see the filament glow.
7. Connect the second channel (channel Y, on some scopes B) to (prepare to) measure the current in the collector  $I_c$   $I_G$ . You can start on sensitivity 2 volts/unit.
8. Make sure that the oscilloscope is set in X–Y mode.
9. Now we start the experiment. Put the reverse bias voltage  $U_g$  to its maximum 10 Volts. After this you put  $U_A$  to approximately 40 Volts. Adjust the reverse bias  $U_g$  downwards till you see the expected current variations on the display of the oscilloscope.
10. Adjust the amplification of  $I_C$  on the amplifier, the same applies to  $U_A$ ,  $U_g$  and the oscilloscope till several minima and maxima appear on the monitor of the scope.
11. Measure the accelerating voltage for the max and min you can identify. This you do from the monitor of the scope.

12. Observe also the following:

- (a) The influence a change of the reverse bias voltage.
- (b) The influence a change of the accelerating potential.
- (c) The influence a change of the voltage over the glowing filament.
- (d) The influence a change of the temperature of the oven. Make changes in steps of 10 °C after a change let the equipment stabilise its temperature for 10 minutes.

How do these influence the current curve on the oscilloscope. Find explanations!

See section 5 regarding details for your report.

## 3 Atomic spectra of Hydrogen and Mercury

### 3.1 The Balmer series of Hydrogen

At the end of the 19th century it was discovered that the elements emit and absorb light at specific wave lengths. Amongst one of the discoveries it was found that light from Hydrogen could be put into a set of different series. A researcher at the university of Uppsala, Jan Rydberg, found that the light in the visible part of the spectra, the Balmer series, could be put into a simple mathematical relation

$$\frac{1}{\lambda} = R_H \left( \frac{1}{n^2} - \frac{1}{m^2} \right), \quad m = 3, 4, \dots \quad (1)$$

Where (for the Balmer series)  $n = 2$ ,  $m = 3, 4, \dots$ ,  $\lambda$  is the wave length of the light,  $R_H$  is Rydberg's constant for Hydrogen. The integer  $m$  is the principal quantum number for states above the final state with principal quantum number  $n = 2$ . To understand the physics of the relation above would still take a couple of decades. Next to the Balmer series there are the Lyman ( $n = 1$ ), Paschen ( $n = 3$ ), and Brackett ( $n = 4$ ) series.

### 3.2 The structure of the atom

A challenge at the end of the 19th century was the structure of the atom. An important experiment was where alpha particles were shot at a thin film made of Gold. The experiment was performed by Geiger and Marsden whom both were Co-workers of Ernest Rutherford in Manchester. The experiments were consistent with the atom having nearly all its mass in a very small part of the centre where also all the positive charge was found.

Rutherford also realised that the positive nucleus was surrounded by the negatively charged electrons. But they could not build a working theory for the atom as according to classical mechanics and electrodynamics the electrons should emit radiation as they are accelerating as they orbit the positively charged nucleus. An electric charge that is accelerated will emit radiation hence the electron will lose energy and eventually the electron will crash into the nucleus. Neither continuous radiation nor crashes were observed. The atom was apparently stable!

The Dane Niels Bohr, with whom Ernest Rutherford had close contacts, eventually came up with a working theory for the Hydrogen atom. It accounts for that light is only emitted at specific wave lengths and also for the stability of the atom. Bohr had made some assumptions about the atom, one that specified that the electron could only have certain specific energies. He also incorporated the ideas of Planck (thermal radiation) and Einstein (photo electric effect) that light could be absorbed or emitted as photons with the energy:

$$E_{\text{photon}} = h\nu = \frac{hc}{\lambda}. \quad (2)$$

The explanation Bohr came up with was interesting but could only be applied to Hydrogen or Hydrogen like atoms. Other atoms like Helium would not fit into Bohr's theory.

Erwin Schrödinger (from Austria) presented a more complete theory (quantum theory) also covering all the atoms not accounted for in Bohr's theory. It should be pointed out that



the development of quantum theory was not a 'one mans job'. Many persons were involved like Niels Bohr, Werner Heisenberg, Erwin Schrödinger, Max Planck, Louis de Broglie, Albert Einstein, Max Born, John von Neumann, Paul Dirac, Wolfgang Pauli and many more. The important work ranged over several years 1925-1931 perhaps peaking at 1927. The quantum theory covered more than just atoms it was in fact a theory for micro 'cosmos'. His equation the Schrödinger equation is as central for small systems as Newton's equations are for large systems. It not only accounted for the energy levels  $E_n$  of the Hydrogen atom

$$E_n = -\frac{W_H}{n^2}, \quad W_H = \left( \frac{2\pi^2 m_e}{h^2} \right) \left( \frac{e^2}{4\pi\epsilon_0} \right)^2, \quad n = 1, 2, \dots \quad (3)$$

but also explained the structure of all atoms, how atoms formed molecules, chemical bonding, the structure of the nucleus, etc. In the above equation  $m_e$  is the mass of the electron,  $e$  its charge and  $n$  is the principal quantum number.

### 3.3 Measurement

A measurement of the wave length of the three visible spectral lines of the Balmer series will make it possible to determine Rydberg's constant  $R_H$ . As the energy of the photon is given by

$$E_{\text{photon}} = E_f - E_i \quad (4)$$

where  $E_f$  is the energy of the final state and  $E_i$  of the initial. In the experiment you run here the final level will be the same for all three lines with the principal quantum number  $n = 2$ . The initial state we do not know but we know that they are members of a series and if you set the lowest (closest to  $n$ ) to  $m$  the next two ones will be  $m + 1$  and  $m + 2$ . This will give you three equations (one for each wave length) but with only two unknowns  $m$  and Rydberg's constant  $R_H$ . We could also have taken  $n$  to be unknown but we set it to  $n = 2$ . As there are three spectral lines but only two unknowns you can calculate  $m$  in several different ways (the actual number of different ways is 3).

Part of this laboratory exercise is to measure the wave lengths of the three lines and solve these equations to find  $m$  for the lines and  $R_H$ . Note that the value you obtain for  $m$  will not be an integer but hopefully you can to a good approximation find an integer close to it.

### 3.4 Measurement of the spectral lines of the Balmer series

You will use a Hydrogen lamp see figure (3) item number 3. In the lamp atomic Hydrogen is formed in a catalytic process from water vapour in the lamp as it ignites. Electrons are accelerated and as they pass through the Hydrogen gas they will excite Hydrogen atoms (same process as in the Franck-Hertz experiment). You will determine the wave lengths of the three spectral lines in the range of visible light. You will use a spectrometer (see figure (3) item number 2) to analyse the light from the Hydrogen lamp. A spectrometer will split the light into its different wave lengths. This is achieved by a diffractive grating that will deflect the light an angle  $\theta$  as a function of its wave length  $\lambda$  and the separation of the lines of the grating  $d$ . It is important that the grating is perpendicular to the incident beam. The grating will give 2 first order ( $k = 1$ , see eq. 5) spectra one to the 'right' and one to

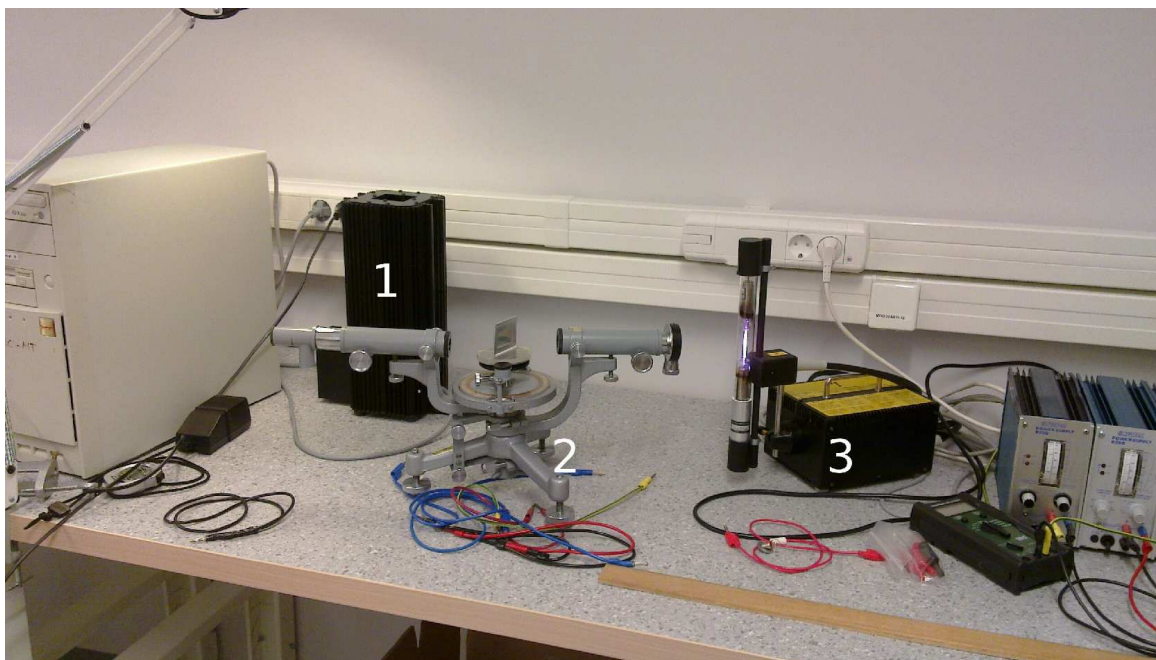


Figure 3: An overview of the setup for the spectral lines experiment. From left to right you see at the number: 1 is the Mercury lamp, 2 is the spectrometer and 3 is the Hydrogen lamp. (Items are not aligned in the photo)

the 'left' as the line up is symmetric along the incident beam. There will spectra of higher order as well ( $k$  larger than one) but they are of no interest to us in this experiment. To take into account that you will not be able to perfectly place the grating perpendicular to the incident beam you will measure both the right and the left angle of deflection ( $\theta_1$  and  $\theta_2$ ) for a certain spectral line. The grating equation (familiar from your first year physics course) will therefore be adjusted to:

$$d(\sin \alpha_1 + \sin \alpha_2) = k\lambda, \quad k = 1, \dots, \quad \alpha_1 = (\theta_1 + \theta_2)/2, \quad \alpha_2 = |\theta_1 - \theta_2|/2 \quad (5)$$

where  $k$  is the order of the spectrum. In this experiment we only measure the first order spectrum. The second order can be found at larger angles of deflection.

### 3.5 Mercury spectra

Next to the Hydrogen lamp you will find a Mercury lamp (see figure (3) item number 1). You will analyse the spectra of the Mercury lamp. You will find about 4 to 5 strong lines in the spectrometer. Measure the wave lengths in the same way as for the Hydrogen spectra.

You have to identify the lines you found in matters of whether it is from ionized (HgII) or neutral (HgI) Mercury, the initial state and the final state of the atom. Find relevant information either in books or out on the internet (most likely the NIST data base).

NOTE and hint: As Mercury is an atom with many electrons it is not sufficient to describe a state of the atom by just its configuration. Information has also to be given on

how spin and angular momentum are aligned. This is done by adding to the configuration the spectroscopic term.

For an introduction to spectroscopic terms you can read : [http://en.wikipedia.org/wiki/Term\\_symbol](http://en.wikipedia.org/wiki/Term_symbol).

It is also covered in the textbook of F0047T.

See section 5 regarding details for your report.

## 4 Numerical integration of the Schrödinger equation

In this part of the laboratory exercise you will solve the Schrödinger equation by simple numerical methods in matlab. As well as training your skills in matlab programming you will get a better understanding of the interplay between eigenvalues and the solution meeting the boundary conditions. You will also gain some insight into the role played by the symmetry of the perturbing potential. A short introduction to matlab is given in the appendix 6.

Matlab is available to students at LTU only in the computer class rooms in either the A or E house. It might be that you can remotely log into these computers but I have to refer you to the help desk for further information. An alternative to matlab is to install **octave** ([www.octave.org](http://www.octave.org)) this is a free to download software and you write matlab code in octave just as if it was matlab. Octave is a Matlab look alike. It is available for windows, Linux, Mac OS X and Sun Solaris. If you download it on your own computer you will be independent of matlab and its limitations of usage.

You start matlab or octave by just typing its name at the prompt in an xterminal. On some systems you can find matlab/octave as an item in a applications menu. There exists also a graphical user interface for octave called koctave or qt octave.

### 4.1 Infinite potential well in one dimension

The stationary Schrödinger equation for a particle in one dimension subjected to a potential  $V(x)$  is given by

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right) \Psi(x) = E \Psi(x). \quad (6)$$

Where  $m$  is the mass of the particle,  $\hbar = 1.0545 \cdot 10^{-34} Js$  and  $E$  is the eigenenergy to the wave function  $\Psi(x)$ .

The next step is to rewrite equation 6 into a dimensionless form. This is achieved if we let  $u = x/L$  and hence  $d^2/dx^2 = d^2/du^2 \cdot 1/L^2$  and change the energy to the dimensionless energy  $E^* = E2mL^2/\hbar^2$  where  $L$  is the width of the well. The potential in dimensionless form is denoted  $W(u)$  and is recovered in a similar manner as the energy  $E$ . The variable  $u$  runs from 0 to 1.

There are good reasons to rewrite the equations into a dimensionless form as the numerical solution will be performed on a more well defined problem (the dimensionless boundary is known etc). Hence you can optimise your code on the dimensionless problem and rescaling to the real world is done afterwards.

$$\left(-\frac{d^2}{du^2} + (W(u) - E^*)\right) \Psi(u) = 0 \quad (7)$$

where the length  $u$  is given in units of  $L$ . The potential  $V(x)$  for a particle in the infinite well is given by

$$V(x) = \begin{cases} 0 & \text{for } 0 \leq x \leq L \\ +\infty & \text{for } x > L, x < 0 \end{cases}$$

The solution of this system is straight forward (you can find it any descent textbook in quantum mechanics).

$$\Psi(u) = \sqrt{\frac{2}{1}} \sin(n\pi u), \text{ where } n = 1, 2, 3, \dots \quad (8)$$

The energies for the dimensionless equation (7) are given by

$$E^* = (n\pi)^2, \text{ where } n = 1, 2, 3, \dots \quad (9)$$

This is in dimensionless units. The series for the energies  $E^*$  starts with  $\pi^2 = 9.8696$ ,  $4\pi^2 = 39.478$ ,  $9\pi^2 = 88.826$  and  $16\pi^2 = 157.914$ . This is in dimensionless units. As you try your program an start with a trial energy it the solution should converge to an eigenvalue. A different eigenvalue is reached if you try a starting trial energy an appropriate bit away from the earlier eigenvalue found. Be confident that your program does this. To get back to real energy's you just reverse the previous expression to  $E = E^* \hbar^2 / 2mL^2$ .

Now we turn to the numerical treatment of equation (7). We will keep it simple and only use the Euler method.

## 4.2 Numerical treatment, Euler method

The strategy is to start the solution at one boundary and integrate out to the other boundary. Only a correct choice of energy  $E$  will make the solution the desired at the other boundary. These correct choices of  $E$  are the eigenvalues.

The starting position  $u = 0.0$  for the integration can be as follows.

$$\text{Initial conditions } \begin{cases} \Psi(u = 0.0) &= 0.0 \\ \Psi'(u = 0.0) &= 5.0 \\ \Psi''(u = 0.0) &= 1.000 * (W(u) - E^*) * \Psi(u = 0.0) = 0.0 \end{cases} \quad (10)$$

The wave function at the boundary has to be zero as the potential is infinite at this location. The second derivative  $\Psi''(u)$  is given by the Schrödinger equation 7. The first derivate  $\Psi'(u)$  can be taken as any nonzero value. There is a reason we can just take a value. The Schrödinger equation 7 is linear and we can multiply the final wave function with a constant and it will still be a solution. There is one restriction however, the wave function has to be normalised according to eq (12). But normalisation is something you can arrange after the integration.

The numerical method you will use is the Euler method. There are other methods of higher accuracy like the Runge–Kutta method but a simple Euler method will do. At the heart of the Euler method taking one iterative forward of step length  $\Delta u$ .

$$\text{Single step in Euler method } \begin{cases} \Psi''(u) &= 1.000 * (W(u) - E^*) * \Psi(u) \\ \Psi'(u + \Delta u) &= \Psi'(u) + \Delta u * \Psi''(u) \\ \Psi(u + \Delta u) &= \Psi(u) + \Delta u * \Psi'(u + \Delta u) \\ u &= u + \Delta u \end{cases} \quad (11)$$

Before we start the integrating procedure we have to make a guess at an appropriate energy  $E^*$ . It is important to understand how the choice of energy  $E^*$ . If the chosen energy is not an eigenenergy of the Schrödinger equation the wave function  $\Psi$  will fail to be zero

at the other end ( $u = 1$ ) of the potential well. The function will either over or under shoot zero at the boundary. An example of this can be seen in figure (4). You have to do some trial and error on how a change of  $E^*$  will change how close the wave function will be to zero at the far end. Be aware there is also difference whether the eigenfunction is even or odd. You can tell whether it is even or odd from the sign of the derivative  $\Psi'(u = 1)$ . If it is the same as at  $u = 0$  the eigenfunction is odd and if it is the the opposite the eigenfunction is even. Once you have sorted this out you can make an appropriate regulating loop in your program that should converge to an eigenvalue  $E^*$  that will meet the boundary condition  $\Psi(u = 1.0) = 0$ .

After this has been achieved you can normalise the wave function so that

$$\int_0^L |\Psi|^2 dx = 1. \quad (12)$$

Note that the normalisation it self does not change the eigenvalues. You can also try to change the initial condition for  $\Psi'(u = 0.0)$  in eq (10). A change of the derivatives initial value will change the 'height' of the eigenfunction but after normalisation it will be the same again.

### 4.3 The perturbed potential

The ordinary one dimensional square potential well has the potential  $V(x) = 0$  inside the well. Once you have your matlab program running it is easy to solve for different perturbing potentials inside the infinite walls. In the previous section you made a program that solves the infinite unperturbed square well.

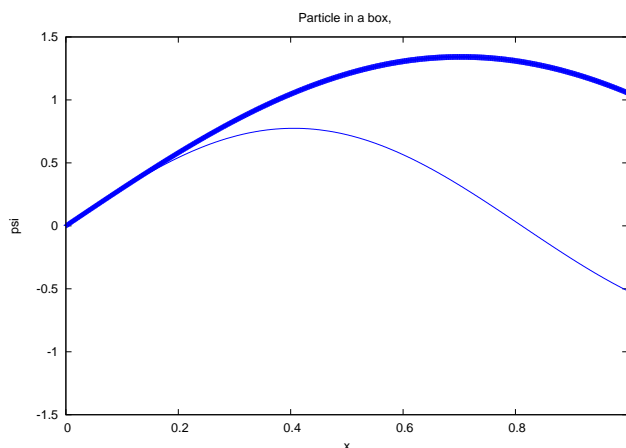


Figure 4: The numerical integrated wave function  $\Psi(u)$  for two different values of initial energy's  $E^*$ . The line graph drawn with a thick line has a too small value of  $E^*$  which gives a small second derivative and this is the reason it is not able to curve down to  $\Psi(L) = 0$ . The second graph drawn with a thin line has a too large value for the energy  $E^*$ . A value of  $E^*$  in between these two would give a  $\Psi(L)$  closer to zero. You can use the value of  $\Psi(L)$  to regulate the next choice for  $E^*$  as you wish to achieve  $\Psi(L) = 0.0$ .

It is now very easy to add perturbations to the system and numerically solve and find the new eigenvalues. In the laboratory exercise you will do a couple of different perturbing potentials.

The coordinates of the infinite walls are  $u = 0$  and  $u = 1$ , the latter corresponds to  $x = L$ . We define four potentials that you will study with a numerical calculation. The potentials are not chosen at random they will demonstrate how symmetry plays an important role to the changes of the new eigenvalues.

The potentials you will investigate are the following five expressed in dimensionless units in the interval running from 0 to 1. In potential (14), (15) and (16) the height of the perturbation is set to 2.0 the only reason for this is to have a clear change but not so large that it is close to the ground state energy. As potential number one we have the standard unperturbed potential

$$\text{Potential 1 } \left\{ \begin{array}{ll} W(u) = 0.0 & \text{for } 0 < u < 1. \end{array} \right. \quad (13)$$

As potential number two we have an even potential with respect to the symmetry line at  $u = 1/2$

$$\text{Potential 2 } \left\{ \begin{array}{lll} W(u) = -1.0 & \text{for } 0 < u < \frac{1}{3} \\ W(u) = 2.0 & \text{for } \frac{1}{3} < u < \frac{2}{3} \\ W(u) = -1.0 & \text{for } \frac{2}{3} < u < 1. \end{array} \right. \quad (14)$$

As potential number three we have an odd potential with respect to the symmetry line at  $u = 1/2$

$$\text{Potential 3 } \left\{ \begin{array}{lll} W(u) = 0.0 & \text{for } 0 < u < \frac{1}{3} \\ W(u) = 2.0 & \text{for } \frac{1}{3} < u < \frac{1}{2} \\ W(u) = -2.0 & \text{for } \frac{1}{2} < u < \frac{2}{3} \\ W(u) = 0.0 & \text{for } \frac{2}{3} < u < 1. \end{array} \right. \quad (15)$$

As potential number four we have a potential with no particular symmetry

$$\text{Potential 4 } \left\{ \begin{array}{lll} W(u) = -0.4 & \text{for } 0 < u < \frac{1}{3} \\ W(u) = 2.0 & \text{for } \frac{1}{3} < u < \frac{1}{2} \\ W(u) = -0.4 & \text{for } \frac{1}{2} < u < 1. \end{array} \right. \quad (16)$$

Now the four potentials are defined that you will compare with each other. They are all constructed in such a way that the average of these four potentials is zero over the full width.

As potential number five we have an even potential with respect to the symmetry line at  $u = 1/2$ . This potential is special as it preserves the area (integral) under the potential function. It is very illustrative to show what happens to the wave function as you let the height of the barrier go to infinity and the width of the central barrier go to zero but the area of the height times the width is preserved.

$$\text{Potential 5 } \left\{ \begin{array}{lll} W(u) = -2.0 & \text{for } 0 < u < \frac{1}{2} - \frac{1}{2b} \\ W(u) = 2.0b - 2.0 & \text{for } \frac{1}{2} - \frac{1}{2b} < u < \frac{1}{2} + \frac{1}{2b} \\ W(u) = -2.0 & \text{for } \frac{1}{2} + \frac{1}{2b} < u < 1. \end{array} \right. \quad (17)$$

Where  $b$  is the height of the barrier and  $1/b$  its width. In this last potential you have to take care as you increase the height the width will decrease. There is a numerical issue here as

the Euler method uses a specific step length  $\Delta u$ . You should take care to ensure that there are a couple of steps inside the width of the barrier, if not the program might completely miss the barrier and your results will be totally wrong.

Now all five potentials are defined. In section 5 you will find the numerical task to perform.

## 4.4 Perturbation calculation, theoretical

As part of the course in Quantum mechanics you follow, you have learnt to make a perturbation calculation to first and second order and you will use this knowledge now in conjunction with the numerical results you just have performed.

Corrections to first order are:

$$E_n^{(1)} = \langle n^{(0)} | H_{\text{perturb}} | n^{(0)} \rangle \quad (18)$$

and corrections to second order are:

$$E_n^{(2)} = \sum_{k, k \neq n} \frac{|\langle k^{(0)} | H_{\text{perturb}} | n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \quad (19)$$

where the sum runs over  $k$ , the  $|n^{(0)}\rangle$  are the unperturbed states for the unperturbed potential (eq. 13). The perturbation  $H_{\text{perturb}}$  are the potentials eq. (14 - 16). The fifth potential eq. (17) cannot be treated by perturbation theory.

Please note the following: As the perturbation potentials are combined of constant patches, you can use the same calculation several times as they only differ for a constant pre factor. The integrals you calculate

$$\langle n^{(0)} | H_{\text{perturb}} | n^{(0)} \rangle = \int_0^1 \sqrt{2} \sin(n\pi u) V(u) \sqrt{2} \sin(n\pi u) du \quad (20)$$

can be organised into patches where the perturbation is constant.



## 5 Your report

Your report must be written on a computer and handed in to me by just a simple email. In the subject line of the email you must include "F0047T". The report should be written in either Swedish or English, this you are free to choose. You can use word, latex (best choice), scientific workplace or any other kind of word processing system. You should take care where you keep your original files, and that all members of the group have a copy of them.

No references to Wikipedia are allowed in your report. Only references to printed articles (in journals submitted to peer review) or printed books. The reason you cannot use Wikipedia is threefold. Firstly there might be a difference of opinion on a certain issue and the author only presents one point of view. Secondly a reference made today to Wikipedia is not necessarily there tomorrow as Wikipedia is an ever changing encyclopedia, even if there is a history of each page. Thirdly you do not know who wrote the page you make a reference to. In itself Wikipedia is excellent, I myself use it often, but you cannot make a reference to it and you have to be aware of its limitations.

Your report should follow the guide lines stated in "**Lathund för rapportskrivning**". You used these guide lines in Fysik 1, 2 and 3. Preferably you use the Latex version.

You may also use the old guide lines given in Torbjörn Löfquist's booklet (Rapportskrivning : en introduktion) which you can find on the home page of the LTU library: <https://www.ltu.se/webbarkiv/BIB/rapport/index.html> (in Swedish).

### 5.1 Franck–Hertz part

You report should contain: (remember it should be a report not just answering the questions below in a punch line like style)

1. A description of the experimental setup.
2. Explain how current, accelerating voltage, reverse bias and collector current should fit together if the laws of classical physics would apply.
3. Using quantum mechanics how would you explain the connection between  $I_C$  and  $U_A$ . Give an account for the values of accelerating voltages for the different maxima and minima, present your results in a table. From these values deduce the excitation energy. *Take great care in your explanation of the experiment. To facilitate your process of understanding you can perform an 'gedanken experiment' like following an electron as it is moving from the source to the collector. Ask yourself questions like, where in the tube will excitations occur, what happens to the electron after exciting a mercury atom, if an electron of constant kinetic energy (like 1eV) would move from the glowing filament to the collector how long would this take, how much is this in comparison to the time it takes to complete one cycle (at 50Hz).*
4. In your report you should also include an analysis of what happens to the current curve if you change the reverse bias, the current in the glowing filament, the maximum acceleration voltage and the temperature of the oven.

## 5.2 Hydrogen and Mercury spectra part

Your report should contain: (remember it should be a report not just answering the questions below in a punch line like style)

1. A description of the experimental setup.
2. In the form of a table give the values for the three visible spectral lines in the Hydrogen spectra for  $\theta_1$  and  $\theta_2$  the principal quantum numbers of the initial and final state and the calculated wave length. Take care to clearly specify data that are results from your measurement, your calculations from data that you perhaps refer to from the literature.
3. Describe how you calculated the wave lengths. Give the set of equations you used to calculate the principle quantum numbers. The calculation of Rydberg's constant. Give also the calculated value for  $m$  as this clearly not will be an integer.
4. Mercury spectra: Firstly is the Mercury ionized or not? In the form of a table give the values for the visible spectral lines in the Mercury spectra for  $\theta_1$  and  $\theta_2$  and the calculated wave lengths (=experimental result). Also state the wave length you identified your experimental result corresponds to and give the spectroscopic terms for the initial and final states for the spectral lines you have identified with information from the internet (NIST) or an appropriate textbook.

## 5.3 Numerical integration of the Schrödinger equation and comparison to a first order perturbation calculation

Your report should contain: (remember it should be a report not just answering the questions below in a punch line like style)

The results you present should be in dimensionless form.

To begin with you have to write a small matlab (or octave) program that solves the Schrödinger equation for a infinite square well. Write your program in a dimensionless form eq. (7). As your program ends let it put in dimensions and give values for the eigenenergies  $E$  in electron volts.

1. Start to make a calculation for potential 1 (eq. (13)) the ordinary square well. Use your program to calculate the four lowest eigenenergies of the potential square well. Verify that your results are correct by equation 9.
2. Perform a numerical calculation of the **six** lowest eigenenergies for potentials 2, 3 and 4 (eq 14 - 16).
3. Present your numerical results in a table for all 5 potentials (eq 13 - 16). Also present your results from the first order perturbation calculation in the same table. Note the number of perturbation calculations is restricted to only six in total marked by 'x' in the table below. A suggestion for a table might be as follows for the potentials eq. (13-16):

Table 1: Suggested table for presentation of numerical results combined with perturbation calculation

Potential	State		energy from matlab	diff to potential 1 (exact solution)	first order correction from perturbation calculation
1	1	even		0.0	
1	2	odd		0.0	
1	3	even		0.0	
.	4	.		0.0	
.	5	.		0.0	
.	6	.		0.0	
2	1	even			x
2	2	odd			x
2	3	even			x
.	4	.			
.	5	.			
.	6	.			
3	1	even			x
3	2	odd			x
3	3	even			x
.	4	.			
.	5	.			
.	6	.			
4	1	even			
4	2	odd			
4	3	even			
.	4	.			
.	5	.			
.	6	.			
5	1	even			
5	2	odd			
5	3	even			
.	4	.			
.	5	.			
.	6	.			

The potentials eq. 13 and 17 will of course contain less columns in their table, in the example here they are left empty. Note this is a suggested table only and you may very well have your own ideas. Just remember to present your results in such a way that you help the reader to understand how the different methods of calculation affects the results.

4. Compare results for potential 2,3 and 4 to the results for potential 1. If you calculate the difference between the perturbed eigenenergy (potential 2, 3 and 4) and the unperturbed (potential 1) eigenenergy your analysis will become simpler. Explain why some of the perturbed eigenenergies change and some not compared to the unperturbed eigenenergies. What role does symmetry play? What can you say about potential 4 (eq. 16).
5. Will the choice of sign in the initial conditions 10 in some way effect your results for say potential 15 or 16? Let instead of  $\Psi'(u = 0) = 5.0$  the initial condition be  $\Psi'(u = 0) = -5.0$ .
6. For potential 3 include the graphs for the eigenfunctions your program has calculated.
7. Potential 5 (eq. 17) set the height in a range  $b = 2000 - 5000$ . Take care that your choice of step length is smaller than the width of the barrier. Calculate the the 4 lowest eigenenergies in dimensionless units and present the graphs of the corresponding eigenfunctions.
8. Include the matlab program as an appendix and also send it to me by email so that I can test your program.
9. Perturbation calculation. You will only make a first order calculation. We restrict the calculation to only potential 2 (eq. 14) and potential 3 (eq. 15) and only the ground state and the two lowest excited states as marked by 'x' in the suggested table (1).
10. Can you say something about the accuracy of the perturbation calculation? How to they compare to the results from the matlab calculation?

## 6 Appendix: Short introduction to Matlab in Swedish

I kursen fysik 1 har du genomfört ett försök med pendeln i klassrummet. Vi skall nu behandla detta försök med hjälp av matlab.

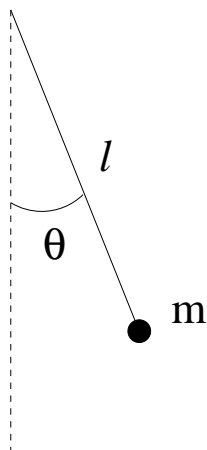


Figure 5: En kropp med massan  $m$  är upphängd i ett snöre med längden  $l$ . Vinkeln  $\theta$  utgör vinkeln mot lodlinjen.

En dimensionsanalys ger att följande variabler är relevanta. Pendellängden  $l$ , vinkeln  $\theta$  och gravitationskonstanten  $g$ , se figur 5. Massan  $m$  är inte relevant (detta behandlades i kursen fysik 1). Då pendeln svänger fram och tillbaka behövs också (för att beskriva rörelsen) vinkelhastigheten, som ges av  $\dot{\theta}$  och vinkelaccelerationen som ges av  $\ddot{\theta}$ . Med skrivsättet  $\dot{\theta}$  menas första derivatan av vinkeln  $\theta$  med avseende på tiden  $t$ , dvs.  $\dot{\theta} = \frac{d\theta}{dt}$ . På motsvarande sätt är andra derivatan  $\ddot{\theta} = \frac{d^2\theta}{dt^2}$ . Newtons andra lag ger följande samband mellan kraften  $F$  och accelerationen  $a$ :  $F = ma$ . Kraften ges av  $F = mg \sin(\theta)$  och accelerationen ges av  $a = l\ddot{\theta}$  vilket insatt i Newtons andra lag ger  $\ddot{\theta} = g \sin(\theta)/l$ . Denna ekvation kallas för en differential ekvation (diff ekvation) och vi skall nu lösa denna ekvation numeriskt med hjälp av matlab/octave.

För att lösa ekvationen

$$\ddot{\theta} = \frac{g \sin(\theta)}{l} \quad (21)$$

numeriskt gör vi på följande vis. Vi behöver startvärden för tiden  $t = 0$ , så kallade begynnelsevillkor. Dessa behövs för  $\theta(t = 0)$  och  $\dot{\theta}(t = 0)$  sedan ges  $\ddot{\theta}$  (vid tiden  $t=0$ ) av ekvation (21). Nu vet vi tre värden vid  $(t = 0)$  och nu kan vi räkna ut nya värden på för  $\theta$  och  $\dot{\theta}$  ett litet tidssteg  $\Delta t$  in i framtiden. Nya värden för  $\theta$  och  $\dot{\theta}$  ges av  $\dot{\theta}(t + \Delta t) = \dot{\theta}(t = 0) + \ddot{\theta} * \Delta t$  och  $\theta(t + \Delta t) = \theta(t = 0) + \dot{\theta} * \Delta t$ , dessa nya värden kan nu på nytt användas i ekvation (21) och ett nytt värde för  $\ddot{\theta}$  erhålles fast nu för ett tidssteg  $(\Delta t)$  framåt i tiden. Vi kan nu låta datorn göra detta upprepade gånger i en iterativ slinga, en så kallade loop. Nedan ses ett exempel på ett sådant program skrivet i matlab/octave. Skriv av detta program eller ladda ner det från kursens hemsida. Använd emacs och spara filen under lämpligt namn med ändelsen .m så att matlab/octave tolkar det som ett skript. Ett exempel på namn kan

vara pendel.m det är viktigt att filnamnet slutar på .m annars tolkar inte matlab/octave programmet filen som ett skript (program).

Lite förklaringar till nedanstående program. Numren som syns till höger är radnummer och hör inte till matlab programmet utan är enbart referenser i texten här, som jag lagt dit. Ett semikolon ; efter ett kommando innebär att kommandot utförs men inget skrivs ut på bildskärmen. Variabeln theta är  $\theta$  och thetaprim är  $\dot{\theta}$  och thetabiss är  $\ddot{\theta}$ . Kommandot clear (rad 1) tar bort gamla variabler, raderna som följer (rad 3 till 6) definierar pendeln. Begynnelsevilkoret är att vi håller pendeln 0.2 radianer ut men i vila och sedan släpper vi den. På raderna 8 till 10 sätts antalet steg i loopen och tidsteget. På rad 12 börjar loopen, rad 14 är ekvation (21). Nya värden för  $\theta$  och  $\dot{\theta}$  ges på raderna 15 och 16 och aktuell tid på rad 17. På rad 18 och 19 sparas aktuell tid och vinkel för att senare när loopen är färdig kunna visas i en figur. Rad 21 är det end som hör ihop med 'for' på rad 12. Rad 23 ritar vinkeln som funktion av tiden med kommandot plot.

clear	1
theta = 0.2 ;	3
thetaprim = 0.0;	4
grav = 9.81 ;	5
mass = 1.0;	6
nstep = 20000 ;	8
deltatime = 0.001;	9
time=0.0;	10
for i = 1:nstep	12
thetabiss = - grav*sin(theta);	14
thetaprim = thetaprim + deltatime*thetabiss;	15
theta = theta + deltatime*thetaprim;	16
time = time + deltatime;	17
tid(i) = time ;	18
vinkel(i) = theta ;	19
end	21
plot(tid,vinkel,'-')	23
pause(0)	24

Det går givetvis att också spara vinkelhastighet och vinkelacceleration i vektorer precis som vinkeln på rad 19. Prova tex att lägga till en rad efter rad 19 som ser ut på följande vis: vinkelhast(i) = thetaprim ; vinkelacc(i) = thetabiss;

Lägg också till motsvarande plot(tid, vinkelhast, '+') eller liknande. Använd hold on/off kommandot för att styra kvarhållandet av tidigare grafer (finns beskrivet på sidan 20).