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Software developed by Katarzyna Holodnik-Malecka
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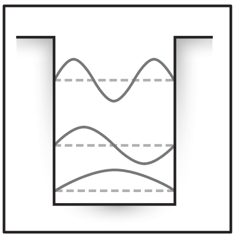
Project 1

Rectangular Finite Quantum Well – Stationary Schrödinger Equation in 1D



In this project, participants utilise the procedure of finding roots of functions to solve the eigenvalue problem of a rectangular quantum well (QWELL code). When considering the rectangular quantum well as the simplest model of a hydrogen atom, the code can be applied to determine its first two to three energy levels, which is the primary exercise in the project. The eigenvalue problem itself, appearing in various areas of physics (such as vibration mechanics, wave optics, and quantum mechanics), will be the subject of a separate project (Project 6) and one of the advanced projects (Project 12), where a rectangular quantum well partially filled with electrons is examined. It is somewhat paradoxical that despite employing the simplest mathematical operations in the current project, it is based on advanced physical concepts, such as quantum mechanics, often unfamiliar to first-year students. Learning the basics of quantum mechanics typically requires a 30-hour course and knowledge of advanced mathematics. Therefore, we will only introduce its fundamental and most straightforward ideas here, just enough to enable the conscious execution of the project.

1.1 Physics Background: Chosen Ideas of Quantum Mechanics

In quantum mechanics, while the physical quantities of interest, such as position or momentum of a particle, remain the same as in classical physics, their representation is entirely different. Focusing on the problem of a single particle, the central object is the quantum state rather than the coordinates in the chosen system (as it would be in classical physics). In the so-called position representation, the quantum state is a particular function of the position variable $\psi(r)$, which, from a mathematical perspective, must meet special conditions of differentiability and integrability. The function itself does not have a physical interpretation, but its squared modulus $|\psi|^2$ does – it represents the probability density of finding the particle at a given point in space, that is becomes a probability when multiplied by the volume element (the Born probabilistic interpretation). Here lies the main difference between classical and quantum physics – the probabilistic nature of the latter, with the concept of probability being inherent to the theory. When measuring a physical quantity, the outcome can only be predicted with a certain probability. The deterministic nature of phenomena, justified in classical physics, no longer holds, and this fact was challenging for many physicists to accept during the early stages of quantum theory development. For instance, Albert Einstein proposed the hidden variables hypothesis, suggesting that there are unknown variables that determine the measurement results. Modern interpretations, such as the Copenhagen Interpretation, go even further, positing that a particle can simultaneously exist in multiple positions with different probabilities (which is entirely impossible in the classical world), and only the act of measurement localises it to a specific position (e.g. the role of the measurement instrument is played by the screen in the ‘electron diffraction on a double slit’ experiment). The same concept applies to other physical quantities, meaning that quantum systems can simultaneously exist in various states of a particular quantity (with different probabilities), and during the measurement, the system selects one of these states. Currently, quantum mechanics is a coherent and complete theory, with the Copenhagen Interpretation being widely accepted, and no scientific evidence has emerged to challenge its validity.

The central and historically first equation for evaluating the state function is the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r,t) = i\hbar\frac{\partial\psi(r,t)}{\partial t}, \tag{1.1.1}$$

where $\hbar = h/2\pi$, h is Planck’s constant, m mass of the particle, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is Laplace’s operator, and $V(r)$ the particle potential energy.

The equation resembles a wave equation, which is why the function $\psi(r)$ is also called the wave function. As we can see, this is a function of both space and time variables. However, when the left-hand side of the equation (potential energy) does not explicitly depend on time, the function can be represented as a product of a space variable and time-dependent parts, with the latter having a known form $\psi(r)e^{i(\omega t)}$ (using the Euler representation of complex numbers, see Appendix A.1). A similar situation has been described (with respective derivation) in Project 6 for the case of a standing wave. If we substitute the factorised

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function into Eq. 1.1.1, we can easily eliminate the time-dependent part, which leads to the stationary Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = \varepsilon\psi(r), \qquad (1.1.2)$$

where $\varepsilon = \hbar\omega$.

This equation is a starting point of the project. From a mathematical point of view it is an eigenvalue problem, the solution to which is a set of pairs: eigenvalues and corresponding eigenfunctions obeying the imposed boundary conditions, $\{(\varepsilon_n, \psi_n(r))\}$. The solutions are indexed with the integer n called the quantum number. The operator appearing on the left-hand side represents the total energy of the particle (Hamiltonian), and the eigenvalue problem leads to eigenenergies and eigenfunctions of the particle. From this an interpretation follows – the quantum system (a particle in a potential well, for example, an electron in the Coulomb potential of a proton) can have only strictly established energies and can occupy corresponding states described by the eigenfunctions. The modulus squared of these functions describes the spatial distribution of probability of finding the particle. It should be added that in quantum mechanics all physical quantities are represented by operators having certain mathematical properties, and the associated eigenvalue problems lead to eigenvalues (possible results of the measurement) and corresponding states. The measurement leads to a collapse of a quantum state into an eigenstate of a given quantity.

Two facts should be pointed out. First, the time-dependent part of the wave function, although it has been separated out, is still present in the full solution, but it does not affect the probability distribution of and eigenstate since its modulus squared equals 1. However, the situation changes if we consider a state being a superposition of a few eigenstates. Then we must not forget about time-dependent parts, and their presence results in time evolution of the probability distribution. The second issue is the normalisation of the wave function, which is necessary since its modulus squared multiplied by the volume element is the probability, and the probability of finding a particle overall must be equal to 1. From mathematical point of view this means that the integral of the modulus squared over the whole considered space must be equal to 1. Such normalisation is always possible since the Schrödinger equation is linear, that is any function being its solution when multiplied by a number still remains the solution.

1.2 Problem: Eigenenergies and Eigenfunctions in Rectangular Finite Quantum Well

In this project we will use the stationary Schrödinger equation (1.1.2) to find eigenvalues and eigenstates of an electron in a rectangular finite quantum well. This is not purely an academic problem since such systems are used to model, for example, semiconductor heterostructures. We describe the system as quasi one-dimensional because the changes of important physical characteristics appear in one direction only. Here, however, we will treat the quantum well as the simplest possible 1D model of the hydrogen atom. Thus Eq. 1.1.2 takes the form

$$\left[-\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=\varepsilon\psi(x), \tag{1.2.1}$$

where potential is equal (Figure 1.1)

$$V(x)=\begin{cases} -V_o & \text{if } -a/2 \le x \le a/2, \\ 0 & \text{if } x < -a/2 \text{ or } x > a/2. \end{cases}$$

In Hartree atomic units, $\hbar = m_e = e = 1$

$$\left[\frac{d^2}{dx^2}+k^2(x)\right]\psi(x)=0, \tag{1.2.2}$$

where $k^2(x) = 2(\varepsilon - V(x))$.

The analytical solutions fall into three categories, two inside the well (Figure 1.1), which differ in symmetry (even and odd), and the third category are the corresponding solutions outside the well

$$\psi(x)=\begin{cases} A\cos(kx) & \text{for } -a/2 \le x \le a/2 \quad (\textit{even}), \\ A\sin(kx) & \text{for } -a/2 \le x \le a/2 \quad (\textit{odd}), \\ B\exp(\mp\kappa x) & \text{for } x < -a/2 \text{ or } x > a/2. \end{cases} \tag{1.2.3}$$

As one can see, the solutions are parametrised by two parameters: k – the wave number (inside the well) and κ – the rate of exponential decrease (outside). It will be shown in the next section

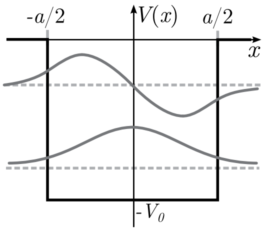

Figure 1.1 A potential well and its solution: the even (lower) and the odd (upper)

that the numerical method will consist of finding the values of these parameters for consecutive eigenstates (thus they will become indexed).

It is worth noting that the eigenfunction (thus also its modulus squared) has finite values outside the well, that is in the region where the kinetic energy of electron is negative. In classical physics a particle must not have negative kinetic energy and that is why we call such a region ‘classically forbidden’ and the phenomenon ‘quantum tunnelling’.

1.3 Numerical Methods: Finding Roots of Characteristic Functions

The condition for the eigenvalue is that the two solutions (inside and outside the region of the well) must join smoothly (Figure 1.2), that is they must have equal values and equal values of their first derivatives at $a/2$ (because of the symmetry of the system it is sufficient to consider only one border). Thus, we have, for even solutions

$$\begin{cases} \pm A\cos(ka/2) = \pm B\exp(-\kappa a/2), \\ \mp Ak\sin(ka/2) = \mp B\kappa\exp(-\kappa a/2), \end{cases} \tag{1.3.1}$$

and for odd solutions

$$\begin{cases} \pm A\sin(ka/2) = \pm B\exp(-\kappa a/2), \\ \pm Ak\cos(ka/2) = \mp B\kappa\exp(-\kappa a/2), \end{cases} \tag{1.3.2}$$

where $k = \sqrt{2(\varepsilon + V_o)}$ and $\kappa = \sqrt{-2\varepsilon}$.

Dividing the first equation by the second one in the above systems, we obtain two conditions, for even (symmetric) and odd (antisymmetric) solutions:

$$\begin{cases} F_{even}(\varepsilon) = \sin(ka/2) - \kappa/k \cdot \cos(ka/2) = 0 \quad (even), \\ F_{odd}(\varepsilon) = \sin(ka/2) + k/\kappa \cdot \cos(ka/2) = 0 \quad (odd). \end{cases} \tag{1.3.3}$$

The eigenvalues ε are found by solving these equations.

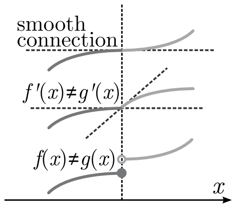

Figure 1.2 The solutions inside and outside the well ($f(x)$ and $g(x)$, respectively) must have same values and equal derivatives at the well border

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1.4 Exercises

Obligatory

1. Using the QWELL code, tabulate functions $F_{even}(\varepsilon)$ and $F_{odd}(\varepsilon)$ These functions correspond to even and odd solutions, respectively, whose zeros are energies of quantum levels. Visualise the functions $F_{even}(\varepsilon)$ and $F_{odd}(\varepsilon)$ in one figure. Repeat the calculation and visualisation of $F_{even}(\varepsilon)$ and $F_{odd}(\varepsilon)$ for three significantly different values of the well parameters, a and V_0 (e.g. wide and shallow well, deep and narrow, intermediate).
2. (Square finite quantum well as a model of the hydrogen atom). Try to fit the first two energy levels to the ones of the hydrogen atom through variation of the parameters a and V_0, by a trial and error method. (Hint: In the beginning set the values $a = 3 Bohr$ and $V_0 = 1 Hartree$.) What is the value of the third energy level? One might try also to fit the first and the third levels. What would be the value of the second level then? Would it be very different from the true value? (Note that in atomic units the energy levels should be $\varepsilon_n = -1/(2n^2)$; since the well is a two-parameter system, it should be possible, in principle, to fit any two levels.)

Challenge

1. Try to construct an algorithm and write a code which automatically finds the parameters of a quantum well with energy levels close to those of the hydrogen atom with arbitrarily low uncertainty.
2. For the found eigenenergies plot the corresponding eigenfunctions and their moduli squared, with the picture of the well in background (do not normalise the functions). Note the effect of quantum tunnelling.

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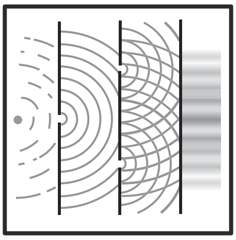
Project 2

Diffraction of Light on a Slit



By working on this project, students will learn numerical differentiation and quadrature procedures. In particular, this project discusses the important issue of convergence with respect to the grid parameter. The numerical quadrature procedure is used to construct the DIFFRACTION code, which simulates diffraction of a scalar wave by a single infinite slit and a system of parallel infinite slits. The code then serves for studying the physical properties of the system.

2.1 Physics Background: Elements of Wave Physics

One can look at a wave as time- and space-dependent variation of a certain physical quantity (pressure, stress in material, displacement of an atom from its equilibrium position, etc.). It is described by a function $\varphi(t, r)$, on which, from a mathematical point of view, special conditions for differentiability are imposed. Some waves require a medium (mechanical), while others do not (electromagnetic, gravitational). The amplitudes in some waves are scalars (like in an acoustic wave), while in others they are vectors (like in an electromagnetic wave). The differential equation for the so-called linear regime (when the response is a linear function of perturbation, like change in volume vs. pressure in air, strain vs. stress in material, or the force acting on an atom in crystal vs. its displacement from equilibrium) is shown in Project 6. Here, we will focus on a certain aspect of wave physics only – the superposition principle which is a consequence of a linear character of the wave equations. Namely, if two waves φ_1 and φ_2 are solutions

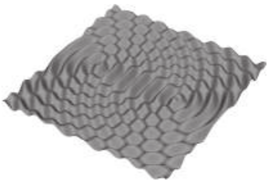


Figure 2.1 We know the principle of superposition from the water waves propagation

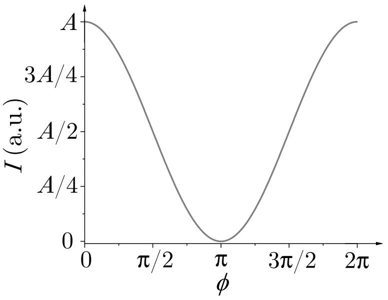


Figure 2.2 The intensity versus the phase difference of two superimposed harmonic oscillations

to wave equation, then also their superposition $A\varphi = \varphi_1 + B\varphi_2$ is (A, B – any variables). Using this principle it is possible to analyse the phenomena connected with the superimposing waves (Figure 2.1), like interference.

We begin with considering an abstract situation when two scalar, harmonic (sinusoidal) oscillations of the same frequency ω and amplitude A, but differing in phase by ϕ, are superimposed in some point in space. We will use the Euler representation of a complex number (see Appendix A.1) in which, for example, the real part describes physical reality. The result of superposition is

$$\varphi(t) = Ae^{(i\omega t)} + Ae^{i(\omega t+\phi)}. \tag{2.1.1}$$

Observations of wave phenomena (e.g. what we see or what we hear) are connected with the wave energy, which is proportional to the amplitude squared. Let us call it intensity (of light or sound) I. Using Equation (2.1.1), after simple algebra we find (Figure 2.2)

$$I = |\varphi(t)|^2 = \varphi(t)\varphi(t)^* = 2A^2[1 + \cos(\phi)], \tag{2.1.2}$$

where the symbol '*' denotes the complex conjugate.

When the effect of the superposition is stable, we call it interference. However, an important condition has to be fulfilled for it to be stable, namely the phase difference ϕ must not vary with time. This condition, combined with the requirement of same frequency form more general condition which we call coherence. In real systems, achieving coherence may be a big problem; for example, in the famous Young's experiment with light diffraction on a double slit, the complexity of the experimental set-up (filter, single slit, double slit) was forced just by the coherence requirement. At present, achieving coherence is one of the main challenges and scientific problems in applications of quantum systems (quantum cryptography, quantum computer).

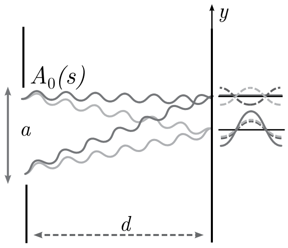


Figure 2.3 Constructive versus destructive interference in a single slit diffraction, a schematic view

The obtained formula for intensity is fundamental and general, and it shows that the effect of interference of two oscillations depends on the phase difference ϕ. There are two types of characteristic extrema: maxima for $\phi = 0 \pm n2\pi$ (n is an integer number) corresponding to constructive interference, and minima for $\phi = \pi \pm n2\pi$ corresponding to destructive interference (zeroth intensity). Besides, there is a big range of intermediate intensities.

Passing to real systems, that is the situation where oscillations depend not only on time but also on spatial variable, we should ask the question what can be the reason for the phase difference ϕ at a certain point in space. Most often the reason is the difference in so-called optical paths, that is the distance from a reference point, of known phase, for each beam, expressed in wave lengths λ. For example, for two point sources of spherical waves the phase difference is connected with the difference in distances from the sources $\phi = k(r_2 - r_1)$, where k is the wave number $k = 2\pi/\lambda$. This is exactly what happens in the Young's experiment (Figure 2.3), which in the history of science became the first irrefutable confirmation of the wave nature of light (although at this time nobody knew what kind of wave is this). A certain funny paradox is that the proof of the wave nature of light was always observed by people, in the form of coloured patterns appearing on spots of oil spilled on the surface of water. The phenomenon is a result of wave interference by division of amplitude (unlike in the Young's experiment, which is based on the division of wavefront), where the phase difference is caused by the difference in optical paths of the part reflected from the upper oil surface and the other part reflected from the oil–water interface. The coherence is most often assured here since the thickness of the oil film is usually smaller than the so-called coherence length of the light beam, that is the length within which the phase differences between chosen points do not depend on time. Presumably, the colours on the oil spots were a great puzzle for people until their origin has been explained. It is worth mentioning that the interference by division of amplitude finds presently significant application in interferometers, that is instruments for precise measurement of length. The Michelson interferometer is an example; its role in the history of science cannot be overvalued, and it was used to disprove the theory of Ether and to detect gravitational waves.

2.2 Problem: Diffraction of a Wave on a Slit

We will apply the superposition principle discussed in the previous section to construct a virtual system of wave diffraction on a certain aperture. A particular case will be an infinite slit with parallel edges. Using this virtual system it will be possible to investigate into the diffraction phenomena on such a slit at various configurations (width of the slit, the distance of the screen). Thus, we consider a plane wave of stabilised phase on a wavefront, falling on a certain aperture. According to Huygens' principle, we can treat the region of the aperture as an infinite and continuous set of point sources of spherical waves. The diffraction phenomenon is a result of the superposition of waves emitted by these sources. To be more exact, the diffraction itself is associated more with the wave deflection, that is, the fact that there is never a sharp shadow of the aperture on the screen. This is because the spherical waves emitted by point sources propagate into the whole space and not along straight lines. We will observe this for the case of a very narrow slit, whose width is much smaller than the wavelength. When additionally the interference takes place, characteristic patterns of brighter and darker regions appear. Generally, the term diffraction is used to denote both the deflection and interference at the same time. Coming back to calculus, we have to sum up the waves emitted by all the point sources, which for the case of their continuous distribution denotes quadrature. We get the diffraction integral

$$D = \int_{\text{Source}} \frac{A_0(s)}{r} \exp\left(-ikr + \phi(s)\right) ds, \tag{2.2.1}$$

where $A_0(s)$ is the amplitude at the elementary source (or more exactly the amplitude density), $\phi(s)$ is the initial phase (at the elementary source), $k = 2\pi/\lambda$ is the wave number, r is the distance from the elementary source to the observation point, and $(A_0(s)/r)$ $\exp(-ikr + \phi(s))$ is the complex amplitude.

It should be noted that the $1/r$ factor holds for a spherical wave, for a cylindrical one (the case considered here) it should be replaced by $1/\sqrt{r}$ because we deal here with cylindrical waves. It should also be explained why there is no time in Eq. 2.2.1, if it is to represent a superposition of elementary waves. This is because in Euler representation