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MATEMATISKA INSTITUTIONEN, STOCKHOLMS UNIVERSITET

Solving the Schrödinger equation by examples

av

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Abstract

In this bachlor diploma, the time-independent Schrödinger equation is derived and studied under the assumption of separable solutions and a real, time-independent potential function. We show that the resulting eigenvalues E are real and bounded below by the minimum of the potential. Furthermore, we examine how solutions to the time-independent equation relate to the full time-dependent Schrödinger equation.

Two examples are treated: the harmonic oscillator, where explicit solutions and eigenvalues are obtained using the ladder operator method, and the finite potential well, where a transcendental equation is derived. Using monotonicity and the Intermediate Value Theorem, we show that this equation has a finite number of solutions depending on the parameter values, and that at least one solution always exists. Finally, the infinite potential well is discussed as a limiting case.

Sammanfattning

I detta kandidatarbete härleds och studeras den tidsoberoende Schrödingerekvationen under antagandet om separabla lösningar och en reel, tidsoberoende potentialfunktion. Vi visar att de resulterande egenvärdena E är reella och begränsade underifrån av potentialens minimum. Vidare undersöks hur lösningar till den tidsoberoende ekvationen relaterar till den fullständiga tidsberoende Schrödingerekvationen.

Två exempel behandlas: den harmoniska oscillationen, där explicita lösningar och egenvärden erhålls med hjälp av stigoperatormetoden, samt den ändliga potentialbrunnen, där en transcendent ekvation härleds. Med monotonicitet och satsen om mellanliggande värden visas att denna ekvation har ett ändligt antal lösningar beroende på parametervärden och att minst en lösning alltid existerar. Slutligen diskuteras den oändliga potentialbrunnen som en gräns.

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Contents

1 Introduction

The Schrödinger equation is a fundamental differential equation in quantum mechanics, with applications ranging from nuclear physics to the electronic structure of molecules. It was formulated by Erwin Schrödinger in the early 20^{th} century and plays a central role in describing how quantum systems evolve.

In many cases, solving the *time-dependent Schrödinger equation* directly can be analytically difficult or even impossible. A common approach is instead to study the *time-independent Schrödinger equation*, which often yields valuable information about the original time-dependent system.

This thesis focuses on the mathematical analysis of the Schrödinger equation in two special cases: harmonic oscillator and the potential well. The main focus is on deriving, analysing, and solving the equation by examples using mathematical tools. We will limit our scope to the one dimensional case.

The structure of the thesis is as follows:

- **Part I:** Derivation of the time-independent Schrödinger equation from the time-dependent form, along with definitions of essential notation and assumptions.
- **Part II:** Proofs of several key properties of the equation that will be used in later sections.
- **Part III:** Solving the harmonic oscillator using Ladder operations, a example with an exact solution.
- **Part IV:** Analysis of the finite and infinite potential wells. The finite case leads to a transcendental equation that cannot be solved explicitly, while the infinite case admits exact analytical solutions.

2 The Schrödinger Equation

We will start by introducing the Schrödinger equation

Definition 2.1. The general time-dependent Schrödinger equation in one spatial dimension is given by

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x,t)\Psi(x,t), \tag{1}$$

where $\hbar$ is Plancks reduced constant, m is the mass parameter, $V(x,t)$ is a known potential function and $\Psi(x,t)$ is unknown.

The function $\Psi(x,t)$ is called the wave-function and the function $V(x,t)$ is called the potential function.

The potential function V describes the interaction. Potential $V \equiv 0$ correspond to when there is no interaction. We will follow the book "Introduction to Quantum Mechanics", [GS18] method to derive the time-independent Schrödinger equation. We begin with the following assumptions:

- The potential V is time independent, $V(x,t) = V(x), x \in \mathbb{R}$.
- The solution of the time-dependent equation is separable: $\Psi(x,t) = \psi(x)\varphi(t)$.
- We use natural units: $\hbar = 1$ and $m = 1$. This simplifies the notation.

Under these assumptions, the derivatives of the wave-function $\Psi(x,t)$ are

$$\frac{\partial\Psi}{\partial t} = \psi(x)\frac{\mathrm{d}\varphi}{\mathrm{d}t}, \quad \frac{\partial^2\Psi}{\partial x^2} = \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\varphi(t). \tag{2}$$

Substituting into the Schrödinger equation yields

$$i\psi(x)\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\frac{1}{2}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\varphi(t) + V(x)\psi(x)\varphi(t). \tag{3}$$

Dividing both sides by $\psi(x)\varphi(t)$, assuming that they are nonzero, we obtain

$$i\frac{1}{\varphi(t)}\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\frac{1}{2\psi(x)}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V(x). \tag{4}$$

The left-hand side depends only on the variable t and the right-hand side only on the variable x, so both must be equal to a constant. Let this constant be E. This gives two separate equations,

$$\frac{d\varphi}{dt} = -iE\varphi(t), \tag{5}$$

$$-\frac{1}{2}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x). \tag{6}$$

All solutions to the first equation are of the form

$$\varphi(t) = Ce^{-iEt}, \tag{7}$$

where C is a constant. The second equation is known as the time-independent Schrödinger equation, which is the primary focus of this work.

Definition 2.2. The equation

$$-\frac{1}{2}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), \quad x \in \mathbb{R} \tag{8}$$

is the time-independent stationary Schrödinger equation in one spatial dimension.

It is often convenient to write the time-independent Schrödinger equation using the Hamiltonian operator:

Definition 2.3. The Hamiltionan differential operator is

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x),$$

acting on functions in the Hilbert space $L^2(\mathbb{R})$ of square-integrable functions.

We can therefore write the time-independent Schrödinger equation as the eigenfunction equation for the Hamiltonian differential operator:

$$H\psi(x) = E\psi(x). \tag{9}$$

In this form, we see that E is an eigenvalue of the operator H, and $\psi(x)$ is the corresponding eigenfunction. We will use this form of the Schrödinger equation in the case of the harmonic oscillation. We will end this section with a definition

Definition 2.4. The function $\psi(x)$ is called the wave-function of the time-independent Schrödinger equation.

When referring to the wave-function it will be the time-independent wave-function, if not specified otherwise. Our main goal will therefore be to find as much information as possible on $\psi(x)$ and E.

3 Properties of the Schrödinger Equation

We will derive some properties of the Schrödinger equation that will be used when working with the examples.

Definition 3.1. We define the inner product on the Hilbert space $L^2(\mathbb{R})$ by

$$\langle \psi, \varphi \rangle := \int_{-\infty}^{\infty} \psi(x)\, \overline{\varphi(x)}\, dx, \tag{10}$$

for all $\psi, \varphi \in L^2(\mathbb{R})$.

Definition 3.2. Let $\Psi(x,t)$ be a wave-function. Its norm is defined by

$$\|\Psi\|^2 = \int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx. \tag{11}$$

Axiom 3.3. Every physically acceptable wave-function must satisfy

$$\|\Psi\|^2 = 1.$$

Remark 3.4. The trivial solution $\Psi(x,t) = 0$ has zero norm and is therefore excluded by the normalization axiom.

Theorem 3.5. *If the wave-function is of the form $\Psi(x,t) = \psi(x)\varphi(t)$ in the time-dependent Schrödniger equation, then the norm, $||\Psi||^2 = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx$, does not depend on t.*

Proof. From the previous section, we know that $\varphi(t) = Ce^{iEt}$. We then have that

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \int_{-\infty}^{\infty} |\psi(x)\varphi(t)|^2 dx = |C|^2 \int_{-\infty}^{\infty} \left(\psi(x)e^{-iEt}\bar{\psi}(x)e^{iEt}\right) dx$$
$$= |C|^2 \int_{-\infty}^{\infty} \left(\psi(x)\bar{\psi}(x)e^{-iEt+iEt}\right) dx = |C|^2 \int_{-\infty}^{\infty} \left(\psi(x)\bar{\psi}(x)\right) dx = |C^2| \int_{-\infty}^{\infty} |\psi(x)|^2 dx. \tag{12}$$

□

Theorem 3.6. *The eigenvalues E of the stationary Schrödinger operator are real*

Proof. We will use inner product to prove this, using its relations and that the Hamiltonian differential operator is Hermitian, that is $< H\psi, \varphi > = < \psi, H\varphi >$.

Then

$$\langle H\psi, \psi\rangle = \langle E\psi, \psi\rangle = E\langle \psi, \psi\rangle. \tag{13}$$

Further

$$\langle H\psi, \psi\rangle = \langle \psi, H\psi\rangle = \langle \psi, E\psi\rangle = \bar{E}\langle \psi, \psi\rangle. \tag{14}$$

Thus, $E\langle\psi,\psi\rangle = \bar{E}\langle\psi,\psi\rangle \implies E = \bar{E}$. Therefore, E must be real. □

Theorem 3.7. *Let $V_{min} = inf(V(x))$, then the eigenvalue $E \geq V_{min}$, when.*

Proof. First, multiply both sides with $\bar{\psi}$ and integrate over $\mathbb{R}$

$$\begin{aligned} -\frac{1}{2}\psi'' + V(x)\psi &= E\psi \\ \implies -\frac{1}{2}\int_{-\infty}^{\infty}\psi''\bar{\psi}dx + \int_{-\infty}^{\infty}V(x)\psi\bar{\psi} &= \int_{-\infty}^{\infty}E\psi\bar{\psi} \\ \iff -\frac{1}{2}\int_{-\infty}^{\infty}\psi''\bar{\psi}dx + \int_{-\infty}^{\infty}V(x)|\psi|^2dx &= E \\ \iff E = \int_{-\infty}^{\infty}\frac{1}{2}|\psi'(x)|^2 + V(x)|\psi(x)|^2dx. \end{aligned} \tag{15}$$

Let $V_{min} = \inf(V(x))$. Then

$$\begin{aligned} E = \int_{-\infty}^{\infty}\frac{1}{2}|\psi'(x)|^2 + V(x)|\psi(x)|^2dx \geq \int_{-\infty}^{\infty}\frac{1}{2}|\psi'(x)|^2 + V_{min}|\psi(x)|^2dx = \\ = \frac{1}{2}\int_{-\infty}^{\infty}|\psi'(x)|^2dx + V_{min} \geq V_{min}. \end{aligned} \tag{16}$$

Thus, we have $E \geq V_{min}$. □

We now have established some properties of the wave-function and the eigenvalue E. With the last theorem, we see that any normilized wave-function in the time-independent case can easily be made a solution to the time-dependent case by multiplying the wave-function by e^{-iEt}.

4 The Harmonic Oscillation

We will, in this part, find the wave-functions and their corresponding values of E to the Schrödinger equation when $V(x)$ is the simple harmonic oscillation, $V(x) = m\omega^2 x^2$. As we have done before, we assume

$$m = \hbar = \omega = 1,$$

and thus we instead have the potential function, $V(x) = \frac{1}{2}x^2$.

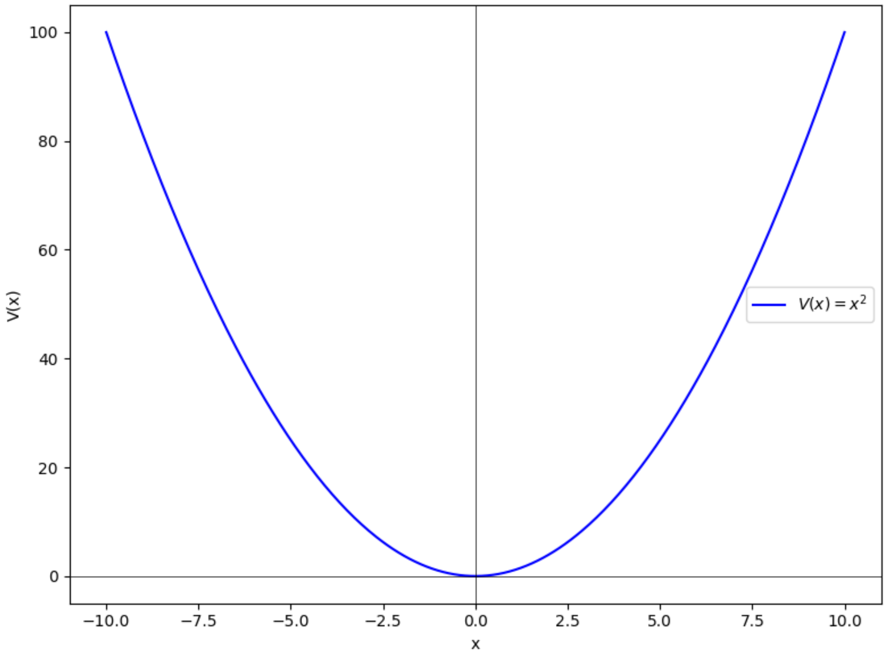

Figure 1: Graph of the finite potential well

Substituting into the Schrödinger equation yields

$$-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + \frac{1}{2}x^2\psi(x) = E\psi(x). \tag{17}$$

or alternatively

$$\frac{1}{2}\Big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2\Big)\psi = E\psi. \tag{18}$$

There are several approaches to this problem, and we will demonstrate one method using Ladder Operations. We will have the same approach as shown in "Introduction to quantum mechanics, Griffiths & Schroeter", chapter 2, [GS18]. We will first define some key properties and show some lemmas before we tackle the Schrödinger equation for simple harmonic oscillation.

Definition 4.1. We define the Lowering Operator as

$$a_- = \frac{1}{\sqrt{2}}\Big(\frac{\mathrm{d}}{\mathrm{d}x} + x\Big) \tag{19}$$

and the Raising Operator as

$$a_+ = \frac{1}{\sqrt{2}}\Big(-\frac{\mathrm{d}}{\mathrm{d}x} + x\Big). \tag{20}$$

Lemma 4.2. *The Hamiltonian H can be written in one of the following forms:*

$$\begin{aligned} H &= a_-a_+ - \frac{1}{2} \\ H &= a_+a_- + \frac{1}{2} \end{aligned} \tag{21}$$

Proof. We see that

$$\begin{aligned} a_+a_-\psi = \frac{1}{2}(-\frac{\mathrm{d}}{\mathrm{d}x} + x)(\frac{\mathrm{d}}{\mathrm{d}x} + x)\psi \\ = \frac{1}{2}(-\frac{\mathrm{d}}{\mathrm{d}x} + x)(\psi' + x\psi) = \frac{1}{2}(-\psi'' + x\psi' - \psi - x\psi' + x^2\psi) \\ = \frac{1}{2}(-\psi'' - \psi + x^2\psi) = \frac{1}{2}(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2)\psi - \frac{1}{2}\psi \\ = H\psi - \frac{1}{2}\psi = (H - \frac{1}{2})\psi. \end{aligned} \tag{22}$$

Therfore, we have that $a_+a_- = H - \frac{1}{2}$. Sloving for H yeilds $H = a_+a_- + \frac{1}{2}$. Analogical calculations can be done for the other case. □

Lemma 4.3.

$$a_-a_+ = a_+a_- + 1. \tag{23}$$

Proof. From previous lemma, we found two ways to express H that must be equal. Thus we have

$$\begin{aligned} a_-a_+ - \frac{1}{2} &= a_+a_- + \frac{1}{2} \\ \iff a_+a_- &= a_+a_- + 1. \end{aligned} \tag{24}$$

□

Now, we have given some definitions and lemmas that will help us in finding the solution to the schrödinger equation. We will now start to find a solution. Our first step is utilizing the lowering and raisng operator:

Theorem 4.4. *If ψ satisfies the Schrödinger equation with Eigenvalue E, then $a_+\psi$ satisfies the Schrödinger equation with Eigenvalue $E+1$.*

If ψ satisfies the Schrödinger equation with Eigenvalue E, then $a_-\psi$ satisfies the Schrödinger equation with Eigenvalue $E-1$.

Proof. We have that

$$\begin{aligned} H(a_+\psi(x)) = (a_+a_- + \frac{1}{2})(a_+\psi(x)) = (a_+a_-a_+ + \frac{1}{2}a_+)\psi(x) \\ = a_+(a_-a_+ + \frac{1}{2})\psi(x) = a_+((a_+a_- + 1 + \frac{1}{2})\psi(x)) \\ = a_+(H+1)\psi(x) = a_+(E+1)\psi(x) = (E+1)(a_+\psi(x)), \end{aligned} \tag{25}$$

where we have in the second line used that $a_-a_+ = a_+a_- + 1$, in the third line used the assumption that ψ satisfies the Schrödinger equation and E is an eigenvalue. For the lowering operation, similar calculations are made.

□

From that lemma, we see that once we have a wave-function, we can use the ladder operators to find other wave-functions with their corresponding eigenvalues. So we now need to find a solution to find a new solution. When taking the lowering operator repeatedly, we lower the value of the eigenvalue. From the previous theorem, we found that E cannot be lower than V_{min}, which is zero, and that E must be real. At some point, the lowering operation must come to a halt, which happens when $E = 0$. Let $\psi_0(x)$ be the ground state, where if we were to lower it once again, we come to the trivial "solution" $\psi(x) = 0, E = 0$(As this solution cannot be normalized, it has no importance more than finding $\psi_0(x)$). We can show the following:

Lemma 4.5. *The ground state $\psi_0(x)$ has the normilized solution*

$$\psi_0(x) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} e^{-\frac{x^2}{2}}, \tag{26}$$

Proof. Reapted use of the lowering operation yields lower potential energy. We thus end up with

$$\begin{aligned} a_-\psi_0(x) &= 0 \\ \iff \frac{1}{\sqrt{2}}(\frac{\mathrm{d}}{\mathrm{d}x} + x)\psi_0(x) &= 0 \\ \iff \frac{\mathrm{d}\psi_0}{\mathrm{d}x} &= -x\psi_0. \end{aligned} \tag{27}$$

Integrating both sides and solve for $\psi_0(x)$, we yeild

$$\psi_0(x) = Ae^{-\frac{x^2}{2}}, \tag{28}$$

where A is a constant, for more details on this method, we refer to [AB19]. Normalizing, we have

$$1 = |A|^2 \int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} dx = |A|^2\sqrt{\pi}. \tag{29}$$

Thus we have that $A = \left(\frac{1}{\pi}\right)^{\frac{1}{4}}$. ☐

Corollary 4.6. *The Eigenvalue for The Ground state is* $E_0 = \frac{1}{2}$.

Proof. Substituting in the ground state in the Schrödinger equation and solving for E and using the fact that $a_-\psi_0 = 0$, yields that $E = \frac{1}{2}$. ☐

We will now formulate the solution.

Theorem 4.7. *The normalised solutions to the Schrödinger equation for the Harmonic oscillation are*

$$\psi_n(x) = A_n a_+^n \psi_0(x) \tag{30}$$

with $E_n = (n + \frac{1}{2})$, *where*

$$\psi_0(x) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} e^{-\frac{x^2}{2}} \tag{31}$$

and A_n *is a normalization constant.*

Proof. We have already shown how to find the ground state $\psi_0(x)$ together with its eigenvalue $E = \frac{1}{2}$. Applying the raising operator repeatedly, we find that

$$\begin{aligned} \psi_n(x) &= A_n a_+^n \psi_0(x) \\ E_n &= (n + \frac{1}{2}), \end{aligned} \tag{32}$$

where A_n is a Normilzing constant such that $\psi_n(x)$ satisfies axiom 3.3 and $n = 1, 2, 3, ...$ □

5 Potential Well

5.1 Single Finite Potential Well

In this section, we will instead see what happens we define the potential function $V(x)$ as the finite potential well, which is

$$V(x) = \begin{cases} V_0 & (x < 0, x > \mathbb{L}) \\ 0 & (0 \leq x \leq \mathbb{L}), \end{cases} \tag{33}$$

for the time-independent Schrödinger equation. This section is heavily inspired by

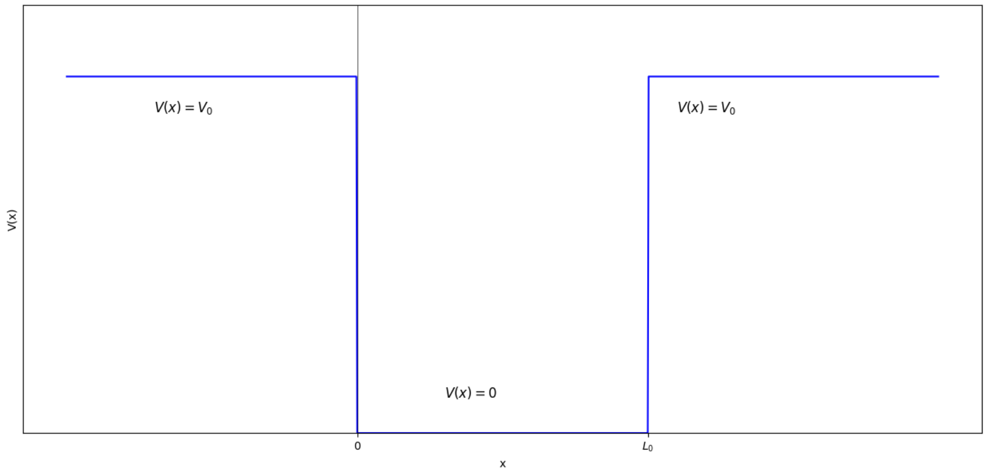

Figure 2: Graph of the finite potential well

Chapter 3.3 in Sara M. McMurry's book Quantum Mechanics [McM94]. In this example, we cannot analytically find the values of E when we have finite depths. However, as we shall see we can find the wave-function and restricions on E. First, we divide the real line into three regions as follows:

$$\begin{aligned} \text{Region I} &:= \{x < 0\}, \\ \text{Region II} &:= \{0 \leq x \leq \mathbb{L}\}, \\ \text{Region III} &:= \{x > \mathbb{L}\}. \end{aligned}$$

In each region, we denote the corresponding wave-function by

$$\psi_I(x), \quad \psi_{II}(x), \quad \text{and} \quad \psi_{III}(x),$$

respectively. We will assume that the eigenvalues E satisfy $E < V_0$, which is referred to as a bound state. In addition, as we saw in theorem 3.6 and 3.7, the values of E are real and greater than 0. And, as usual, we assume that $\hbar = m = 1$. Finally, we have that for both V_0 and $\mathbb{L}$ that they are positive constants. For the finite potential well the wave-function is given bys in the following.

Lemma 5.1. *The General solution in their respective region for the Schrödinger equation is*

$$\begin{aligned} \psi_I(x) &= Ce^{\gamma x}, \quad x < 0 \\ \psi_{II}(x) &= A \cdot \sin{(kx)} + C \cdot \cos{(kx)}, \quad 0 \leq x \leq \mathbb{L} \\ \psi_{III}(x) &= Ge^{-\gamma x}, \quad x > \mathbb{L} \end{aligned} \tag{34}$$

where $A, B, C, G \in \mathbb{R}$ *and with* $k^2 := 2E \geq 0$, $\gamma^2 := 2(V_0 - E)$

Proof of Theorem 5.1. We start by defining

$$\begin{aligned} k^2 &:= 2E \\ \gamma^2 &:= 2(V_0 - E). \end{aligned} \tag{35}$$

As E is always positive, we see that $k^2 \geq 0$. We can also see that for γ^2, it also needs to be larger than 0. We start by finding a solution in Region II. Our differential equation in this region is

$$\begin{aligned} -\frac{1}{2}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} &= E\psi(x) \\ \iff \frac{\partial^2\psi}{\partial x^2} &= -k^2\psi(x). \end{aligned} \tag{36}$$

This have the general solution.

$$\psi_{II}(x) = A \cdot \sin{(kx)} + B \cdot \cos{(kx)}, \quad 0 \leq x \leq \mathbb{L}, \tag{37}$$

where $A, B \in \mathbb{R}$. A method to find can for example be seen in "Ordinary Differential Equations" by Andersson and Böiers [AB19].

Instead, for Regions I and II, we have that the Time-Independent Schrödinger equation is

$$\begin{aligned} \frac{-1}{2}\frac{\mathrm{d}}{\mathrm{d}x^2}\psi(x) + V_0\psi(x) &= E\psi(x) \\ \iff \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} &= \gamma^2\psi(x), \end{aligned} \tag{38}$$

where $\gamma^2 = 2(V_0 - E)$. A general solution to the differential equation is given by

$$\begin{aligned} \psi_I(x) &= Ce^{\gamma x} + De^{-\gamma x}, \quad x < 0 \\ \psi_{III}(x) &= Fe^{\gamma x} + Ge^{-\gamma x}, \quad x > \mathbb{L}, \end{aligned} \tag{39}$$

for their respective region. Now, we use axiom 3.3 of normalisation of the solution. In our case, that implies that

$$\begin{aligned} x \to -\infty &\implies \psi_I(x) \to 0 \\ x \to \infty &\implies \psi_{III}(x) \to 0. \end{aligned} \tag{40}$$

For that to be possible, we must have that $D = 0$ and $F = 0$. □

Now, we have only taken into consideration that the solution can be normalized. We have, however, not taken into account that it should be continuous. We must also take into account the following relations to have a valid continous solution

$$\begin{aligned} \psi_I(0) = \psi_{II}(0), &\quad \psi_I'(0) = \psi_{II}'(0) \\ \psi_{III}(\mathbb{L}) = \psi_{II}(\mathbb{L}), &\quad \psi_{III}'(\mathbb{L}) = \psi_{II}'(\mathbb{L}). \end{aligned} \tag{41}$$

With this we make the following theorem

Theorem 5.2. *For the finite potential well, the values of E must satisfy*

$$2\cot(k\mathbb{L}) = \frac{k}{\gamma} - \frac{\gamma}{k}. \tag{42}$$

Proof. The Condition $\psi_I(0) = \psi_{II}(0)$ gives us

$$Ce^{\gamma 0} = A\sin(k0) + B\cos(k0) \implies C = B. \tag{43}$$

The condition $\psi_I'(0) = \psi_{II}'(0)$ give

$$\gamma Ce^{\gamma 0} = Ak\cos(k0) - Bk\sin(k0) \implies A = \frac{\gamma C}{k}. \tag{44}$$

The condition $\psi_{III}(\mathbb{L}) = \psi_{II}(\mathbb{L})$ gives

$$A\sin(k\mathbb{L}) + B\cos(k\mathbb{L}) = Ge^{-\gamma\mathbb{L}} \iff \frac{\gamma C}{k}\sin(k\mathbb{L}) + C\cos(k\mathbb{L}) = Ge^{-\gamma\mathbb{L}}. \tag{45}$$

The condition $\psi'_{III}(\mathbb{L}) = \psi'_{II}(\mathbb{L})$ gives

$$kA\cos(k\mathbb{L}) - kB\sin(k\mathbb{L}) = -Ge^{-\gamma\mathbb{L}} \implies -C\cos(k\mathbb{L}) + \frac{k}{\gamma}C\sin(k\mathbb{L}) = Ge^{-\gamma\mathbb{L}}. \tag{46}$$

We can now combine the implications of the last two conditions, and we obtain

$$\begin{aligned}\frac{\gamma C}{k}\sin(k\mathbb{L}) + C\cos(k\mathbb{L}) &= -C\cos(k\mathbb{L}) + \frac{k}{\gamma}C\sin(k\mathbb{L}) \\ \iff 2\cot(k\mathbb{L}) &= \frac{k}{\gamma} - \frac{\gamma}{k}.\end{aligned} \tag{47}$$

□

Now we have obtained an equation that only has E as an unknown. Unfortunately, we cannot solve for E and obtain an explicit solution. To find values of E, numerical methods must be used. However, we can draw some conclusions from it analytically, as we shall see. We will treat E as a variable. Then we define each side of the equation as

$$\begin{aligned} y(E) &= 2\cot(\sqrt{2\mathbb{L}^2 E}), \\ g(E) &= \sqrt{\frac{E}{V_0 - E}} - \sqrt{\frac{V_0 - E}{E}}. \end{aligned} \tag{48}$$

Now, we are looking for the intersections of these two graphs and, thus, allowed values of E.

Both functions are continuous in the interval $(0, V_0)$. First, we see that $y(E)$ is a periodic function, and we shall show the following:

Lemma 5.3. *For each interval*

$$\left(\frac{\pi^2 n^2}{2\mathbb{L}^2}, \frac{\pi^2(n+1)^2}{2\mathbb{L}^2}\right), \quad n \in 0, 1, 2, 3...$$

where the right side of the interval is smaller or equal to V_0, there exists exactly one solution. In addition, if the interval is

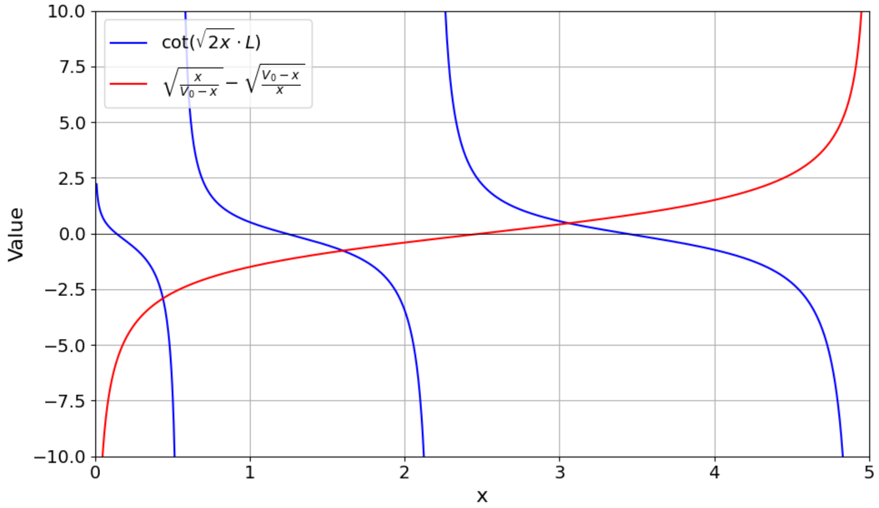

Figure 3: Graph of y and g when $\mathbb{L} = 3, V_0 = 5$

$$\left(\frac{\pi^2 n^2}{2\mathbb{L}^2}, V_0\right)$$

where $V_0 \leq \frac{\pi^2(n+1)^2}{2\mathbb{L}^2}$, there exists exactly one solution.

But first, we shall show the following theorem.

Theorem 5.4. *Let $f, g : (a, b) \to \mathbb{R}$ be continuous functions. Furthermore, let f be strictly decreasing and g strictly increasing on (a, b). Let*

$$\begin{aligned} \lim_{x \to a^+} (f(x) - g(x)) > 0 \\ \lim_{x \to b^-} (f(x) - g(x)) < 0. \end{aligned} \tag{49}$$

Then there exist a unique x_0 such that $f(x_0) = g(x_0)$.

Proof. First we define $h(x) := f(x) - g(x)$. As both f and g are contious, so will $h(x)$. Further $h(x)$ will be strictly decreasing as,

$$\begin{aligned} x_1 < x_2 \implies f(x_1) > f(x_2), g(x_1) < g(x_2) \\ \implies f(x_1) - g(x_1) > f(x_2) - g(x_2) = h(x_1) > h(x_2). \end{aligned} \tag{50}$$

By assumptions, we have that $\lim_{x \to a^+} h(x) > 0$ and $\lim_{x \to b^-} h(x) < 0$. Since $h(x)$ is continuous, by the Intermediate Value Theorem, there must exist a point $x_0 \in (a, b)$

such that

$$h(x_0) = 0 \iff f(x_0) = g(x_0). \tag{51}$$

Now, suppose there exist $x_1, x_2 \in (a, b)$ such that $x_1 < x_2$, $f(x_1) = g(x_1)$ and $f(x_2) = g(x_2)$. Then $h(x_1) = h(x_2) = 0$. But since $h(x)$ is strictly decreasing in the interval (a, b), it contradicts $h(x_1) = h(x_2)$. Thus the point $h(x_0) = 0$ is unique. □

We now can show the proof of the lemma 5.3.

Proof. First we see that $y(E)$ have a period of

$$\sqrt{2\mathbb{L}^2 E} = \pi n \implies E = \frac{\pi^2 n^2}{2\mathbb{L}^2}, n \in 0, 1, 2, 3... \tag{52}$$

In each interval, $y(E)$ is strictly decreasing from $+\infty$ to $-\infty$, as $\cot(x)$ is, and $2\mathbb{L}^2 E$ only increases in value, only with different amplitude than x.

For $g(E)$, its derivative is

$$g'(E) = \frac{\frac{E}{(V_0-E)^2} + \frac{1}{V_0-E}}{2\sqrt{\frac{E}{V_0-E}}} + \frac{\frac{1}{E} + \frac{V_0-E}{E^2}}{2\sqrt{\frac{V_0-E}{E}}}. \tag{53}$$

As $0 < E < V_0$, we see that $g'(E) > 0$ and thus monotonically increase the interval $0 < E < V_0$. Now for each interval

$$\left(\frac{\pi^2 n^2}{2\mathbb{L}^2}, \frac{\pi^2 (n+1)^2}{2\mathbb{L}^2}\right),$$

there must exist one intersection and thus one solution, by the previous theorem. So if the whole interval is covered by E, then there exists one solution.

But what if V_0 is in one of these interval so only a part is defined? Then there are two cases. Either when

$$\frac{\pi^2 n^2}{2\mathbb{L}^2} < V_0 < \frac{\pi^2 (n+1)^2}{2\mathbb{L}^2}, \tag{54}$$

for some non-negative integer number n or

$$0 < V_0 < \frac{\pi^2}{2\mathbb{L}^2}. \tag{55}$$

Now in the first case, $y(E)$ will go from $+\infty$ to some number, call it a. We also see for $g(E)$ that

$$\lim_{E\to V_0} \sqrt{\frac{E}{V_0 - E}} - \sqrt{\frac{V_0 - E}{E}} \longrightarrow +\infty. \tag{56}$$

Thus $g(E)$ will go from a number b to $+\infty$. And now by theorem 5.4, there exist one point where they cross and, therefore, a solution. In the second case, $g(E)$ will instead have the limit

$$\lim_{E\to 0} g(E) = -\infty. \tag{57}$$

We see that the criterion of theorem 5.4 holds and thus a solution exists in that interval. □

Now the interesting question is: how many solutions exist?

Theorem 5.5. *For the finite potential well there exists*

$$\left\lceil \frac{\mathbb{L}\sqrt{2V_0}}{\pi} \right\rceil$$

number of bound states.

Proof. As we saw before, every interval contains a solution. Then we have that for the largest n such that the next interval is larger than V_0 that

$$\frac{\pi^2 n^2}{2\mathbb{L}^2} < V_0 \implies n < \frac{\mathbb{L}\sqrt{2V_0}}{\pi}. \tag{58}$$

With this, we know that there exist n full intervals of $y(E)$ and thus n solutions. But between $\frac{\pi^2 n^2}{2\mathbb{L}^2}$ and V_0, we implement the previous theorem to find an additional solution. The ceiling function ensures that the solution is taken into account if V_0 isn't equal to one of the endpoints of an interval. □

Corollary 5.6. *In the finite potential well, there will always exist at least one bound solution to the Schrödinger equation.*

Proof. This will have the same style as the proof of the existence and uniqueness of a solution in each interval. Let V_0 and $\mathbb{L}$ be fixed and positive. If $V_0 < \frac{\pi^2}{2\mathbb{L}^2}$, then we proved that a solution exists. If instead $V_0 > \frac{\pi^2}{2\mathbb{L}^2}$, then by the lemma, we have at least that the interval $(\frac{\pi^2 0^2}{2\mathbb{L}^2}, \frac{\pi^2 1^2}{2\mathbb{L}^2})$ has a solution. □

We conclude this section here. We found the form of the wave-function and how many solutions exist, but it is impossible to get explicit formulas for the eigenvalues.

5.2 Single Infinite Potential Well

We will now see how the solution changes when we let $V_0 \to \infty$ for the potential well.

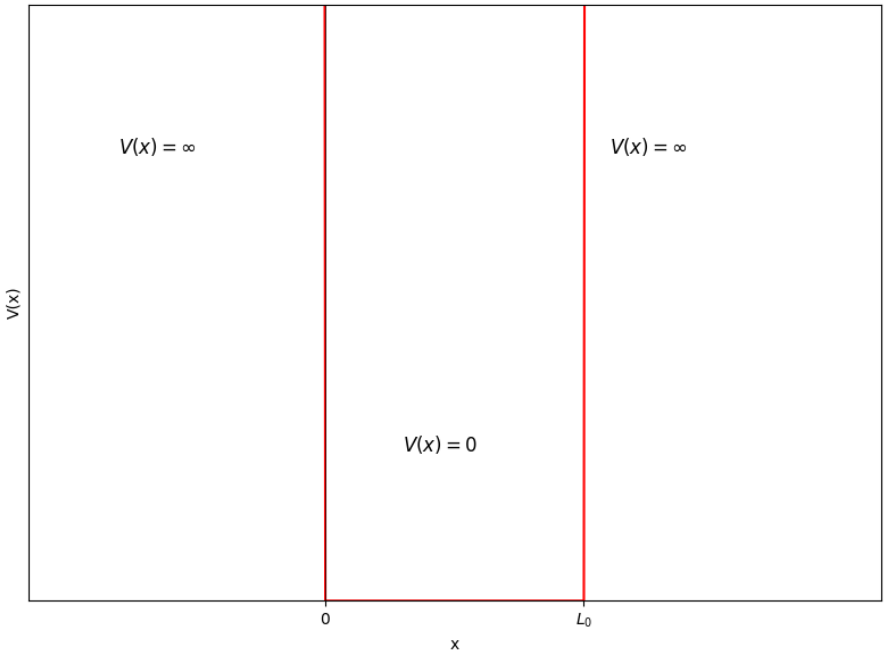

Figure 4: Graph of the finite potential well

In this case, the wave-function and its eigenvalue E can be found explicitly as we shall see. We summarise the result in the following Theorem:

Theorem 5.7. *When $V_0 \to \infty$ for the potential well, then the normalised solution to the Schrödinger equation is*

$$\begin{aligned} \psi_{II}(x) = \sqrt{\frac{2}{\mathbb{L}}} \sin\left(\frac{n\pi x}{\mathbb{L}}\right), \quad 0 \leq x \leq \mathbb{L} \\ \psi_I(x) = 0, \quad x < 0 \\ \psi_{III}(x) = 0, \quad x > \mathbb{L} \end{aligned} \tag{59}$$

where $n \in \{1, 2, 3, ...\}$, with allowed values of E being

$$E_n = \frac{n^2\pi^2}{2\mathbb{L}^2}, n = 1, 2, 3, ... \tag{60}$$

Proof. First, we notice that when $V_0 \to \infty$, then $\gamma \to \infty$. From the finite case, we found the solution when only considering that the solution can be normlized to be

$$\begin{aligned} \psi_I(x) &= Ce^{\gamma x}, \quad x < 0 \\ \psi_{II}(x) &= A \cdot \sin(kx) + B \cdot \cos(kx), \quad 0 \leq x \leq \mathbb{L} \\ \psi_{III}(x) &= Ge^{-\gamma x}, \quad x > \mathbb{L}. \end{aligned} \tag{61}$$

As $\gamma \to \infty$ we see that both $\psi_I(x)$ and $\psi_{III}(x)$ must be identically equal to 0. For $\psi_{II}(x)$, its derivative no longer needs to be continuous and finite at the boundaries of Region II. But we have the condition that at the boundaries, we have

$$\psi_{III}(0) = \psi_{III}(\mathbb{L}) = 0. \tag{62}$$

Thus, we yield at $x = 0$ that

$$A\cos(0) - B\sin(0) = 0 \iff A = 0. \tag{63}$$

If we instead look at $x = \mathbb{L}$, we have that

$$\psi_{III}(\mathbb{L}) = B\sin(k\mathbb{L}) = 0. \tag{64}$$

Since $\sin(n\pi) = 0$, for non negative integers, it follows that

$$k\mathbb{L} = n\pi \iff k = n\frac{\pi}{\mathbb{L}}. \tag{65}$$

By substitution our new expression of k into our definition of k, as seen in (33), we obtain

$$\frac{n^2\pi^2}{\mathbb{L}^2} = 2E \iff E_n = \frac{n^2\pi^2}{2\mathbb{L}^2}, \quad n = 1, 2, 3, ... \tag{66}$$

Notice that we now have calculated E_n. For our function over Region II, we find that with the condition on $x = \mathbb{L}$ that

$$\psi(x) = B\sin\Big(\frac{n\pi x}{\mathbb{L}}\Big). \tag{67}$$

With our new way of writting k, we can substitute it in in the sinus function. We end the proof by finding B such that $\psi_{II}(x)$ is normilized. We then have that

$$1 = \int_0^{\mathbb{L}} |\psi_n(x)|^2 = B^2 \int_0^{\mathbb{L}} \sin^2\left(\frac{n\pi x}{\mathbb{L}}\right) = B^2\frac{\mathbb{L}}{2}. \tag{68}$$

Solving for B we yeild that $B = \sqrt{\frac{2}{\mathbb{L}}}$. Thus we have that

$$\begin{aligned} \psi(x) = \sqrt{\frac{2}{\mathbb{L}}} \sin\left(\frac{n\pi x}{\mathbb{L}}\right), \quad 0 \leq x \leq \mathbb{L} \\ \psi(x) = 0, \quad x < 0, x > \mathbb{L}. \end{aligned} \tag{69}$$

□

Remark 5.8. Looking at the allowed values of E, we see that it matches the interval edges from the finite case.

6 Conclusion

In this diploma, we have derived and studied the time-independent Schrödinger equation under the assumptions of a separable solution and a real, time-independent potential function. We proved that the values of E are real and bounded below by the minimum of the potential function, and how solutions to the time-independent case are connected to the time-dependent Schrödinger equation.

We then analysed two examples to illustrate these properties. For the harmonic oscillator, we obtained explicit solutions and their corresponding values of E using the Ladder operations method. For the finite potential well in the bound case where $E < V_0$, we derived a transcendental equation and proved, using monotonicity and the Intermediate Value Theorem, that this equation admits a finite number of solutions, depending on the parameters $\mathbb{L}$ and V_0 and the existence of atleast one. Lastly, we derived the solutions to the infinite potential well.

This work demonstrates how techniques in analysis and algebra can be used to establish the existence and properties of solutions to a class of second-order differential equations with boundary conditions. Various examples of further studies include other ways to solve the harmonic oscillation, for example, with Power series, higher-dimensional spatial coordinates, or numerical approaches for potentials that do not allow explicit solutions.

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