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Bachelor Thesis

Self-Adjoint Energy and Momentum Operators for a Particle in a Box

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Abstract

In this thesis, a 2-parameter family of self-adjoint extensions of the Hamiltonian for a particle in a 1-d box is considered to generalize the standard treatment with Dirichlet boundary conditions. Within this more general setting, it is shown that the standard momentum operator $-i\partial_x$ does not qualify as a physical observable. In turn, an alternative momentum operator $\hat{p}_R$ with a corresponding quantized spectrum is derived from a lattice treatment. Its construction consists in a symmetrized forward-backward next-to-nearest neighbor derivative over two lattice spacings. Moreover, it is also proven that the Ehrenfest theorem, relating the expectation values of position and momentum, only holds when replacing $\hat{p} = -i\partial_x$ with the new momentum operator $\hat{p}_R$. Throughout this entire thesis, the subtle but crucial difference between Hermiticity and self-adjointness of linear operators is illustrated.

Contents

Chapter 1

Introduction

A particle with mass M confined to the inside of a finite box is probably the first concrete system any physics student encounters in his or her first lecture on quantum mechanics. Seemingly straightforward from a mathematical point of view, it nicely illustrates the most fundamental principles of quantum mechanics. This straightforwardness, however, only results from assumptions that seem physically reasonable, but are in fact not the whole story. When one detaches oneself from these assumptions and begins from a much more general starting point, mathematical subtleties with great physical implications arise. The apparently simple particle in a box turns out to be a very interesting and highly non-trivial issue, and the goal of this thesis is to illustrate these subtle details.

The thesis proceeds as follows: In this first chapter, the aim of this thesis is presented, and the most important concepts of quantum mechanics as well as its mathematical framework used in this thesis are briefly recapitulated. Hopefully, most of these concepts look familiar to the reader.
In chapter 2, the Hamiltonian[1] for a particle in a box will be treated, but in a much more general fashion compared to what is presented in most undergraduate lectures, closely following and carrying forward the approach presented in [1].
In chapter 3, the standard momentum operator $\hat{p} = -i\hbar\partial_x$ is shown not to be suitable in the most general situation as it is not Hermitean[2], let alone self-adjoint. Consequently, a new concept for momentum, which was first presented in [2], will be discussed.
Applying the results from the previous two chapters, chapter 4 will be devoted to the applicability of Ehrenfest's[3] theorem, a general statement on expectation values that is valid in the infinite volume but which does not trivially generalize to the case of a particle in a box.
Chapter 5 will conclude the discussion and give an outlook to open questions that are yet to be answered.

For notational convenience, we will work in natural units where $\hbar = 1$ throughout the whole thesis. Moreover, we'll use the notation ∂_t and ∂_x for partial derivatives with respect to time or position.

1.1 Aim of the Thesis

The aim of this thesis is to illustrate the mathematical subtlety differentiating between Hermiticity and self-adjointness of linear operators, which is crucial for the framework of quantum mechanics to be applicable. In systems with spatial boundaries, not all "standard" operators are per se self-adjoint, and thus the measurement of the quantities they represent is a non-trivial issue.

[1] After Sir William Rowan Hamilton (1805-1865), Irish physicist and mathematician.
[2] Charles Hermite (1822-1901), French mathematician
[3] Paul Ehrenfest (1880-1933), Austrian physicist.

Specifically, the kinetic energy and the momentum operator for a particle in a finite interval are treated. Under general boundary conditions, the goal is to find self-adjoint extensions of the kinetic energy operator, which are characterized by two extension parameters. Moreover, one will see that under these conditions, the momentum operator $-i\partial_x$ is not even Hermitean, and thus an alternative concept for a momentum operator introduced in [2] shall be discussed. The plausibility of this new momentum operator should show itself by comparing momentum distributions in energy eigenstates within the old and the new picture and by discussing their implications on the validity of Ehrenfest's theorem.

1.2 Operators in Quantum Mechanics

In quantum mechanics, the state of any quantum mechanical system is described by its wave function $|\Psi(t)\rangle$ living in Hilbert[4] space, and the evolution of the wave function is governed by the time-dependent Schrödinger[5] equation [3],

$$i\partial_t |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle , \tag{1.1}$$

where $\hat{H}$ is the Hamilton operator of the considered system. This equation is a prime example of an equation involving operators, which play a fundamental role in quantum mechanics: Every physical observable, be it position, momentum, or energy, is described by a corresponding linear, self-adjoint operator, which is characterized by its action and its domain [4]. What the operator does to the wave function it acts upon is governed by its action, whilst its domain describes the subset of Hilbert space on which the operator can act.
Although most introductory courses in quantum mechanics only pay little attention to the notion of domains, they play an important role when it comes to distinguish *Hermitean* from *self-adjoint* operators, as will be done in section 1.3. Only self-adjointness, not Hermiticity alone, guarantees that an operator $\hat{A}$ has a complete set of orthonormal eigenstates with real eigenvalues, as proven in [5]. In the case of a discrete spectrum, for example,

$$\hat{A} |\psi_n\rangle = \lambda_n |\psi_n\rangle , \quad \lambda_n \in \mathbb{R} \ \ \forall n \in \mathbb{N} \tag{1.2}$$

any wave function $|\Psi\rangle$ in Hilbert space could be decomposed into the basis of eigenstates $|\psi_n\rangle$ of $\hat{A}$

$$|\Psi\rangle = \sum_n c_n |\psi_n\rangle , \qquad \{c_n\}_{n\in\mathbb{N}} \subset \mathbb{C}. \tag{1.3}$$

Most of the time in quantum mechanics, the domains of operators are characterized by criteria concerning differentiability and square-integrability of derivatives: The operator of kinetic energy, for example, contains a second derivative with respect to position, and thus can only act upon wave functions that are at least twice differentiable and whose second derivatives are still square-integrable. In the present case, where a system of finite volume with boundaries is considered, boundary conditions further restrict the domain of an operator.

Before continuing with the definitions of Hermiticity and self-adjointness, the used notation in this thesis is briefly revisited. So far, Dirac[6] notation was tacitly used to represent the state of a system by a ket $|\Psi(t)\rangle$ in an abstract Hilbert space $\mathcal{H}$. For the usual treatment of a particle in an interval Ω, the considered Hilbert space is the set of all square-integrable functions on Ω, denoted by $\mathcal{H} = L^2(\Omega)$. For explicit calculations, one can project these states into position basis to obtain a wave function of x (and t):

$$\Psi(x,t) = \langle x|\Psi(t)\rangle . \tag{1.4}$$

[4]David Hilbert (1862-1943), German mathematician.
[5]Erwin Rudolf Josef Alexander Schrödinger (1887-1961), Austrian physicist.
[6]Paul Adrien Maurice Dirac (1902-1984), British physicist.

In the first three chapters, the time evolution of the system will not be of interest, so the variable t will be omitted to simplify the notation wherever it isn't needed.
The (complex) inner product between two wave functions (in one dimension) is defined as

$$\langle\chi|\Psi\rangle \equiv \int_{-\infty}^{\infty} dx\, \chi(x)^* \Psi(x), \tag{1.5}$$

which can be used to obtain the expectation value of an operator $\hat{A}$ in a state $|\Psi\rangle$

$$\langle\hat{A}\rangle \equiv \langle\Psi|\hat{A}|\Psi\rangle \equiv \langle\Psi|\hat{A}\Psi\rangle = \int_{-\infty}^{\infty} dx\, \Psi(x)^* A\Psi(x). \tag{1.6}$$

Here, A is meant to be the representation of $\hat{A}$ in position basis.

1.3 Hermiticity versus Self-Adjointness

Without proof, it has so far been stated that only self-adjointness guarantees that an operator has a complete set of eigenstates with real eigenvalues. Hermiticity alone does not suffice for that purpose, contrary to what is sometimes suggested in introductory courses. The reason for the necessity of a complete set of eigenstates lies within the interpretation of quantum mechanics, as illustrated in the following example of a Hamiltonian $\hat{H}$ with discrete spectrum. If the Hamiltonian is indeed self-adjoint and thus has a complete set of eigenstates $\{|\psi_n\rangle\}_{n\in\mathbb{N}}$ with corresponding energy eigenvalues E_n, $\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle$, then every physical state $|\Psi\rangle$ can be expanded as

$$|\Psi\rangle = \sum_n c_n\,|\psi_n\rangle\,. \tag{1.7}$$

According to the Copenhagen interpretation of quantum mechanics, a physical measurement of the energy would yield E_n with probability $|c_n|^2$, which also implies the normalization requirement $\sum_n |c_n|^2 = 1$ [3]. Hence, completeness (and the reality of the eigenvalues) prevents physical measurements from being ill-defined in this interpretation.

Now consider an operator $\hat{A}$ with domain $D(\hat{A})$ in a Hilbert space $\mathcal{H}$. The adjoint $\hat{A}^\dagger$ of $\hat{A}$ is defined such that

$$\langle\hat{A}^\dagger\chi|\Psi\rangle = \langle\chi|\hat{A}\Psi\rangle \tag{1.8}$$

for all $|\chi\rangle$ and $|\Psi\rangle$. As such, $\hat{A}^\dagger$ acts upon bras, whereas $\hat{A}$ acts upon kets, and they do not necessarily have the same domains as they can be regarded as two separate operators.
The operator $\hat{A}$ is said to be Hermitean (or symmetric) if

$$\langle\hat{A}\chi|\Psi\rangle = \langle\chi|\hat{A}\Psi\rangle\,, \tag{1.9}$$

or equivalently, $\hat{A}^\dagger = \hat{A}$, i.e. the action of the operator and its adjoint is the same when acting on wave functions in $D(\hat{A})$.

In finite-dimensional Hilbert spaces, operators can be represented by matrices, which can act upon every vector in Hilbert space. In infinite-dimensional Hilbert spaces, containing, for example, functions on a continuous but finite interval or the real axis, an operator $\hat{A}$ may not be able to act on the entire Hilbert space: $D(\hat{A}) \subsetneq \mathcal{H}$.
Furthermore, a Hermitean operator $\hat{A}$ is said to be self-adjoint if and only if it satisfies

$$D(\hat{A}^\dagger) = D(\hat{A}), \tag{1.10}$$

i.e. it is Hermitean and the domain coincides with the domain of its adjoint.
From the above considerations, it is clear that in finite-dimensional Hilbert spaces, the two properties are the same. In infinite-dimensional spaces, this is generally not the case. This subtlety already arises in the treatment of the particle in a box under general conditions.

1.4 Ehrenfest Theorem in the Infinite Volume

In the last part of this thesis, the validity of the Ehrenfest theorem for a particle in a box will be thoroughly analyzed. For now, the theorem for a system in the infinite volume and thus without boundaries will be stated and proved.
Let $\hat{A}$ be a self-adjoint operator with domain $D(\hat{A})$ and let $|\Psi(t)\rangle \in D(\hat{A}) \cap D(\hat{H})$ be a wave function upon which $\hat{A}$ and $\hat{H}$ can act. Here, one should also assume that $\hat{H}\,|\Psi(t)\rangle \in D(\hat{A})$ and $\hat{A}\,|\Psi(t)\rangle \in D(\hat{H})$ [6]. Ehrenfests theorem then states that the total time derivative of the expectation value of $\hat{A}$ satisfies

$$\frac{d}{dt}\,\langle \hat{A}\rangle = i\,\langle [\hat{H},\hat{A}]\rangle + \langle \partial_t \hat{A}\rangle\,, \tag{1.11}$$

where the commutator

$$[\hat{H},\hat{A}] \equiv \hat{H}\hat{A} - \hat{A}\hat{H} \tag{1.12}$$

is introduced. The proof of this statement is simple and straightforward:
By using the product rule, one immediately finds

$$\frac{d}{dt}\,\langle \hat{A}\rangle = \frac{d}{dt}\,\langle \Psi(t)|\hat{A}|\Psi(t)\rangle = \langle \partial_t\Psi(t)|\hat{A}|\Psi(t)\rangle + \langle \Psi(t)|\partial_t\hat{A}|\Psi(t)\rangle + \langle \Psi(t)|\hat{A}|\partial_t\Psi(t)\rangle \tag{1.13}$$

The time-dependent Schrödinger equation (1.1) implies $\partial_t\,|\Psi(t)\rangle = -i\hat{H}\,|\Psi(t)\rangle$, and by exploiting the properties of the complex scalar product and the definition of expectation values, this reduces the above expression to

$$\frac{d}{dt}\,\langle \hat{A}\rangle = i\left(\langle \hat{H}\Psi(t)|\hat{A}|\Psi(t)\rangle - \langle \Psi(t)|\hat{A}|\hat{H}\Psi(t)\rangle\right) + \langle \partial_t\hat{A}\rangle\,. \tag{1.14}$$

Lastly, by using that the Hamiltonian is assumed to be Hermitean (1.9), one obtains

$$\frac{d}{dt}\,\langle \hat{A}\rangle = i\,\langle \Psi(t)|\hat{H}\hat{A} - \hat{A}\hat{H}|\Psi(t)\rangle + \langle \partial_t\hat{A}\rangle = i\,\langle [\hat{H},\hat{A}]\rangle + \langle \partial_t\hat{A}\rangle\,, \tag{1.15}$$

which proves the assertion. Notice however that the commutator is only well-defined due to the assumptions $\hat{H}\,|\Psi(t)\rangle \in D(\hat{A})$ and $\hat{A}\,|\Psi(t)\rangle \in D(\hat{H})$. If this is not the case, [6] gives an alternative expression that does not involve commutators.

So far, the relation to the infinite volume has not yet been drawn. In such a system, there are no boundary conditions that further restrict the domains of the considered operators. In a lot of cases, one chooses $\hat{A} \in \{\hat{x},\hat{p},\hat{H}\}$, and these operators have compatible domains in the infinite volume such that the commutators in (1.11) are well-defined.

One case that will be of particular interest is $\hat{A} = \hat{x}$. As $\hat{x}$ does not explicitly depend on time, only the commutator term remains. If one assumes a Hamiltonian of the form

$$\hat{H} = -\frac{1}{2M}\,\partial_x^2 + V(x) = \frac{\hat{p}^2}{2M} + V(x) \tag{1.16}$$

and uses the common relation $[\hat{p},\hat{x}] = -i$, one retrieves

$$[\hat{H},\hat{x}] = \frac{1}{2M}[\hat{p}^2,\hat{x}] = \frac{1}{2M}(\hat{p}[\hat{p},\hat{x}] + [\hat{p},\hat{x}]\hat{p}]) = -\frac{i}{M}\hat{p}. \tag{1.17}$$

Inserting all these relations into (1.11), one finally obtains

$$M\frac{d\,\langle \hat{x}\rangle}{dt} = \langle \hat{p}\rangle\,, \tag{1.18}$$

which is nothing else but the quantum mechanical analogue of the classical relation between position and momentum.

Chapter 2

The Hamiltonian for a Particle in a Box

In this chapter, the standard textbook problem of a particle with mass M confined to a finite interval $\Omega = [-L/2, L/2]$, but otherwise experiencing no potential, is revisited. Such a potential is given by

$$V(x) = \begin{cases} 0, & x \in \Omega \\ \infty, & \text{else} \end{cases} \tag{2.1}$$

and the corresponding Hamilton operator of the system is

$$H = -\frac{1}{2M}\partial_x^2 + V(x). \tag{2.2}$$

The form of the potential immediately requires that the wave function solving the time-independent Schrödinger equation

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle \tag{2.3}$$

vanishes for $|x| > L/2$. The boundary conditions $\Psi(x)$ should satisfy at $x = \pm L/2$, however, are not determined by the potential. It is the requirement of self-adjointness that will lead to appropriate boundary conditions. In the standard treatment, one requires that the wave function vanishes at the boundaries $\Psi(\pm L/2) = 0$ in order to keep the wave function continuous. Nonetheless, this requirement is no necessity from a physical point of view, and the reason for this will be discussed in this chapter.

Therefore, in the next step, the most general boundary conditions which guarantee that $\hat{H}$ is self-adjoint will be motivated. In several examples, the spectrum of $\hat{H}$ will be derived in order to illustrate its dependence on the so-called extension parameters that appear in the boundary conditions. The procedure closely follows the one presented in [1] as well as in [2].

2.1 Self-Adjointness and Robin Boundary Conditions

Before one checks for self-adjointness of $\hat{H}$, one will have to verify Hermiticity. Using partial integration twice, one can check whether $\hat{H}$ satisfies (1.9). The explicit calculation gives

$$\begin{aligned}
\langle\chi|\hat{H}\Psi\rangle &= -\frac{1}{2M}\int_{-L/2}^{L/2} dx\,\chi(x)^*\partial_x^2\Psi(x) \\
&= -\frac{1}{2M}[\chi^*(x)\partial_x\Psi(x)]\Big|_{-L/2}^{L/2} + \frac{1}{2M}\int_{-L/2}^{L/2} dx\,\partial_x\chi(x)^*\partial_x\Psi(x) \\
&= -\frac{1}{2M}[\chi(x)^*\partial_x\Psi(x) - \partial_x\chi(x)^*\Psi(x)]\Big|_{-L/2}^{L/2} - \frac{1}{2M}\int_{-L/2}^{L/2} dx\,\partial_x^2\chi(x)^*\Psi(x) \\
&= -\frac{1}{2M}[\chi(x)^*\partial_x\Psi(x) - \partial_x\chi(x)^*\Psi(x)]\Big|_{-L/2}^{L/2} + \langle\hat{H}\chi|\Psi\rangle
\end{aligned} \tag{2.4}$$

In order for $\hat{H}$ to be Hermitean, this leads to the condition

$$[\chi(x)^*\partial_x\Psi(x) - \partial_x\chi(x)^*\Psi(x)]\Big|_{-L/2}^{L/2} = 0. \tag{2.5}$$

In this treatment, the two boundaries should be considered as two independent points in space, hence the most general, physical boundary conditions cannot connect the wave function at these two points, i.e. they should be *local*. Furthermore, due to the linearity of quantum mechanics, the conditions should as well be *linear* and only contain derivatives of at most first order, as higher orders do not appear in the condition (2.5). This naturally leads to the most general so-called Robin[1] boundary conditions [2]:

$$\gamma_\pm\Psi(\pm L/2) \pm \partial_x\Psi(\pm L/2) = 0, \qquad \gamma_\pm \in \mathbb{C}. \tag{2.6}$$

Notice that these conditions only restrict the domain $D(\hat{H})$, not $D(\hat{H}^\dagger)$.
If one would assume $\gamma_\pm \in \mathbb{R}$, then these are exactly the conditions that imply that the probability current

$$j(x) = \frac{1}{2Mi}(\Psi(x)^*\partial_x\Psi(x) - \partial_x\Psi(x)^*\Psi(x)) \tag{2.7}$$

does not leak outside the box, $j(\pm L/2) = 0$ [1]. From a physical point of view, this is the only necessary constraint on the boundary conditions, as probability must be conserved.

Inserting the Robin boundary conditions in (1.9), one finds

$$[\partial_x\chi(L/2)^* + \gamma_+\chi(L/2)^*]\Psi(L/2) - [\partial_x\chi(-L/2)^* - \gamma_-\chi(-L/2)^*]\Psi(-L/2) = 0. \tag{2.8}$$

As the values $\Psi(\pm L/2)$ are still unrestricted, this requires

$$\gamma_+^*\chi(L/2) + \partial_x\chi(L/2) = 0, \qquad \gamma_-^*\chi(-L/2) - \partial_x\chi(-L/2) = 0, \tag{2.9}$$

which are identically the conditions (2.6) for $\langle\chi| \in D(\hat{H}^\dagger)$ but with parameters $\gamma_\pm^*$. Until now, the domains $D(\hat{H})$ and $D(\hat{H}^\dagger)$ contain the functions whose second derivatives are square-integrable and which satisfy (2.6) or (2.9) respectively. In order for $\hat{H}$ to be self-adjoint, the two domains must coincide, $D(\hat{H}) = D(\hat{H}^\dagger)$, which implies

$$\gamma_\pm = \gamma_\pm^* \quad \Rightarrow \quad \gamma_\pm \in \mathbb{R}. \tag{2.10}$$

At this point, one has come full circle: the self-adjointness of $\hat{H}$ is what guarantees the conservation of probability.

The two real-valued parameters $\gamma_\pm$ characterize a 2-parameter family of so-called self-adjoint extensions of $\hat{H}$ – each choice of $\gamma_\pm$ gives rise to a new physical situation. The textbook case with $\Psi(\pm L/2) = 0$ results from choosing $\gamma_\pm \to \infty$, also referred to as Dirichlet[2] boundary conditions. Another frequently used special case of (2.6) is $\gamma_\pm = 0$, which implies $\partial_x\Psi(\pm L/2) = 0$ and which are known as Neumann[3] boundary conditions.

[1] Victor Gustave Robin (1855-1897), French mathematician.
[2] Johann Peter Gustav Lejeune Dirichlet (1805-1859), German mathematician.
[3] Karl Gottfried Neumann (1832-1925), German mathematician.

2.2 Quantization Conditions

With the appropriate boundary conditions (2.6), one is now in a position to solve (2.3)

$$\begin{aligned} \partial_x^2\Psi(x) + 2ME\Psi(x) = 0, \qquad & x \in \Omega, \\ \gamma_\pm\Psi(x) \pm \partial_x\Psi(x) = 0, \qquad & x = \pm L/2. \end{aligned} \tag{2.11}$$

Before one actually does that, it is useful to first consider what implications the boundary conditions have on the energy spectrum. The first striking implication is that not only strictly positive energies are allowed, but also negative or zero energy eigenstates can arise, as will be shown below. The physical interpretation of such states will be discussed in section 2.3. For now, the infinite number of positive energy eigenvalues will be considered with respect to their quantization condition. Furthermore, the extension parameter combinations for which there are zero-energy eigenstates shall be determined.

Starting with $E > 0$, the general solution to (2.11) is

$$\Psi(x) = A\exp(ikx) + B\exp(-ikx), \qquad k = \sqrt{2ME} > 0. \tag{2.12}$$

Imposing both boundary conditions, a straightforward calculation[4] leads to a quantization condition for k:

$$\exp(2ikL) = \frac{(\gamma_+ - ik)(\gamma_- - ik)}{(\gamma_+ + ik)(\gamma_- + ik)} \in S^1 = \{z \in \mathbb{C} : |z| = 1\}. \tag{2.13}$$

In the case of Dirichlet boundary conditions, $\gamma_\pm \to \infty$, one immediately obtains the usual result:

$$\exp(2ikL) = 1 = \exp(2in\pi), \quad n \in \mathbb{Z} \quad \Rightarrow k = \frac{\pi}{L}n, \quad E_n = \frac{\pi^2 n^2}{2ML^2}, \quad n \in \mathbb{N}^{>0}. \tag{2.14}$$

Consider now $E = 0$. The general solution to

$$\partial_x^2\Psi(x) = 0 \tag{2.15}$$

is obviously

$$\Psi(x) = Ax + B, \qquad A, B \in \mathbb{C}. \tag{2.16}$$

By again imposing the boundary conditions, one finds

$$\begin{aligned} \gamma_-\left(-\frac{AL}{2} + B\right) - A = 0, \\ \gamma_+\left(\frac{AL}{2} + B\right) + A = 0. \end{aligned} \tag{2.17}$$

These equations imply

$$\gamma_+\gamma_- L + \gamma_+ + \gamma_- = 0, \tag{2.18}$$

which is the condition onto $\gamma_\pm$ for the existence of an energy eigenstate with $E = 0$.

In particular, Dirichlet boundary conditions would imply $L = 0$, and hence they do not allow a zero-energy eigenstate. Neumann conditions, on the other hand, satisfy (2.18), and the corresponding constant eigenstate is

$$\Psi(x) = \frac{1}{\sqrt{L}}. \tag{2.19}$$

[4] See Appendix A.1

2.3 Spectra and Eigenstates of the Hamiltonian

At this point, different extension parameter combinations are investigated and the corresponding spectra and eigenfunctions are derived. In section 2.3.1, the results from a case treated in [1] are very briefly summarized, and the presented procedure is extended to the subsequent cases in more detail, leading to rather surprising results.

2.3.1 Parity Preserving Boundary Conditions: $\gamma_+ = \gamma_-$

The most natural and intuitive choice of extension parameters is probably the one that preserves spatial parity. In this case, both walls of the box behave in the same way, and they thus contribute the same parameter: $\gamma_+ = \gamma_- \equiv \gamma \in \mathbb{R}$. As the system is symmetric under parity, one may immediately choose even or odd eigenfunctions [1].
For $E = k_n^2/2M > 0$, the even solutions are

$$\Psi_n(x) = A\cos(k_n x), \qquad n \in \{0, 2, 4, ...\}. \tag{2.20}$$

By imposing the boundary conditions in (2.11) or by carefully exploiting (2.13), one finds that the k_n satisfy

$$\frac{\gamma}{k_n} = \tan\left(\frac{k_n L}{2}\right). \tag{2.21}$$

Similarly, the odd solutions

$$\Psi_n(x) = A\sin(k_n x), \qquad n \in \{1, 3, 5, ...\} \tag{2.22}$$

imply

$$\frac{\gamma}{k_n} = -\cot\left(\frac{k_n L}{2}\right). \tag{2.23}$$

The two transcendental equations (2.21) and (2.23) are easily solved in two special cases, namely those with Dirichlet or Neumann boundary conditions:

$$\begin{aligned} \gamma \to \infty \Rightarrow k_n &= \frac{\pi}{L} n, \qquad n \in \{1, 2, 3, ...\}, \\ \gamma = 0 \Rightarrow k_n &= \frac{\pi}{L} n, \qquad n \in \{0, 1, 2, ...\}. \end{aligned} \tag{2.24}$$

For arbitrary γ, numerically solving these equations shows that $k_n(\gamma)$ is a strictly increasing function, for which [1] gives an analytical proof.

The next thing to consider are eigenstates with $E = 0$. Here, the condition (2.18) reduces to

$$\gamma(\gamma L + 2) = 0. \tag{2.25}$$

Hence, such eigenstates only exist for $\gamma = 0$ or $\gamma = -2/L$. Imposing the boundary conditions onto the general solution (2.16) and normalizing the wave function, one straightforwardly obtains

$$\begin{aligned} \gamma = 0 &\Rightarrow \Psi_{E=0}(x) = \frac{1}{\sqrt{L}}, \\ \gamma = -\frac{2}{L} &\Rightarrow \Psi_{E=0}(x) = \sqrt{\frac{12}{L^3}}\, x. \end{aligned} \tag{2.26}$$

These linear wave functions are a first new feature to which general Robin boundary conditions have led.

Lastly, one can consider eigenstates with $E < 0$. The equation

$$\partial_x^2 \Psi(x) - \kappa^2 \Psi(x) = 0, \qquad \kappa^2 = -2ME > 0 \tag{2.27}$$

has the general solution

$$\Psi(x) = A\exp(\kappa x) + B\exp(-\kappa x), \tag{2.28}$$

which gives rise to the even and odd combinations

$$\Psi^e_{E<0}(x) = A\cosh(\kappa x), \qquad \Psi^o_{E<0}(x) = A\sinh(\kappa x). \tag{2.29}$$

Analogous to what was done before, the even eigenstate implies

$$\frac{\gamma}{\kappa} = -\tanh\left(\frac{\kappa L}{2}\right), \tag{2.30}$$

which has exactly one positive solution for $\gamma < 0$. The odd eigenstate, on the other hand, leads to

$$\frac{\gamma}{\kappa} = -\coth\left(\frac{\kappa L}{2}\right), \tag{2.31}$$

which only has exactly one positive solution for $\gamma < -2/L$.
One thus sees that for $\gamma < -2/L$, there are two states with negative energy, and the energy diverges to negative infinity for $\gamma \to -\infty$ [1]. The behavior of such eigenstates is analyzed in more detail in the subsequent sections.

2.3.2 Partial Neumann Boundary Conditions: $\gamma_- = 0$

In a second example, Neumann boundary conditions are fixed at the left boundary, $\gamma_- = 0$ and hence $\partial_x\Psi(-L/2) = 0$, whilst the other parameter is arbitrary, $\gamma_+ \equiv \gamma$. This situation does in general not preserve parity, and one should not expect eigenstates of purely even or odd parity.

For the eigenstates with $E > 0$, one can use (2.13) with $\gamma_- = 0$ to obtain the quantization condition

$$\exp(2ikL) = -\frac{\gamma - ik}{\gamma + ik}. \tag{2.32}$$

Rearranging this equation, one finds

$$\frac{\gamma}{k} = \tan(kL). \tag{2.33}$$

The solutions in the case $\gamma = 0$ have already been found to be integer multiples of π/L. For $\gamma \to \infty$, however, the possible values of k and the corresponding energies are

$$k_n = \frac{\pi}{L}\left(n + \tfrac{1}{2}\right), \qquad E_n = \frac{\pi^2\left(n+\frac{1}{2}\right)^2}{2ML^2}, \qquad n \in \{0, 1, 2, ...\}, \tag{2.34}$$

i.e. the spectrum is quantized in terms of odd multiples of a half.
The condition (2.18) for the existence of a zero-energy eigenstate reduces to $\gamma = 0$, hence, only then there is such a state.

When it comes to $E < 0$, one starts off with the general solution

$$\Psi(x) = A\exp(\kappa x) + B\exp(-\kappa x). \tag{2.35}$$

If one imposes $\partial_x\Psi(-L/2) = 0$, one finds

$$\kappa\left(A\exp\left(-\frac{\kappa L}{2}\right) - B\exp\left(\frac{\kappa L}{2}\right)\right) = 0 \Rightarrow A = \exp(\kappa L)B. \tag{2.36}$$

By further requiring $\gamma_+\Psi(L/2) + \partial_x\Psi(L/2) = 0$ and using the relation between A and B, the condition on κ is found:

$$\gamma_+\Psi(L/2) + \partial_x\Psi(L/2) = 0, \quad A = \exp(\kappa L)B \Rightarrow \frac{\gamma}{\kappa} = -\tanh(\kappa L). \tag{2.37}$$

As $\kappa > 0$, there is exactly one solution for κ if and only if $\gamma < 0$, which approaches negative infinity as $\gamma \to -\infty$. For $\gamma > 0$, there are no eigenstates with negative energy. The energy spectrum as a function of $\arctan(\gamma L) \in [-\pi/2, \pi/2]$ (which is equivalent to $\gamma \in [-\infty, \infty]$) is shown in Fig. 2.1. It is obvious to see that E_n is again a strictly increasing function of γ for all n. Apart from the additional negative energy ground state, the spectrum for $\gamma \to -\infty$ is the same as for $\gamma \to \infty$.

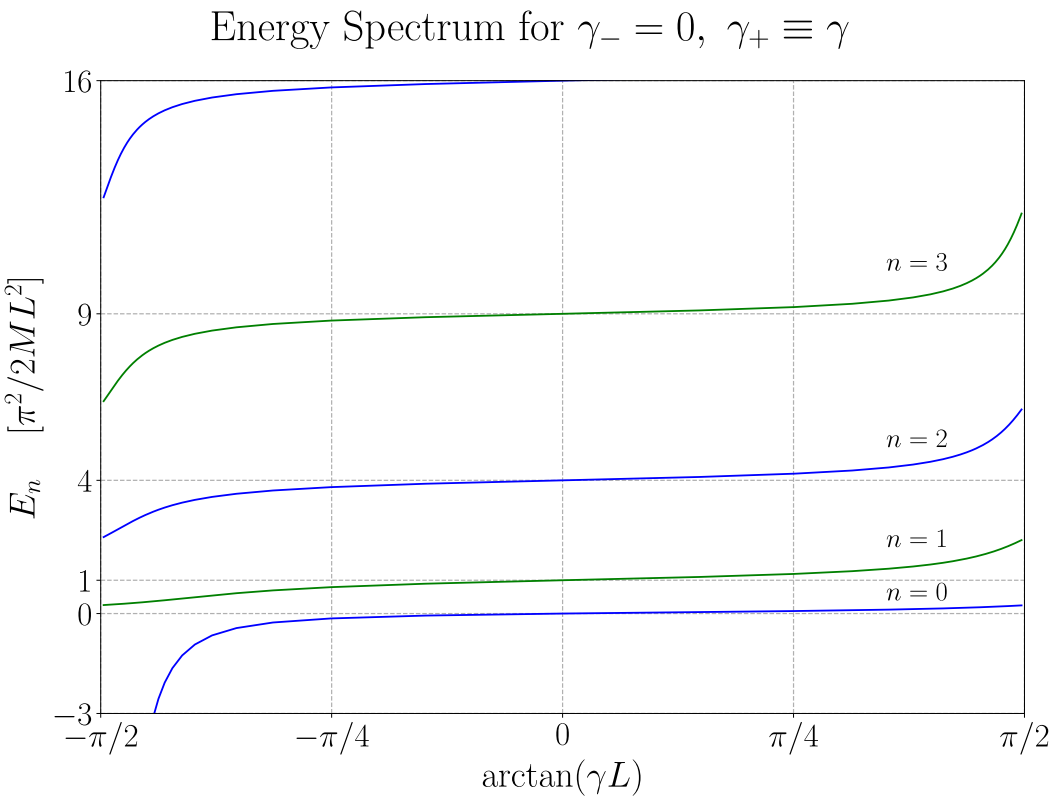


Figure 2.1: Energy spectrum in the case $\gamma_- = 0,\ \gamma_+ \equiv \gamma$ for $n \in \{0, 1, 2, 3, 4\}$, as a function of $\arctan(\gamma L)$ found by numerically solving (2.33) and (2.37).

Of further interest are the explicit eigenstates. Starting with $E > 0$ and the general solution $\Psi_n(x) = A\exp(ik_n x) + B\exp(-ik_n x)$, the boundary condition on the left side implies[5]

$$ik_n\left(A\exp\left(-\frac{ik_nL}{2}\right) - B\exp\left(\frac{ik_nL}{2}\right)\right) = 0 \Rightarrow A = \exp(ik_nL)B. \tag{2.38}$$

Having said that, one retrieves

$$\begin{aligned}\Psi_n(x) &= A\exp(ik_nx) + B\exp(-ik_nx) = B(\exp(ik_n(x+L) + \exp(-ik_nx)) \\ &= B\exp\left(\frac{ik_nL}{2}\right)\left(\exp\left(ik_n\left(x+\tfrac{L}{2}\right)\right) + \exp\left(-ik_n\left(x+\tfrac{L}{2}\right)\right)\right) \\ &= C\cos\left(k_n\left(x+\tfrac{L}{2}\right)\right).\end{aligned} \tag{2.39}$$

By now requiring normalization, $\langle\Psi_n|\Psi_n\rangle = 1$, C can be determined to find

$$\Psi_n(x) = \sqrt{\frac{2k_n}{k_nL + \sin(k_nL)\cos(k_nL)}}\cos\left(k_n\left(x+\tfrac{L}{2}\right)\right). \tag{2.40}$$

The $E = 0$ eigenstate follows directly from

$$\Psi_0(x) = Ax + B, \quad \partial_x\Psi(L/2) = A = 0 \Rightarrow \Psi_0(x) = B = \frac{1}{\sqrt{L}}. \tag{2.41}$$

[5]Notice that applying the second boundary condition would only lead to condition (2.32).

by normalization.
Lastly, where it exists, the single eigenstate with negative energy is found by recalling (2.36):

$$\begin{aligned}\Psi_0(x) &= A\exp(\kappa x) + B\exp(-\kappa x) = B(\exp(\kappa(x+L)) + \exp(-\kappa x)) \\ &= B\exp\left(\frac{\kappa L}{2}\right)\left(\exp\left(\kappa\left(x+\tfrac{L}{2}\right)\right) + \exp\left(-\kappa\left(x+\tfrac{L}{2}\right)\right)\right) \\ &= C\cosh\left(\kappa\left(x+\tfrac{L}{2}\right)\right).\end{aligned} \tag{2.42}$$

As before, normalization determines C and implies

$$\Psi_0(x) = \sqrt{\frac{4\kappa}{2\kappa L + \sinh(\kappa L)}}\cosh\left(\kappa\left(x+\tfrac{L}{2}\right)\right). \tag{2.43}$$

The first few eigenstates for different values of γ are illustrated in Fig. 2.2. The column with $\gamma = -1/L$ is included purely to show the functional form of the ground state for negative but finite γ. Other than that, it doesn't present any specialty.

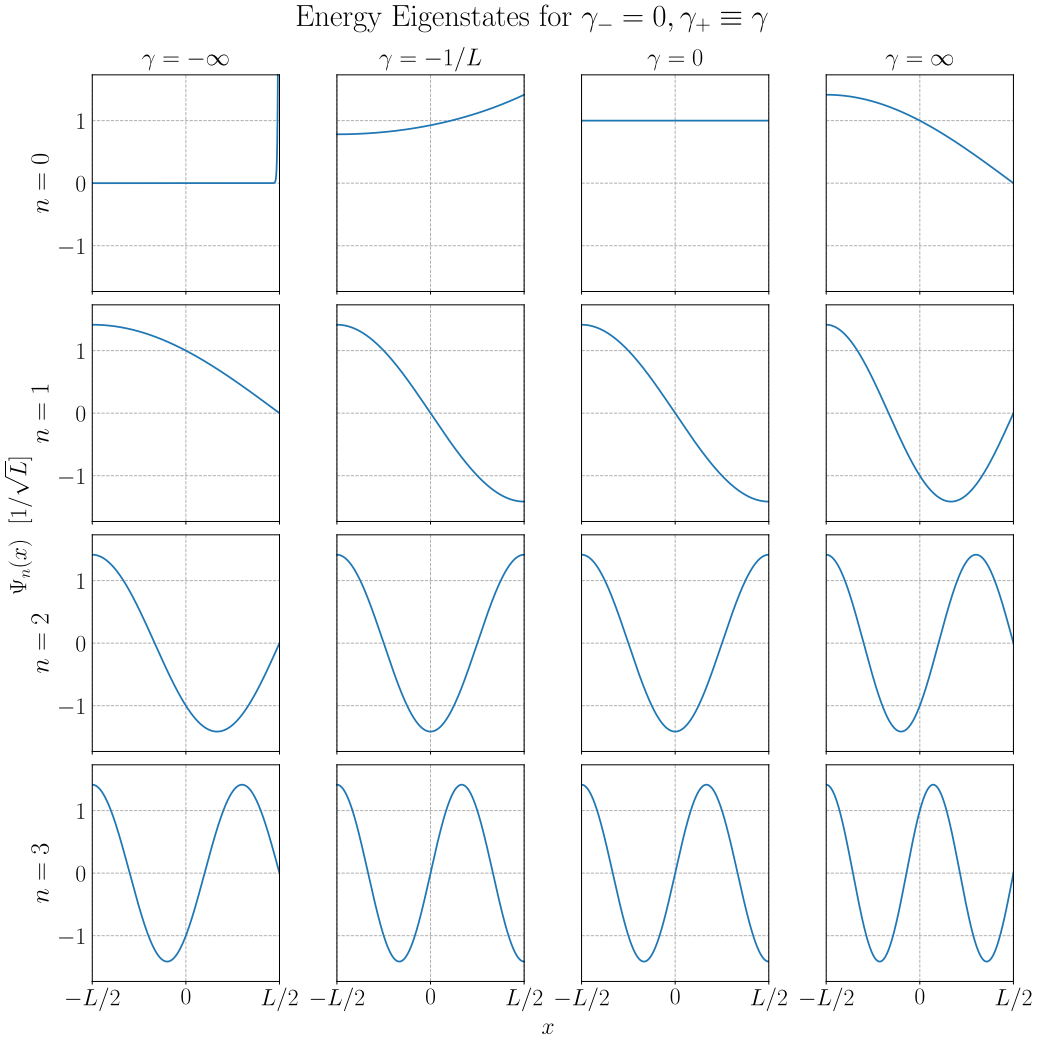


Figure 2.2: The first four energy eigenstates in case of $\gamma_- = 0, \gamma_+ \equiv \gamma$. Notice that the y-axis is in units of $1/\sqrt{L}$. Rather remarkable are the ground states for $\gamma \leq 0$, as they do not present the usual oscillatory behavior. The ground state for $\gamma \to -\infty$ resembles a δ-function that is localized at the right boundary.

As was to be expected from the energy spectrum, the eigenstates in the cases $\gamma \to \infty$ and $\gamma \to -\infty$ differ only with respect to the additional ground state with negative energy. For large but finite negative γ, the ground state seems to represent a particle that "sticks" to the wall and has a large negative energy. In the actual limit $\gamma \to -\infty$, the wave function somewhat degenerates in a δ-function-like fashion since

$$\begin{aligned} \lim_{\gamma\to-\infty} \Psi_0(x) = 0 \quad \forall\ x \in [-L/2, L/2), \\ \lim_{\gamma\to-\infty} \langle\Psi_0|\Psi_0\rangle = 1. \end{aligned} \tag{2.44}$$

For this reason, it is difficult to say how meaningful the ground state is in this limit from a physical point of view. For finite γ, however, there is nothing that prevents one from saying that the particle is simply localized close to the wall of the box.

2.3.3 The Special Case $\gamma_- = -\gamma_+$

The so far treated cases both showed energy eigenvalues E_n that were strictly monotonously increasing with γ. To show that this is not necessarily true for all choices of extension parameters, one can just consider the still quite natural case $\gamma_+ = -\gamma_- \equiv \gamma$. Although this last example is somewhat similar to the parity conserving case, it leads to rather different results.

First, consider $E > 0$. For $\gamma_+ = -\gamma_-$, eq. (2.13) simplifies tremendously,

$$\exp(2ikL) = 1 \Rightarrow k = \frac{\pi}{L}n, \quad n \in \{1, 2, 3, ...\}. \tag{2.45}$$

Contrary to the case that preserves parity, the condition $\exp(2ikL) = 1$ arises independent of γ, not only for $\gamma \to \pm\infty$. Therefore, the positive energy spectrum does not depend on γ.

Second, to give rise to an $E = 0$ eigenstate, the condition to satisfy (2.18) reduces to

$$\gamma^2 L = 0 \Rightarrow \gamma = 0, \tag{2.46}$$

which gives the known result for Neumann boundary conditions.

Lastly, to obtain the eigenstates with $E < 0$, one again starts with the general solution (2.35) and imposes the boundary conditions:

$$\begin{aligned} \gamma\left(A\exp\left(\frac{\kappa L}{2}\right) + B\exp\left(-\frac{\kappa L}{2}\right)\right) + \kappa\left(A\exp\left(\frac{\kappa L}{2}\right) - B\exp\left(-\frac{\kappa L}{2}\right)\right) = 0, \\ \gamma\left(A\exp\left(-\frac{\kappa L}{2}\right) + B\exp\left(\frac{\kappa L}{2}\right)\right) + \kappa\left(A\exp\left(-\frac{\kappa L}{2}\right) - B\exp\left(\frac{\kappa L}{2}\right)\right) = 0. \end{aligned} \tag{2.47}$$

Once adding and once subtracting these equations from each other, one finds

$$\begin{aligned} (\gamma(A+B) + \kappa(A-B))\cosh\left(\frac{\kappa L}{2}\right) = 0, \\ (\gamma(A+B) + \kappa(A-B))\sinh\left(\frac{\kappa L}{2}\right) = 0. \end{aligned} \tag{2.48}$$

This immediately implies

$$\gamma(A+B) + \kappa(A-B) = 0 \quad \overset{(*)}{\Rightarrow} \quad \kappa = \frac{\gamma(A+B)}{(B-A)}. \tag{2.49}$$

In the implication (*), it was used that $A \neq B$, as this would eventually lead to $\kappa = 0$, which is not possible by assumption. Inserting (2.49) in one of the equations (2.47), one then obtains

$$\frac{\gamma AB}{B-A}\sinh\left(\frac{\kappa L}{2}\right) = 0 \quad \Rightarrow \quad A = 0 \vee B = 0 \quad \overset{(2.49)}{\Rightarrow} 0 < \kappa = \pm\gamma. \tag{2.50}$$

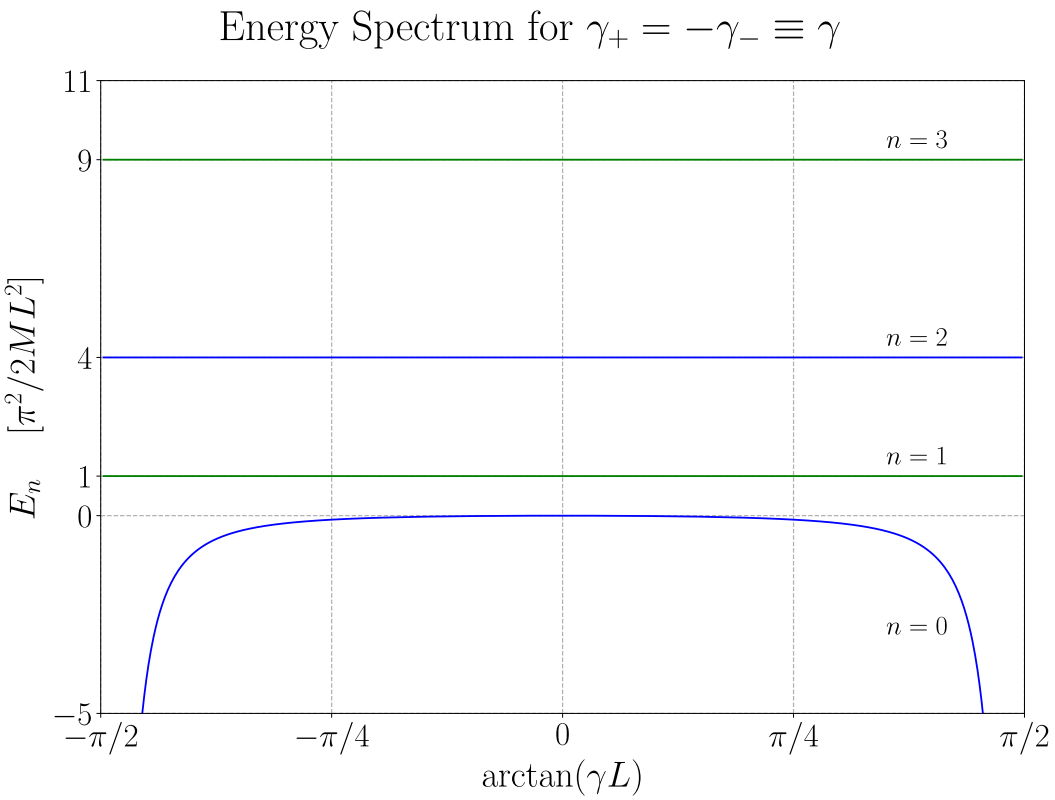


Figure 2.3: Energy spectrum for $\gamma_+ = -\gamma_- \equiv \gamma$ as a function of $\arctan(\gamma L)$.

Hence, there is a negative energy state for all $\gamma \neq 0$. The first few eigenvalues of the spectrum as a function of $\arctan(\gamma L)$ are illustrated in Fig. 2.3.
Whilst the positive energies are independent of γ, the negative energies of the spectrum behave like $E_0 = -\gamma^2/2M$. In particular, this shows a completely different behavior than what was seen for $\gamma_+ = \gamma_-$.

The last goal of this chapter is to derive the corresponding eigenstates. Starting with the positive energy eigenstates $\Psi_n(x) = A\exp(ik_n x) + B\exp(-ik_n x)$, one uses the boundary condition at $x = L/2$ to obtain

$$\gamma\left(A\exp\left(\frac{ik_nL}{2}\right) + B\exp\left(-\frac{ik_nL}{2}\right)\right) + \left(A\exp\left(-\frac{ik_nL}{2}\right) - B\exp\left(\frac{ik_nL}{2}\right)\right) = 0$$
$$\Rightarrow B = -(-1)^n\frac{\gamma + ik_n}{\gamma - ik_n}A. \tag{2.51}$$

Since all k_n are integer multiples of π/L irrespective of γ, the normalization is particularly simple:

$$\Psi_n(x) = \frac{1}{\sqrt{2L}}\left(\exp(ik_nx) - (-1)^n\frac{\gamma + ik_n}{\gamma - ik_n}\exp(-ik_nx)\right). \tag{2.52}$$

To obtain the negative energy eigenstate, one reconsiders equations (2.35) and (2.49). If $A = 0$, one finds $\kappa = \gamma$, whilst $B = 0$ implies $\kappa = -\gamma$. In any case, the eigenfunction takes the form $\Psi_0(x) = C\exp(-\gamma x)$. Normalization is straightforward and gives

$$\Psi_0(x) = \sqrt{\frac{\gamma}{\sinh(\gamma L)}}\exp(-\gamma x). \tag{2.53}$$

In the limit $\gamma \to 0$, this reduces to the known constant eigenstate $\Psi_0(x) = 1/\sqrt{L}$ with $E = 0$.

The ground state and the first three excited states are shown in Fig. 2.4 for different values of γ. All the excited states present the familiar oscillatory behavior, whilst all ground states are described by an exponential function. In this case, both limits $\gamma \to \pm\infty$ lead to a degenerate wave function that could be interpreted as being localized at a boundary of the box.

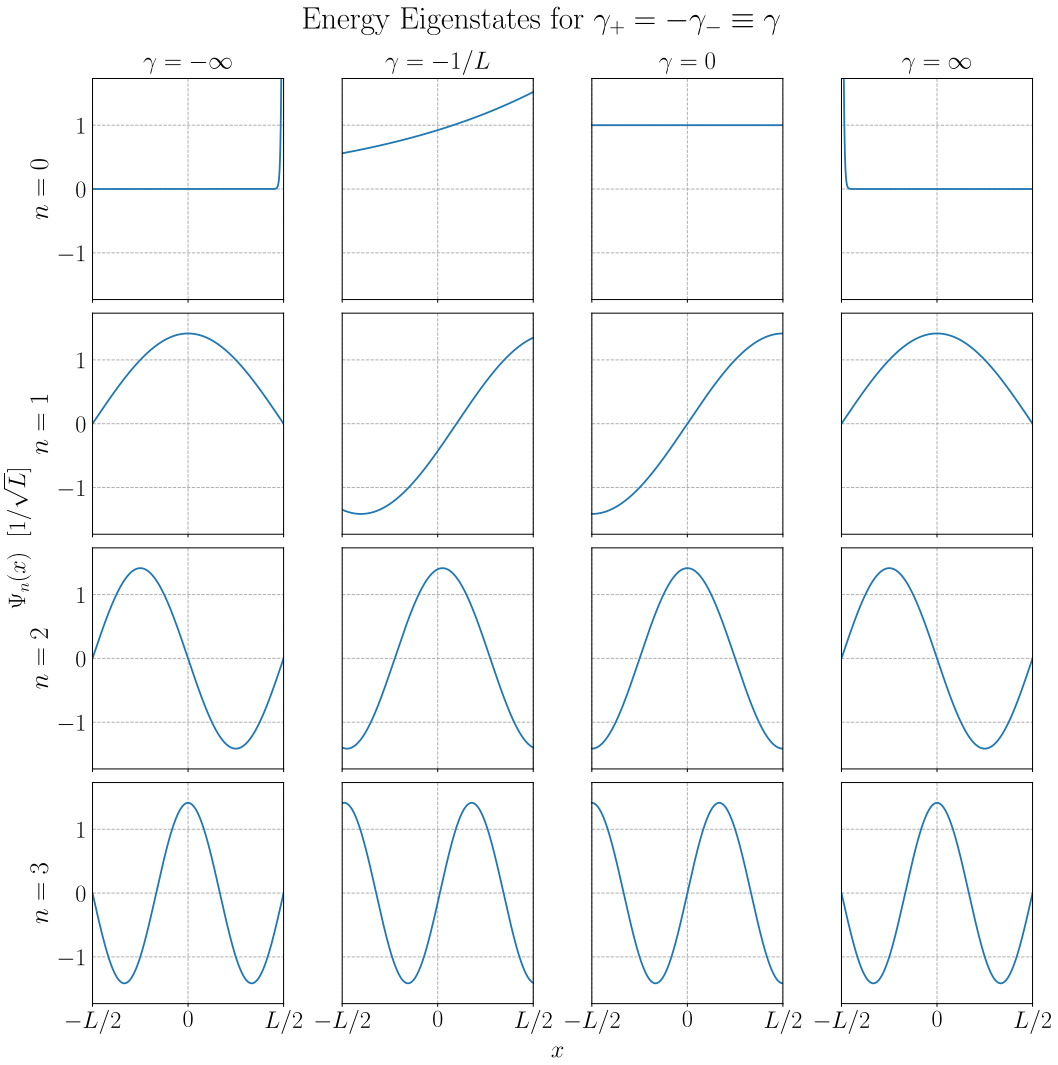


Figure 2.4: First four eigenstates of $\hat{H}$ in the case $\gamma_+ = -\gamma_- \equiv \gamma$. Notice that the y-axis is in units of $1/\sqrt{L}$.

Chapter 3

Momentum for a Particle in a Box

In the previous chapter, the treatment of a particle in a box was generalized in the sense that more general boundary conditions (2.6) were introduced, of which the standard textbook problem is just a special case.
In particular, one of the main results was that the wave function does not need to vanish at the boundaries of the box. Remarkably, this has tremendous implications for the concept of momentum and its operator $\hat{p} = -i\partial_x$, which will be discussed in this chapter.

3.1 Non-Hermiticity of $-i\partial_x$

In the infinite volume, the domains of $\hat{H}$ or $\hat{p}$ are purely determined by differentiability and square-integrability of derivatives; there are no boundary conditions that would further restrict the domain. As the kinetic term of $\hat{H}$ includes a second order derivative while $\hat{p}$ only contains one of first order, the domain of $\hat{H}$ certainly lies within the domain of $\hat{p}$. In particular, $\hat{H}$ is Hermitean within $D(\hat{p})$, which is shown in most quantum mechanics lectures.

Whether this assertion is true in the finite box can easily be checked. Let $|\Psi\rangle\,,\ |\chi\rangle \in D(\hat{H})$ such that they satisfy (2.6). Then

$$\begin{aligned}\langle \hat{p}^\dagger \chi|\Psi\rangle \equiv \langle \chi|\hat{p}\Psi\rangle &= \int_{-L/2}^{L/2} dx\, \chi(x)^*(-i\partial_x)\Psi(x) \\ &= -i[\chi(x)^*\Psi(x)]\Big|_{-L/2}^{L/2} + \int_{-L/2}^{L/2} dx\, (-i\partial_x\chi(x))^*\Psi(x) \\ &= -i[\chi(x)^*\Psi(x)]\Big|_{-L/2}^{L/2} + \langle \hat{p}\chi|\Psi\rangle\,.\end{aligned} \tag{3.1}$$

In order for $\hat{p}$ to be Hermitean, one needs

$$\chi(L/2)^*\Psi(L/2) - \chi(-L/2)^*\Psi(-L/2) = 0. \tag{3.2}$$

In the standard treatment where one sets $\Psi(\pm L/2) = 0$, this condition is satisfied, so $\hat{p}$ is indeed Hermitean. As there would be no further restrictions on $\chi(x)$ since the condition on $\Psi(x)$ is enough to fulfill (3.2), one finds $D(\hat{p}) \subset D(\hat{p}^\dagger)$, and the momentum operator would not be self-adjoint. This renders momentum measurements ill-defined.

For wave functions satisfying (2.6), the values at $x = \pm L/2$ are still arbitrary in general, so (3.2) is not guaranteed to be satisfied. In conclusion, $\hat{p}$ is not even Hermitean within the domain of $\hat{H}$, let alone self-adjoint.

Nevertheless, there are circumstances under which the operator with action $\hat{p} = -i\partial_x$ can be adapted such that it is self-adjoint. As discussed in [1, 7], imposing the *linear* (yet *non-local*) boundary condition

$$\Psi(L/2) = \lambda\Psi(-L/2), \qquad \lambda \in \mathbb{C} \tag{3.3}$$

onto the wave functions within $D(\hat{p})$ leads to a family of self-adjoint extensions of the momentum operator. By inserting this boundary condition into (3.2), one obtains

$$\left(\chi(L/2)^* - \frac{1}{\lambda}\chi(-L/2)^*\right)\Psi(L/2) = 0. \tag{3.4}$$

Again due to the arbitrariness of $\Psi(L/2)$, this requires

$$\chi(L/2) = \frac{1}{\lambda^*}\chi(-L/2), \tag{3.5}$$

which is nothing else but the boundary condition (3.3) with parameter $1/\lambda^*$, restricting $D(\hat{p}^\dagger)$. Similar to the treatment of the Hamiltonian, one now finds

$$D(\hat{p}) = D(\hat{p}^\dagger) \quad \Rightarrow \quad \lambda = \frac{1}{\lambda^*} \quad \Rightarrow \quad |\lambda| = 1. \tag{3.6}$$

Therefore, λ can only be some phase $\exp(i\theta)$ and the probability density $|\Psi|^2$ turns out to be periodic

$$|\Psi(L/2)|^2 = |\exp(i\theta)\Psi(-L/2)|^2 = |\Psi(-L/2)|^2. \tag{3.7}$$

Periodic boundary conditions are thus the only way to obtain a self-adjoint momentum operator with action $-i\partial_x$. Yet, this is no solution to the presented problem, as the goal is to distinguish the boundaries and to not violate locality.

3.2 A New Concept for Momentum

As the usual momentum operator $\hat{p} = -i\partial_x$ is neither self-adjoint nor Hermitean in the most general setting, it is thus of interest to find a momentum operator that is. A first such attempt was made in [2], and it turns out that these newly introduced self-adjoint momentum operator extensions lead to similar results to what one would expect from the usual concept.
In this section, a motivation (rather than a derivation) of this concept will be given, as it is presented in [2].

3.2.1 Motivation of $\hat{p} = \hat{p}_R + i\hat{p}_I$

A possible step to obtain a new candidate for a momentum operator is to discretize the interval Ω by introducing a lattice. In this way, the considered Hilbert space becomes finite-dimensional, the operators become matrices and the difference between Hermiticity and self-adjointness evaporates as discussed in section 1.3. After having a satisfactory treatment of the lattice, one can then try to take the limit where the lattice spacing approaches zero and the lattice turns into the continuous interval, to obtain a corresponding description of the initial situation.
The lattice proposed in [2] takes an odd number N of lattice points with spacing a given by

$$\begin{aligned} x_m = n_m a, \qquad N = \frac{L}{a}, \qquad n_m &\in \left\{-\frac{N-1}{2}, -\frac{N-3}{2}, ..., 0, ..., \frac{N-3}{2}, \frac{N-1}{2}\right\} \\ &= \left\{-\frac{N}{2} + \frac{2m-1}{2} \in \mathbb{Z} \;\middle|\; m \in \{1, 2, ..., N\}\right\}, \end{aligned} \tag{3.8}$$

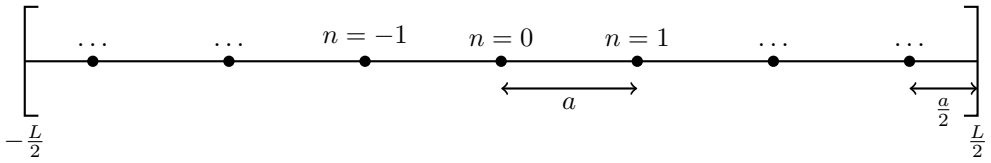


Figure 3.1: Lattice in the interval $\Omega = [-L/2, L/2]$ with $N = 7$ lattice points. By choosing N odd, the boundaries of the interval do not coincide with any lattice points.

and is shown in Fig. 3.1 for $N = 7$.

On such a lattice, the wave function is represented by an N-dimensional vector

$$\langle x|\Psi\rangle = (\Psi_{x_1}\ \Psi_{x_1} \dots \Psi_{x_N})^T \equiv \Psi_x, \tag{3.9}$$

which contains the N values of the wave function on the lattice.
Notice already that one can distinguish between odd and even lattice points (odd and even n_m), which one cannot do in the continuum. This will play an important role in the transition from the lattice to the interval.

To find a suitable momentum operator, one should incorporate a discretized first derivative. As pointed out in [2], one can and has to distinguish between backward (B) and forward (F) derivatives, which take the discretized form

$$\begin{aligned} \Psi'_B(x_m) &\equiv \frac{\Psi(x_m) - \Psi(x_m - a)}{a} \equiv \frac{\Psi_{x_m} - \Psi_{x_{m-1}}}{a}, \\ \Psi'_F(x_m) &\equiv \frac{\Psi(x_m + a) - \Psi(x_m)}{a} \equiv \frac{\Psi_{x_{m+1}} - \Psi_{x_m}}{a}. \end{aligned} \tag{3.10}$$

The operators p_F and p_B representing $(-i)$ times a forward or backward derivative are thus given by the matrices

$$\begin{aligned} \hat{p}_F &= -\frac{i}{a} \begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 & 0 \\ 0 & 0 & -1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -1 & 1 & 0 \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \\ 0 & 0 & 0 & \dots & 0 & 0 & \lambda_+ \end{pmatrix} \\ \hat{p}_B &= -\frac{i}{a} \begin{pmatrix} -\lambda_- & 0 & 0 & \dots & 0 & 0 & 0 \\ -1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & -1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & 0 & \dots & -1 & 1 & 0 \\ 0 & 0 & 0 & \dots & 0 & -1 & 1 \end{pmatrix} \end{aligned} \tag{3.11}$$

The forward derivative at x_N as well as the backward derivative at x_1 are not defined, since they would require non-existing lattice points outside the interval. For this reason, the parameters $\lambda_\pm \in \mathbb{C}$ are introduced to allow for a general but local action of the operator at the boundaries [2]. As will be seen below, these parameters will turn into extension parameters for the momentum operator, analogous to $\gamma_\pm$ for the Hamiltonian.
By considering $(p_{F,B})^\dagger = (p^*_{F,B})^T$, one immediately recognizes that both are not Hermitean[1].

[1] A matrix A is said to be Hermitean if it is equal to its adjoint (which is the complex conjugate of its transpose), $A = A^\dagger \equiv (A^*)^T$

Under the assumption $\lambda_\pm \in i\mathbb{R}$, which will be justified in section 3.2.2, one can use these operators to construct (anti-)Hermitean linear combinations

$$\begin{aligned}
\hat{p}_R &\equiv \frac{1}{4}(\hat{p}_F + \hat{p}_F^\dagger + \hat{p}_B + \hat{p}_B^\dagger) \\
&= -\frac{i}{2a}\begin{pmatrix} -\lambda_- & 1 & 0 & \dots & 0 & 0 & 0 \\ -1 & 0 & 1 & \dots & 0 & 0 & 0 \\ 0 & -1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & 0 & \dots & -1 & 0 & 1 \\ 0 & 0 & 0 & \dots & 0 & -1 & \lambda_+ \end{pmatrix}, \\
i\hat{p}_I &\equiv \frac{1}{4}(\hat{p}_F - \hat{p}_F^\dagger + \hat{p}_B - \hat{p}_B^\dagger) \\
&= \frac{i}{2a}\mathrm{diag}(1, 0, ..., 0, -1).
\end{aligned} \tag{3.12}$$

By construction, $\hat{p}_R$ is Hermitean whilst $i\hat{p}_I$ is anti-Hermitean. Together, they constitute the (non-Hermitean) momentum operator

$$\hat{p} \equiv \frac{\hat{p}_F + \hat{p}_B}{2} = \hat{p}_R + i\hat{p}_I, \tag{3.13}$$

which has a Hermitean component $\hat{p}_R$ and which can be regarded as an averaged forward-backward derivative. In the transition to the continuum, one will see that only $\hat{p}_R$ acts "within the interval", in the sense that $\hat{p}_I$ reduces to δ-functions at the boundaries [2]. For this reason, $\hat{p}_R$ qualifies as the desired physical (i.e. self-adjoint) momentum operator, so one should carefully analyze its properties. Notice that although $i\hat{p}_I$ is anti-Hermitean, $\hat{p}_I$ alone is Hermitean and thus self-adjoint, so it also represents a physical observable which is part of the new momentum concept.

The most important property of $\hat{p}_R$ follows from solving the eigenvalue equation

$$\hat{p}_R\phi_{k,x} = \tilde{k}\phi_{k,x}. \tag{3.14}$$

The eigenstates $\phi_{k,x}$ and eigenvalues $\tilde{k}$ with $x = na$ are given by [2]

$$\begin{aligned}
\tilde{k} &= \frac{\sin(ka)}{a}, \\
\phi_{k,x} &= \begin{cases} A\exp(ikx) + B\exp(-ikx), & n \text{ even}, \\ A\exp(ikx) - B\exp(-ikx), & n \text{ odd}, \end{cases}
\end{aligned} \tag{3.15}$$

where k satisfies the quantization condition

$$\exp(2ikL) = \frac{[1 + \lambda_+\exp(ika)][1 - \lambda_-\exp(ika)]}{[\exp(ika) - \lambda_+][\exp(ika) + \lambda_-]}. \tag{3.16}$$

Remarkably, the eigenfunctions of $\hat{p}_R$ explicitly depend on whether n is even or odd. In order to obtain a corresponding candidate for $\hat{p}_R$ in the continuum, one should try to carry over this distinction between even and odd degrees of freedom. As the real axis cannot be divided into odd and even numbers, this is not straightforward.
The following calculation should by no means be regarded as a rigorous derivation, but rather as a motivation to postulate a new concept for momentum. One way to introduce even and odd degrees of freedom in the continuum is to postulate a two-component wave function

$$\langle x|\Psi\rangle = \Psi(x) = \begin{pmatrix} \Psi_e(x) \\ \Psi_o(x) \end{pmatrix}, \tag{3.17}$$

containing an even and an odd component, which are both functions on Ω. As such, $|\Psi\rangle$ lives in an "extended" or "doubled" Hilbert space $\mathcal{H}_{\text{ext}} = L^2(\Omega) \times \mathbb{C}^2$ of the square-integrable functions on the doubly-covered interval Ω. In this Hilbert space, operators are represented by 2×2-matrices.
To gain an intuition on how the corresponding 2×2-matrix of $\hat{p}_R$ must look, one can consider the limit $a \to 0$ of its action on the components of the wave function. At first, consider the action on a component at a position $x \in (-L/2, L/2)$. In the limit $a \to 0$, this position x corresponds to an $x_m = an_m$ with $m \neq 1, N$ (where one automatically also has $N, m \to \infty$, keeping an_m fixed). If one tries to find the action on the even component, then m must be even such that x_m is an even lattice point[2]. The same is true for the odd component. For an even m, one thus has

$$\hat{p}_R \Psi_e\big|_x = \lim_{a\to0}(\hat{p}_R\Psi_x)_m = -i \lim_{a\to0}\left(\frac{1}{2a}\left(\Psi_{x_{m+1}} - \Psi_{x_{m-1}}\right)\right). \tag{3.18}$$

As $x_{m\pm1} = x_m \pm a$ are odd lattice points, they turn out to be represented by the odd component $\Psi_o(x)$ and one finds

$$\begin{aligned}\frac{1}{2a}\left(\Psi_{x_{m+1}} - \Psi_{x_{m-1}}\right) &= \frac{1}{2a}\left(\Psi_o(x+a) - \Psi_o(x-a)\right)\\ &= \frac{1}{2}\left(\frac{\Psi_o(x+a) - \Psi_o(x)}{a} + \frac{\Psi_o(x) - \Psi_o(x-a)}{a}\right)\\ &\overset{(3.10)}{=} \frac{1}{2}(\Psi'_{o,F}(x) + \Psi'_{o,B}(x)),\end{aligned} \tag{3.19}$$

and therefore

$$\hat{p}_R \Psi_e\big|_x = -i \lim_{a\to0}\left(\frac{1}{2}(\Psi'_{o,F}(x) + \Psi'_{o,B}(x))\right). \tag{3.20}$$

In the limit $a \to 0$, the discrete forward and backward derivatives turn into right-hand and left-hand derivatives, which coincide for differentiable functions. For differentiable $\Psi_o(x)$, one thus obtains

$$\hat{p}_R \Psi_e\big|_x = -i\partial_x \Psi_o\big|_x.$$

Analogously,

$$\hat{p}_R \Psi_o\big|_x = -i\partial_x \Psi_e\big|_x, \tag{3.21}$$

and hence

$$\hat{p}_R = \begin{pmatrix} 0 & -i\partial_x \\ -i\partial_x & 0 \end{pmatrix} = -i\sigma_1\partial_x, \tag{3.22}$$

where σ_1 is known as the first Pauli[3] matrix. The action of $\hat{p}_R$ on the wave function at x_1 and x_N manifests itself in a set of boundary conditions [2], as these points converge to the boundaries for $a \to 0$. The explicit form of the boundary conditions will follow from the requirement that $\hat{p}_R$ should be self-adjoint, which is discussed in section 3.2.2.
The continuum analogue of $\hat{p}_I$ is much more obvious. If one assumes that $(N-1)/2$ is still even such that the outmost lattice points are even, then $\hat{p}_I$ in eq. (3.12) can be represented as [2]

$$\hat{p}_I = \frac{1}{2}\lim_{\epsilon\to0}\begin{pmatrix} \delta(x + \frac{L}{2} - \epsilon) - \delta(x - \frac{L}{2} + \epsilon) & 0 \\ 0 & 0 \end{pmatrix}. \tag{3.23}$$

Using this heuristic motivation, one can *postulate* a new concept for momentum, as is done in [2]. On the Hilbert space $\mathcal{H}_{\text{ext}}$ of two-component wave functions $\Psi(x) = (\Psi_e(x),\ \Psi_o(x))^T$, the momentum operator shall take the form

$$\hat{p} = \hat{p}_R + i\hat{p}_I = \begin{pmatrix} 0 & -i\partial_x \\ -i\partial_x & 0 \end{pmatrix} + \frac{i}{2}\lim_{\epsilon\to0}\begin{pmatrix} \delta(x + \frac{L}{2} - \epsilon) - \delta(x - \frac{L}{2} + \epsilon) & 0 \\ 0 & 0 \end{pmatrix}, \tag{3.24}$$

[2]Simply due to the argument that the even degrees of freedom, namely the even lattice points, should be absorbed in the even component of the continuum wave function.
[3]Wolfgang Ernst Pauli (1900-1958), Austrian physicist.

where only $\hat{p}_R$ is supposed to represent the *physical* (and hence self-adjoint) momentum operator. Whether and under what circumstances $\hat{p}_R$ is indeed self-adjoint will be discussed in the next section.

3.2.2 Self-Adjointness and Extension Parameters

The original momentum operator $\hat{p} = -i\partial_x$ has now been replaced with $\hat{p}_R = -i\sigma_1\partial_x$ which acts in an extended Hilbert space. In this new Hilbert space, the inner product is adapted in the natural way

$$\langle\chi|\Psi\rangle = \int_{-L/2}^{L/2} dx \begin{pmatrix}\chi_e^*(x)\\ \chi_o^*(x)\end{pmatrix}^T \begin{pmatrix}\Psi_e(x)\\ \Psi_o(x)\end{pmatrix} = \int_{-L/2}^{L/2} dx\,[\chi_e^*(x)\Psi_e(x) + \chi_o^*(x)\Psi_o(x)]. \tag{3.25}$$

Hermiticity is investigated in the same way as before. One calculates

$$\begin{aligned}
\langle\hat{p}_R^\dagger\chi|\Psi\rangle \equiv \langle\chi|\hat{p}_R\Psi\rangle &= \int_{-L/2}^{L/2} dx \begin{pmatrix}\chi_e^*(x)\\ \chi_o^*(x)\end{pmatrix}^T \begin{pmatrix}0 & -i\partial_x\\ -i\partial_x & 0\end{pmatrix} \begin{pmatrix}\Psi_e(x)\\ \Psi_o(x)\end{pmatrix}\\
&= -i\int_{-L/2}^{L/2} dx \left[\begin{pmatrix}\chi_e^*(x)\\ \chi_o^*(x)\end{pmatrix}^T \begin{pmatrix}\partial_x\Psi_o(x)\\ \partial_x\Psi_e(x)\end{pmatrix}\right]\\
&= -i\int_{-L/2}^{L/2} dx\,[\chi_e^*(x)\partial_x\Psi_o(x) + \chi_o^*(x)\partial_x\Psi_e(x)]\\
&= -i[\chi_e^*(x)\Psi_o(x) + \chi_o^*(x)\Psi_e(x)]\big|_{-L/2}^{L/2} + i\int_{-L/2}^{L/2} dx\,[\partial_x\chi_e^*(x)\Psi_o(x) + \partial_x\chi_o^*(x)\Psi_e(x)]\\
&= -i[\chi_e^*(x)\Psi_o(x) + \chi_o^*(x)\Psi_e(x)]\big|_{-L/2}^{L/2} + \langle\hat{p}_R\chi|\Psi\rangle\,.
\end{aligned} \tag{3.26}$$

Hermiticity of $\hat{p}_R$ hence requires

$$-i[\chi_e^*(x)\Psi_o(x) + \chi_o^*(x)\Psi_e(x)]\big|_{-L/2}^{L/2} = 0. \tag{3.27}$$

The most general *linear* and *local*[4] boundary condition one can impose on $\Psi(x)$ reads [2]

$$\Psi_o(\pm L/2) = \lambda_\pm\Psi_e(\pm L/2), \qquad \lambda_\pm \in \mathbb{C}. \tag{3.28}$$

Inserting these conditions in (3.27), one obtains

$$(\lambda_+\chi_e^*(L/2) + \chi_o^*(L/2))\Psi_e(L/2) - (\lambda_-\chi_e^*(-L/2) + \chi_o^*(-L/2))\Psi_e(-L/2) = 0 \tag{3.29}$$

As the values $\Psi_e(\pm L/2)$ are arbitrary, one needs

$$\chi_o(\pm L/2) = -\lambda_\pm^*\chi_e(\pm L/2), \tag{3.30}$$

which is nothing but condition (3.28) for $\chi(x)$ with parameters $-\lambda_\pm^*$. Therefore, $\hat{p}_R$ is self-adjoint if

$$D(\hat{p}_R) = D(\hat{p}_R^\dagger) \;\Rightarrow\; \lambda_\pm = -\lambda_\pm^* \;\Rightarrow\; \lambda_\pm \in i\mathbb{R}. \tag{3.31}$$

Although a priori there was no connection between the parameters in (3.12) and those in (3.28), requiring self-adjointness of $\hat{p}_R$ led to the tacit assumption $\lambda_\pm \in i\mathbb{R}$ one used to obtain the operators on the lattice. This justifies the claim that the parameters introduced in the operator $\hat{p}_R$ in (3.12) manifest themselves in a set of boundary conditions when transitioning into the continuum.

[4] Now that one has two degrees of freedom at both boundaries, there is a possibility for a general *local* boundary condition, which was not the case in the one-component treatment.

3.2.3 Spectrum of $\hat{p}_R$

The next step in the discussion of $\hat{p}_R$ is the derivation of its spectrum and its eigenfunctions $\phi_k(x)$, i.e. the eigenvalue problem

$$\hat{p}_R\phi_k(x) = k\phi_k(x). \tag{3.32}$$

A formal treatment of this eigenvalue problem is given in Appendix A.2. The solutions look identical to the ones on the lattice, and they read

$$\langle x|\phi_k\rangle \equiv \phi_k(x) = \begin{pmatrix} A\exp(ikx) + B\exp(-ikx) \\ A\exp(ikx) - B\exp(-ikx) \end{pmatrix}. \tag{3.33}$$

Acting with $\hat{p}_R$ on $\phi_k(x)$, one indeed finds

$$\begin{aligned} \hat{p}_R\phi_k(x) = -i\partial_x \begin{pmatrix} A\exp(ikx) - B\exp(-ikx) \\ A\exp(ikx) + B\exp(-ikx) \end{pmatrix} &= k \begin{pmatrix} A\exp(ikx) + B\exp(-ikx) \\ A\exp(ikx) - B\exp(-ikx) \end{pmatrix} \\ &= k\phi_k(x), \end{aligned} \tag{3.34}$$

so $\phi_k(x)$ is indeed an eigenfunction of $\hat{p}_R$ with eigenvalue k. By applying the boundary conditions (3.28), one has

$$\begin{aligned} A\exp\left(\frac{ikL}{2}\right) - B\exp\left(-\frac{ikL}{2}\right) &= \lambda_+\left(A\exp\left(\frac{ikL}{2}\right) + B\exp\left(-\frac{ikL}{2}\right)\right) \\ A\exp\left(-\frac{ikL}{2}\right) - B\exp\left(\frac{ikL}{2}\right) &= \lambda_-\left(A\exp\left(-\frac{ikL}{2}\right) + B\exp\left(\frac{ikL}{2}\right)\right). \end{aligned} \tag{3.35}$$

The first one of these relations implies

$$A(1-\lambda_+) = B\exp(-ikL)(1+\lambda_+), \tag{3.36}$$

which, together with the second relation and the fact that $1 \pm \lambda_\mp \neq 0$, leads to the quantization condition

$$\exp(2ikL) = \frac{(1+\lambda_+)(1-\lambda_-)}{(1-\lambda_+)(1+\lambda_-)}. \tag{3.37}$$

This agrees with condition (3.16) in the limit $a \to 0$, which further suggests that this two-component formulation is indeed the analogue of the lattice description.
Normalization of $\phi_k(x)$ (see Appendix A.3) finally leads to

$$\phi_k(x) = \frac{1}{2\sqrt{L}} \begin{pmatrix} \exp(ikx) + \sigma\exp(-ikx) \\ \exp(ikx) - \sigma\exp(-ikx) \end{pmatrix}, \qquad \sigma \equiv \exp(ikL)\frac{1-\lambda_+}{1+\lambda_+} \tag{3.38}$$

Surprisingly, the new concept for momentum of a particle in a box leads to the quantization of momentum. However, this is merely a consequence of the self-adjointness requirement. If one would choose to settle for the non-local momentum treatment proposed in the end of section 3.1, a similar quantization condition would arise. In this case, where the momentum operator would be $-i\partial_x$, the eigenstates are easily found to be $\phi_k(x) = A\exp(\pm ikx)$. Imposing $\phi_k(L/2) = \exp(i\theta)\phi_k(-L/2)$ would then imply

$$\exp(ikL) = \exp(i\theta) \;\Rightarrow\; k = \frac{\theta}{L} + \frac{2\pi}{L}n, \qquad n \in \mathbb{Z}. \tag{3.39}$$

Lastly, it is crucial to notice that in general, the eigenfunctions of $\hat{p}_R$ do not live within the domain of the Hamiltonian (which will have to be slightly adapted in the extended Hilbert space), since $\phi_{k,o}$ and $\phi_{k,e}$ do not necessarily satisfy the boundary conditions (2.6) of the Hamiltonian. Consequently, $\hat{p}_R$ will not be able to simply act within the entire domain

of the adapted Hamiltonian. However, as $\hat{p}_R$ is now self-adjoint, it has a complete set of eigenfunctions, and the identity operator can be written as

$$\mathbb{1} = \sum_k |\phi_k\rangle \langle\phi_k| . \tag{3.40}$$

With that, the action of $\hat{p}_R$ on an arbitrary $|\Psi\rangle$ can be defined by projecting $|\Psi\rangle$ onto the eigenfunctions of $\hat{p}_R$

$$\hat{p}_R |\Psi\rangle \equiv \hat{p}_R \mathbb{1} |\Psi\rangle = \sum_k \hat{p}_R |\phi_k\rangle \langle\phi_k|\Psi\rangle = \sum_k k \langle\phi_k|\Psi\rangle |\phi_k\rangle . \tag{3.41}$$

3.3 The Hamiltonian in the Extended Hilbert Space

To find a momentum operator that is suitable in the given context, a wave function containing an even and an odd component was introduced. The treatment of the Hamiltonian alone did not suggest that such a distinction was necessary, as one already had self-adjoint Hamiltonians in the initial setting. If one would like to talk about momentum and energy at the same time, it is inevitable to adapt the Hamiltonian, i.e. to find its analogue in $\mathcal{H}_{\text{ext}}$. Before one does that, it is useful to note that any wave function $\Psi(x) = (\Psi_e(x),\ \Psi_o(x))^T$ can be decomposed in a component $\Psi^+(x)$ which satisfies $\Psi^+_e(x) = \Psi^+_o(x)$ and a component $\Psi^-(x)$ which satisfies $\Psi^-_e(x) = -\Psi^-_o(x)$,

$$\Psi(x) = \begin{pmatrix} \Psi_e(x) \\ \Psi_o(x) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \Psi_e(x) + \Psi_o(x) \\ \Psi_e(x) + \Psi_o(x) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Psi_e(x) - \Psi_o(x) \\ -(\Psi_e(x) - \Psi_o(x)) \end{pmatrix} \equiv \Psi^+(x) + \Psi^-(x). \tag{3.42}$$

As the Hamiltonian in the initial Hilbert space is self-adjoint, it provides one with a basis $\{\Psi_n(x)\}_{n\in\mathbb{N}}$ such that any $\Psi_{e,o}(x)$ can be written as a superposition of the $\Psi_n(x)$. In the "doubled" Hilbert space, the set $\{(\Psi_n(x),\ \Psi_n(x))^T\}_{n\in\mathbb{N}}$ then obviously provides one with a basis of the subspace of all $\Psi^+(x)$. The same applies to the subspace of all $\Psi^-(x)$ where the set $\{(\Psi_n(x),\ -\Psi_n(x))^T\}_{n\in\mathbb{N}}$ can be chosen as a basis. Due to (3.42), it follows easily that the combined set $\{(\Psi_n(x),\ \pm\Psi_n(x))^T\}_{n\in\mathbb{N}}$ constitutes a basis of the entire Hilbert space. If one would now naively introduce a Hamiltonian of the form

$$\hat{H}_{\text{ext}} \equiv \begin{pmatrix} \hat{H} & 0 \\ 0 & \hat{H} \end{pmatrix} \tag{3.43}$$

where $\hat{H}$ is the usual Hamiltonian, one would immediately find degeneracy in the spectrum of $\hat{H}_{\text{ext}}$, since

$$\hat{H}\Psi_n(x) = E_n\Psi_n(x) \ \Rightarrow\ \hat{H}_{\text{ext}} \begin{pmatrix} \Psi_n(x) \\ \pm\Psi_n(x) \end{pmatrix} \equiv \hat{H}_{\text{ext}}\Psi^\pm_n(x) = E_n\Psi^\pm_n(x). \tag{3.44}$$

Apparently, $\hat{H}_{\text{ext}}$ is not exactly the Hamiltonian one is looking for, as degeneracy is a feature the initial Hamiltonian did not have. Intuitively, only the energy eigenstates of the form $\Psi^+(x)$ seem to agree with the prior discussion, as the energy description did not distinguish even and odd degrees of freedom. As proposed in [2], a more sensible Hamiltonian is

$$\hat{H}(\mu) \equiv \begin{pmatrix} \hat{H} & 0 \\ 0 & \hat{H} \end{pmatrix} + \frac{\mu}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \equiv \begin{pmatrix} \hat{H} & 0 \\ 0 & \hat{H} \end{pmatrix} + \mu\hat{P}_- \tag{3.45}$$

when $\mu \to \infty$. The operator $\hat{P}_-$ is a projection operator with the property $\hat{P}_-\Psi^+(x) = 0$ and $\hat{P}_-\Psi^-(x) = \Psi^-(x)$. Having said that, the Hamiltonian in (3.45) retains the same eigenfunctions, but has a different spectrum, namely

$$\hat{H}(\mu)\Psi^+_n(x) = E_n\Psi^+_n(x), \qquad \hat{H}(\mu)\Psi^-_n(x) = (E_n + \mu)\Psi^-_n(x). \tag{3.46}$$

In the limit $\mu \to \infty$, only the states Ψ_n^+ have finite energies, and they are thus considered as the "physical" states, whilst the states Ψ_n^- seem to be unphysical with diverging energies.

The origin of this issue can be found when one also treats the Hamiltonian on the lattice. There, one finds solutions that treat odd and even points the same, but also such that treat them differently. These latter solutions have energies that diverge in the limit $a \to 0$, just the same as with the above suggested Hamiltonian. As this shall be of no major importance, it will not be further discussed here. A more thorough analysis is given in Appendix B.

If one accepts the states $\Psi^+(x)$ as the physical states, one can omit $\mu\hat{P}_-$ in the Hamiltonian such that it agrees with the naively chosen $\hat{H}_{\text{ext}}$. From now on, this Hamiltonian will simply be denoted by $\hat{H}$.
Apart from the action that is given by its functional form, one should further consider the domain $D(\hat{H})$ that is characterized by the boundary conditions on $\Psi(x)$. Although there is an even larger number of possible extension parameters for $\hat{H}$ that guarantee its self-adjointness (as there are more degrees of freedom) [2], their choice should be such that the boundary conditions are equivalent to those in the original treatment, namely Robin boundary conditions. This is discussed in more depth in [2]. In short, one finds that Robin boundary conditions for $\Psi^+(x)$ are obtained if the extension parameters are chosen such that they support $\Psi_o^+(x) = \Psi_e^+(x)$. This gives another reasoning for why the states $\Psi^+(x)$ should be regarded as the physical states.

3.4 Momentum Measurements and Distributions in Energy Eigenstates

Now that one is equipped with a self-adjoint momentum operator, one can try to meaningfully talk about momentum measurements. Such a measurement would put the state of the system into an eigenstate of momentum, and as the discussion below will show, this inevitably transfers an infinite amount of energy to the particle[5], no matter which concept for momentum is applied, and both concepts require that the initial Hilbert space must be extended.

Before considering the situation for $\hat{p}_R$, it pays off to see what happens with the usual operator $-i\partial_x$. This operator is only self-adjoint when $L \to \infty$, i.e. when one considers the whole real line. Consequently, one needs to extend the Hilbert space from $L^2(\Omega)$ to $L^2(\mathbb{R})$. The momentum eigenfunctions are then given by $\phi_k(x) = \exp(ikx)$ where k is the *unquantized* momentum. As this wave function lives on the entire real axis, its energy would be infinitely large as $\langle\phi|V|\phi\rangle \to \infty$ since $V \to \infty$ for $x \notin \Omega$ [2].
Prior to the measurement, the wave function $\Psi(x)$ of the system vanishes outside the box and its Fourier[6] transform

$$\tilde{\Psi}(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \exp(-ikx)\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-L/2}^{L/2} dx\, \exp(-ikx)\Psi(x) \tag{3.47}$$

gives the probability distribution $|\tilde{\Psi}(k)|^2$ of momentum [2]. The probability to measure a momentum in the infinitesimal range $[k_0, k_0 + dk]$, for example, would be

$$P(k \in [k_0, k_0 + dk]) = |\tilde{\Psi}(k_0)|^2 dk. \tag{3.48}$$

The situation is different when one considers the new momentum concept $\hat{p}_R$. In order to obtain this self-adjoint momentum operator, one had to extend the Hilbert space from $L^2(\Omega)$

[5] Obviously, a practical measurement can only transfer a *finite* amount of energy to the particle. This comes hand in hand with the fact that an infinitely deep potential well is only a mathematical idealization – any real potential barrier must be finitely large.

[6] Jean Baptiste Joseph Fourier (1768-1830), French mathematician and physicist.

to $L^2(\Omega) \times \mathbb{C}^2$. Its eigenfunctions were found to be

$$\phi_k(x) = \frac{1}{2\sqrt{L}} \left(\begin{pmatrix} \exp(ik_n x) \\ \exp(ik_n x) \end{pmatrix} + \sigma \begin{pmatrix} \exp(-ik_n x) \\ -\exp(-ik_n x) \end{pmatrix} \right) \equiv \phi_k^+(x) + \phi_k^-(x) \tag{3.49}$$

with the quantized momentum eigenvalues k_n satisfying (3.37). If one now performs a measurement of momentum, the wave function again collapses into a momentum eigenstate $|\phi_k\rangle$. As every momentum eigenstate also contains a component $|\phi_k^-\rangle$ that has infinite energy for $\mu \to \infty$, such an idealized measurement again transfers an infinite amount of energy to the particle. Obviously, these infinite energies arise only from mathematical idealizations, as in practice there cannot be an infinite amount of energy. This matter will be further discussed at the end of this section. For now, our main interest concerns the momentum distributions. As the eigenvalues of $\hat{p}_R$ are quantized, a measurement can only yield a discrete set of results, namely the momenta k_n. In order to find out what the probability to measure a momentum k_n in a physical state $|\Psi\rangle = |\Psi^+\rangle$ is, one first uses the self-adjointness of $\hat{p}_R$ to write $|\Psi\rangle$ as a superposition of momentum eigenstates

$$|\Psi\rangle = \mathbb{1}\,|\Psi\rangle = \sum_k \langle\phi_k|\Psi\rangle\,|\phi_k\rangle\,. \tag{3.50}$$

The probability to measure k_n is now simply given by the square of the projection coefficient

$$P(k_n) = |\langle\phi_k|\Psi\rangle|^2. \tag{3.51}$$

In the region of all physical states $|\Psi^+\rangle$, there is a useful relation that exploits the fact $\langle\chi^-|\Psi^+\rangle = 0$. As the given $|\Psi\rangle$ lies within this region, one finds[7]

$$\langle\phi_k|\Psi\rangle = \langle\phi_k^+|\Psi\rangle = \frac{1}{\sqrt{2L}} \int_{-L/2}^{L/2} dx\, \exp(-ik_n x)\Psi(x) = \sqrt{\frac{\pi}{L}}\tilde{\Psi}(k_n). \tag{3.52}$$

Hence, the probability to measure k_n with the new momentum concept is proportional to the absolute value squared of the Fourier transform of $\Psi(x)$ evaluated at k_n. This seems to agree with what one could expect from the classical treatment.

To illustrate these relationships a bit further, some explicit examples will be presented. First, assume $\lambda_+ = \lambda_-$, such that (3.37) reduces to

$$\exp(2ik_n L) = 1 \;\Rightarrow\; k_n = \frac{\pi}{L}n, \qquad n \in \mathbb{Z}. \tag{3.53}$$

As shown in [2], this choice preserves the parity of the situation, since it guarantees that $\hat{p}_R$ (or in fact even $\hat{p} = \hat{p}_R + i\hat{p}_I$) changes its sign under a parity transformation, as momentum usually does. The first example will treat Dirichlet boundary conditions, for which the physical energy eigenstates are given by

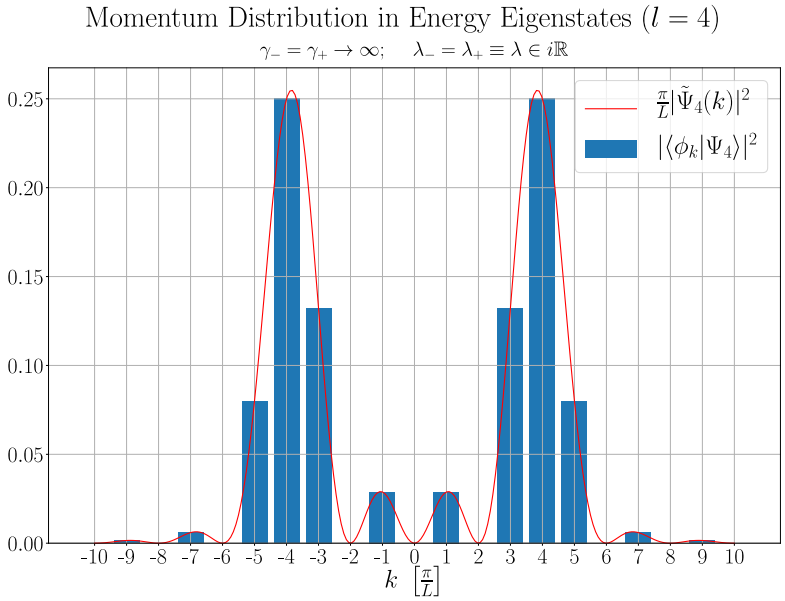
$$\Psi_l(x) = \frac{1}{\sqrt{L}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{cases} \cos\left(\frac{l\pi x}{L}\right), & l \text{ odd}, \\ \sin\left(\frac{l\pi x}{L}\right), & l \text{ even}. \end{cases} \tag{3.54}$$

It is then straightforward to calculate [2]

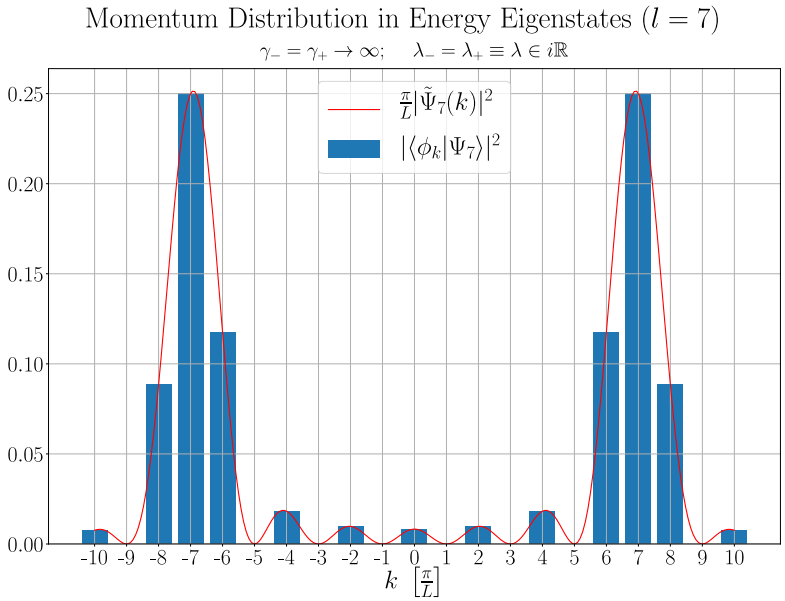
$$|\langle\phi_k|\Psi_l\rangle|^2 = \begin{cases} \frac{1}{4}, & n = \pm l, \\ 0, & (-1)^{n+l} = 1, \\ \frac{4l^2}{\pi^2(l^2-n^2)^2}, & (-1)^{n+l} = -1. \end{cases} \tag{3.55}$$

[7] Here, it is assumed that the two-component wave function is of the form $\langle x|\Psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \Psi(x) \\ \Psi(x) \end{pmatrix}$ where $\Psi(x)$ is properly normalized in the one-component framework.

A direct comparison between these momentum distributions and the corresponding Fourier transforms of $\Psi_l(x)$ for $l \in \{4, 7\}$ is given in Fig. 3.2. As one would already expect from the classical analysis with the non-self-adjoint momentum operator $-i\partial_x$, the momentum eigenvalue $k_{\max}$ with the highest probability of being measured is the one such that $k_{\max}^2/2M = E_l$. Interestingly, the probability to measure some other momentum value whose quantum number n has the same parity as l vanishes.
The plausibility of $\hat{p}_R$ is further established by the fact that the probabilities are normalized, i.e. $\sum_k |\langle\phi_k|\Psi_l\rangle|^2 = 1$ for all l [8].



(a) Momentum distribution for the third excited state with Dirichlet boundary conditions.



(b) Momentum distribution for the sixth excited state with Dirichlet boundary conditions.

Figure 3.2: Momentum distributions in different energy eigenstates in case of Dirichlet boundary conditions, compared to the Fourier transforms of the corresponding eigenstates.

The next examples illustrate the momentum distribution in energy eigenstates with $E = 0$. The constant ground state in case of Neumann boundary conditions

$$\Psi_0(x) = \frac{1}{\sqrt{2L}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{3.56}$$

yields the momentum distribution

$$|\langle \phi_k | \Psi_0 \rangle|^2 = \begin{cases} \dfrac{2}{n^2\pi^2}, & n \text{ odd}, \\ 0, & n \neq 0 \text{ even}, \\ \dfrac{1}{2}, & n = 0. \end{cases} \tag{3.57}$$

Although $\Psi_0(x)$ is an even function, there are no other momentum eigenstates with even n that contribute to this zero-energy ground state other than $n = 0$. Furthermore, using $\sum_{n>0 \text{ odd}} n^{-2} = \pi^2/8$, one can again verify that the probabilities are properly normalized. Due to the fact that one has $E = 0$ for this eigenstate, it seems rather unsurprising that $k = 0$ is the most probable momentum eigenvalue to measure. As the next example will show, pure intuition can yet be misleading.

Apart from the constant eigenstate with $E = 0$ given in (3.56) and the eigenstates with the affine components $\Psi_{0;e,o}(x) = Ax + B$, $A \neq 0 \neq B$, there exists also a purely linear eigenstate with zero energy. This state arises when one chooses $\gamma_- = \gamma_+ = -2/L$, and it is given by

$$\Psi_0(x) = \sqrt{\frac{6}{L^3}} \begin{pmatrix} x \\ x \end{pmatrix}. \tag{3.58}$$

In this case, the (again normalized) momentum distribution is given by

$$|\langle \phi_k | \Psi_0 \rangle|^2 = \begin{cases} \dfrac{24}{n^4\pi^4}, & n \text{ odd}, \\ \dfrac{6}{n^2\pi^2}, & n \neq 0 \text{ even}, \\ 0, & n = 0, \end{cases} \tag{3.59}$$

suggesting that the most probable outcome of a momentum measurement is $\pm\pi/L$, whilst all other odd momentum modes are suppressed. Surprisingly, the least probable value to obtain is actually $k = 0$.
Analogous to Fig. 3.2, the momentum distributions for these two examples are presented in Fig. 3.3.

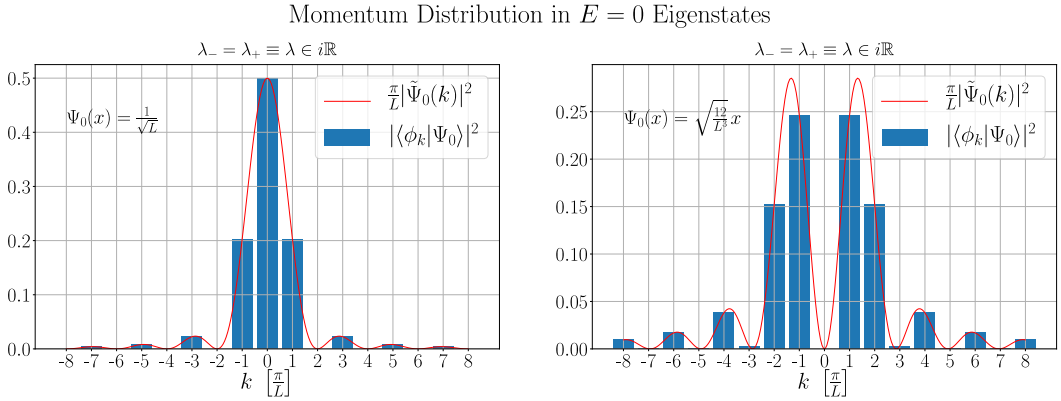


Figure 3.3: Momentum distributions in constant or linear energy eigenstates with $E = 0$, compared to the Fourier transforms of the respective states.

Until now, only a mathematically idealized situation has been described, since a potential that is infinite almost everywhere in space is not realizable in a laboratory. In a practical experiment, one can only construct relatively high, but finite potential barriers, such that the energy to escape the well is much higher than the energy of the particle itself. Nonetheless, quantum mechanics allows for a non-zero probability to find the particle outside the box. From a theoretical point of view, an idealized measurement of the old momentum operator $-i\partial_x$ would indeed catapult the particle outside the box, but by doing so, the experimenter would transfer an infinite amount of energy to the particle. This is due to the fact that mathematically, to measure $-i\partial_x$, one would have to extend the Hilbert space in the infrared (long distance scale) by sending $L \to \infty$, which results in $\langle\Psi|V|\Psi\rangle \to \infty$, since only for $L \to \infty$, $-i\partial_x$ is really self-adjoint and thus measurable.
If one could really prevent the particle from escaping the box, maybe because physical space actually ended at the boundaries, one would have to extend the Hilbert space in the ultraviolet (short distance scale) to obtain the self-adjoint momentum operator $\hat{p}_R$ [8]. Again, a momentum measurement would transfer an infinite amount of energy to the particle. This time, however, this would happen in the ultraviolet, as the $|\phi_k^-\rangle$-component of the momentum eigenstates contributes a diverging amount of energy.

As should be obvious by now, this idealized description of perfectly confined particles can only be used to approximate a real experiment, as only a finite amount of energy is available at all times. It really depends on how the experimental apparatus behaves. If one can (almost) guarantee that the particle will remain inside the box, the new concept involving $\hat{p}_R$ might be more suitable to describe the system [2]. This a priori requires that one can actually measure $\hat{p}_R$ in a laboratory, which is an issue that has not been and will not be discussed in this thesis at all.

At last, as emphasized in [8], one should remark that the construction of $\hat{p}_R$ assumed a physically meaningful ultraviolet sensitivity, which first presented itself in the distinction between odd and even degrees of freedom. In the transition from the lattice to the continuum, this sensitivity remained in the sense that one found energy eigenstates $|\Psi_n^-\rangle$ that have energies at the scale $1/a$. For $\hat{p}_R$ to be a sensible concept, this cut-off scale must exist; in experimental situations, this cut-off does indeed exist [8].

Chapter 4

Ehrenfest Theorem in the Finite Interval

This chapter will revisit Ehrenfest's theorem, which has been discussed in section 1.4 for the infinite volume. In order to arrive at the form (1.11), one had to consider the compatibility of the involved operator domains. In the infinite volume, one particularly had

$$M\frac{d\langle\hat{x}\rangle}{dt} = \langle\hat{p}\rangle\,, \tag{4.1}$$

i.e. the expectation value of momentum is equal to the mass M times the time-derivative of the expectation value of position – just as one would expect from classical physics. As the domains are further restricted by boundary conditions for operators in the finite volume, here, this relation does not necessarily hold anymore. The question this chapter is supposed to answer is whether (4.1) does hold for a particle in a box and/or if $\hat{p} = -i\partial_x$ has to be replaced by $\hat{p}_R$ for it to be true.

4.1 The Relation Between $\langle -i\partial_x\rangle$ and $\langle\hat{p}_R\rangle$

By now, one is equipped with two concepts for momentum: The usual momentum operator $\hat{p} = -i\partial_x$ which is in general only self-adjoint in the infinite volume, and the newly introduced momentum operator $\hat{p}_R = -i\sigma_1\partial_x$ that is self-adjoint but requires a larger Hilbert space. To find out which of these operators should appear in (4.1), it is useful to first find a relation between the expectation values $\langle -i\partial_x\rangle$ and $\langle\hat{p}_R\rangle$ for physical states with $\Psi_e(x) = \Psi_o(x)$.

To do so, it will be necessary to know the quantized eigenvalues k_n of $\hat{p}_R$, which follow from the quantization condition (3.37)

$$\begin{aligned}\exp(2ik_nL) = \frac{(1+\lambda_+)(1-\lambda_-)}{(1-\lambda_+)(1+\lambda_-)} &\equiv \exp(2i\theta L)\\ \Rightarrow k_n &= \frac{\pi}{L}n + \theta\end{aligned} \tag{4.2}$$

Consider now a physical (i.e. finite-energy) state

$$\langle x|\Psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}\Psi(x)\\ \Psi(x)\end{pmatrix} \tag{4.3}$$

where $\Psi(x)$ is some differentiable wave function. As this state lies within the physical subset of the doubled Hilbert space, the two-component analogue of $-i\partial_x$ (which acts on a one-component function) is simply $-i\mathbb{1}\partial_x$. Furthermore, as before, only the $\langle\phi_k^+|$ contributes in

projections in this region of Hilbert space. Having said that, one first finds

$$\begin{aligned}
\langle\phi_k|\partial_x\Psi\rangle &= \frac{1}{2\sqrt{2L}}\int_{-L/2}^{L/2} dx \begin{pmatrix}\exp(-ikx)\\ \exp(-ikx)\end{pmatrix}^T \begin{pmatrix}\partial_x & 0\\ 0 & \partial_x\end{pmatrix}\begin{pmatrix}\Psi(x)\\ \Psi(x)\end{pmatrix}\\
&= \frac{1}{\sqrt{2L}}\int_{-L/2}^{L/2} dx\, \exp(-ikx)\partial_x\Psi(x)\\
&= \frac{1}{\sqrt{2L}}\exp(-ikx)\Psi(x)\big|_{-L/2}^{L/2} + \frac{1}{\sqrt{2L}}\int_{-L/2}^{L/2} dx\, ik\exp(-ikx)\Psi(x)\\
&= \frac{1}{\sqrt{2L}}\left(\Psi(L/2)\exp\left(-\frac{ikL}{2}\right) - \Psi(-L/2)\exp\left(\frac{ikL}{2}\right)\right) + ik\,\langle\phi_k|\Psi\rangle\,.
\end{aligned} \tag{4.4}$$

With this relation, one can compute the expectation value of ∂_x and relate it to $\langle\hat{p}_R\rangle$ if one works with a projection onto the eigenfunctions $|\phi_k\rangle$

$$\begin{aligned}
\langle\partial_x\rangle \equiv \langle\Psi|\partial_x\Psi\rangle &= \sum_k \langle\Psi|\phi_k\rangle\,\langle\phi_k|\partial_x\Psi\rangle\\
&= \sum_k ik\,\langle\Psi|\phi_k\rangle\,\langle\phi_k|\Psi\rangle + \frac{1}{\sqrt{2L}}\sum_k \langle\Psi|\phi_k\rangle\left(\Psi(\tfrac{L}{2})\exp\left(-\frac{ikL}{2}\right) - \Psi(-\tfrac{L}{2})\exp\left(\frac{ikL}{2}\right)\right)\\
&= i\,\langle\hat{p}_R\rangle + \frac{1}{2L}\int_{-L/2}^{L/2} dx\,\Psi^*(x)\left(\Psi(\tfrac{L}{2})\sum_k \exp(ik(x-\tfrac{L}{2})) - \Psi(-\tfrac{L}{2})\sum_k\exp(ik(x+\tfrac{L}{2}))\right).
\end{aligned} \tag{4.5}$$

To evaluate this expression, Poisson's[1] summation formula, which states that [9]

$$\frac{1}{T}\sum_{n\in\mathbb{Z}}\exp\left(2\pi i n\tfrac{t}{T}\right) = \sum_{m\in\mathbb{Z}}\delta(t-mT), \tag{4.6}$$

implies

$$\begin{aligned}
\sum_k \exp(ik(x\pm\tfrac{L}{2})) &\overset{(4.2)}{=} \sum_{n\in\mathbb{Z}}\exp(i\tfrac{\pi}{L}n(x\pm\tfrac{L}{2}))\exp(i\theta(x\pm\tfrac{L}{2}))\\
&\overset{(4.6)}{=} 2L\exp(i\theta(x\pm\tfrac{L}{2}))\sum_{m\in\mathbb{Z}}\delta(x\pm\tfrac{L}{2}-2mL)
\end{aligned} \tag{4.7}$$

This now reduces (4.5) to[2]

$$\begin{aligned}
\langle\partial_x\rangle = i\,\langle\hat{p}_R\rangle + \int_{-L/2}^{L/2} dx\,\Psi^*(x)\Big(&\Psi(\tfrac{L}{2})\exp(i\theta(x-\tfrac{L}{2}))\sum_{m\in\mathbb{Z}}\delta(x-\tfrac{L}{2}-2mL)\\
&- \Psi(-\tfrac{L}{2})\exp(i\theta(x+\tfrac{L}{2}))\sum_{m\in\mathbb{Z}}\delta(x+\tfrac{L}{2}-2mL)\Big)\\
&= i\,\langle\hat{p}_R\rangle + \frac{1}{2}(|\Psi(L/2)|^2 - \Psi(-L/2)|^2).
\end{aligned} \tag{4.8}$$

[1] Siméon Denis Poisson (1781-1840), French mathematician.

[2] The factor $\frac{1}{2}$ in the last term of the equation is rather subtle from an analytical standpoint as it arises from having a δ-function on the boundary of the integration area, but one can easily verify it by considering the convergence behavior of the sum of exponential terms for $n\to\infty$ in (4.6), which is best done graphically.

Taking a closer look at the expression in parentheses, one recognizes it as minus the expectation value of $\hat{p}_I$, since

$$\begin{aligned}\langle\Psi|\hat{p}_I|\Psi\rangle &= \frac{1}{2}\lim_{\epsilon\to 0}\int_{-L/2}^{L/2} dx \begin{pmatrix}\Psi^*(x)\\ \Psi^*(x)\end{pmatrix}\begin{pmatrix}\delta(x+\frac{L}{2}-\epsilon)-\delta(x-\frac{L}{2}+\epsilon) & 0\\ 0 & 0\end{pmatrix}\begin{pmatrix}\Psi(x)\\ \Psi(x)\end{pmatrix}\\ &= \frac{1}{2}\lim_{\epsilon\to 0}\int_{-L/2}^{L/2} dx\,(\delta(x+\tfrac{L}{2}-\epsilon)-\delta(x-\tfrac{L}{2}+\epsilon))|\Psi(x)|^2\\ &= \frac{1}{2}(|\Psi(-L/2)|^2-|\Psi(L/2)|^2)\end{aligned} \tag{4.9}$$

such that

$$\langle -i\partial_x\rangle = \langle\hat{p}_R\rangle + i\,\langle\hat{p}_I\rangle\,. \tag{4.10}$$

In particular, this shows that $\langle -i\partial_x\rangle \neq \langle\hat{p}_R\rangle$ whenever the probability density $|\Psi(x)|^2$ does not satisfy periodic boundary conditions, i.e. when $\langle\hat{p}_I\rangle \neq 0$. One special case where $\hat{p}_R$ and $-i\partial_x$ have the same expectation value are Dirichlet boundary conditions, which to some degree explains why the standard textbook treatment seems to be consistent, especially with respect to Ehrenfest's theorem that will be discussed in the next section.

4.2 Validity of Ehrenfest's Theorem for a Particle in a Box

With relation (4.10) in one's toolbox, one can now explicitly check whether Ehrenfest's theorem (4.1) is valid and if so, which concept for momentum should be applied.
Consider a finite energy solution $|\Psi(t)\rangle = |\Psi^+(t)\rangle$ to Schrödinger's equation

$$i\partial_t\,|\Psi(t)\rangle = \hat{H}\,|\Psi(t)\rangle\,. \tag{4.11}$$

With the help of (4.11) and the self-adjointness of $\hat{H}$, one can express the time-derivative of the expectation value of position as

$$\begin{aligned}\frac{d}{dt}\langle\hat{x}\rangle \equiv \frac{d}{dt}\langle\Psi(t)|\hat{x}|\Psi(t)\rangle &= \langle\partial_t\Psi(t)|\hat{x}|\Psi(t)\rangle + \langle\Psi(t)|\hat{x}|\partial_t\Psi(t)\rangle\\ &= i\,\langle\hat{H}^\dagger\Psi(t)|\hat{x}|\Psi(t)\rangle - i\,\langle\Psi(t)|\hat{x}|\hat{H}\Psi(t)\rangle\\ &= i(\langle\hat{H}\Psi(t)|\hat{x}|\Psi(t)\rangle - \langle\Psi(t)|\hat{x}|\hat{H}\Psi(t)\rangle).\end{aligned} \tag{4.12}$$

Using $\hat{H} = -\frac{1}{2M}\partial_x^2$, one obtains

$$\begin{aligned}\langle\hat{H}\Psi(t)|\hat{x}|\Psi(t)\rangle - \langle\Psi(t)|\hat{x}|\hat{H}\Psi(t)\rangle &= -\frac{1}{2M}\int_{-L/2}^{L/2} dx\,[(\partial_x^2\Psi^*)x\Psi - \Psi^* x\partial_x^2\Psi]\\ &= -\frac{1}{2M}\int_{-L/2}^{L/2} dx\,[-(\partial_x\Psi^*)(\Psi+x\partial_x\Psi) - \Psi^* x\partial_x^2\Psi] - \frac{1}{2M}(\partial_x\Psi^*)x\Psi\Big|_{-L/2}^{L/2}\\ &= -\frac{1}{2M}\int_{-L/2}^{L/2} dx\,[\Psi^*(2\partial_x\Psi + x\partial_x^2\Psi) - \Psi^* x\partial_x^2\Psi]\\ &\quad -\frac{1}{2M}[(\partial_x\Psi^*)x\Psi - \Psi^*(\Psi+x\partial_x\Psi)]\Big|_{-L/2}^{L/2}\\ &= \frac{1}{M}\langle -\partial_x\rangle - \frac{1}{2M}[(\partial_x\Psi^*)x\Psi - \Psi^*(\Psi+x\partial_x\Psi)]\Big|_{-L/2}^{L/2}.\end{aligned} \tag{4.13}$$

The boundary term that was created by partial integration can be simplified by exploiting the boundary conditions (2.6)

$$\begin{aligned}
&((\partial_x\Psi^*)x\Psi - \Psi^*(\Psi + x\partial_x\Psi)\big|_{-L/2}^{L/2} \\
&\quad= \frac{L}{2}\partial_x\Psi^*(\tfrac{L}{2})\Psi(\tfrac{L}{2}) - \Psi^*(\tfrac{L}{2})\Psi(\tfrac{L}{2}) - \frac{L}{2}\Psi^*(\tfrac{L}{2})\partial_x\Psi(\tfrac{L}{2}) \\
&\quad+ \frac{L}{2}\partial_x\Psi^*(-\tfrac{L}{2})\Psi(-\tfrac{L}{2}) + \Psi^*(-\tfrac{L}{2})\Psi(-\tfrac{L}{2}) - \frac{L}{2}\Psi^*(-\tfrac{L}{2})\partial_x\Psi(-\tfrac{L}{2}) \\
&\quad\overset{(2.6)}{=} -\frac{L}{2}\gamma_+\Psi^*(\tfrac{L}{2})\Psi(\tfrac{L}{2}) - \Psi^*(\tfrac{L}{2})\Psi(\tfrac{L}{2}) + \frac{L}{2}\Psi^*(\tfrac{L}{2})\gamma_+\Psi(\tfrac{L}{2}) \\
&\quad+ \frac{L}{2}\gamma_-\Psi^*(-\tfrac{L}{2})\Psi(-\tfrac{L}{2}) + \Psi^*(-\tfrac{L}{2})\Psi(-\tfrac{L}{2}) - \frac{L}{2}\Psi^*(-\tfrac{L}{2})\gamma_-\Psi(-\tfrac{L}{2}) \\
&\quad= |\Psi(-\tfrac{L}{2})|^2 - |\Psi(\tfrac{L}{2})|^2 \\
&\quad= 2\langle\Psi|\hat{p}_I|\Psi\rangle = 2\langle\hat{p}_I\rangle\,.
\end{aligned} \tag{4.14}$$

Putting together (4.13) and (4.14), one finally finds

$$\begin{aligned}
M\frac{d\langle\hat{x}\rangle}{dt} &= iM(\langle\hat{H}\Psi(t)|\hat{x}|\Psi(t)\rangle + \langle\Psi(t)|\hat{x}|\hat{H}\Psi(t)\rangle) \\
&= \langle -i\partial_x\rangle - i\langle\hat{p}_I\rangle = \langle\hat{p}_R\rangle\,.
\end{aligned} \tag{4.15}$$

This proves Ehrenfest's theorem for all extension parameters $\gamma_\pm \in \mathbb{R},\ \lambda_\pm \in i\mathbb{R}$ when one identifies $\hat{p}_R$ as the physical momentum operator[3].

In particular, this also means that the Ehrenfest theorem holds even for the usual momentum operator $-i\partial_x$ when one has $\langle\hat{p}_I\rangle = 0$, i.e. when the probability distribution $|\Psi(x)|^2$ has the same value at both boundaries. This is indeed the case for Dirichlet boundary conditions. For general Robin boundary conditions, on the other hand, the proof of Ehrenfest's theorem as given in section 1.4 already breaks down when introducing the commutator between $\hat{x}$ and $\hat{H}$, since $x\Psi(x)$ would generally not satisfy the same boundary conditions as $\Psi(x)$ and hence $\hat{x}\,|\Psi\rangle \notin D(\hat{H})$ such that $[\hat{H},\hat{x}]$ is ill-defined.
Although at this point, the proof of Ehrenfest's theorem has already failed due to an ill-defined commutator, there is another issue worth mentioning. The step that identifies $-\partial_x^2$ as $\hat{p}^2$ when $\hat{p} = -i\partial_x$ is legitimate only in the infinite volume. In the finite volume, ∂_x^2 and $\hat{p}$ have domains characterized by completely different boundary conditions, and there is no reason to identify $-\partial_x^2 = \hat{p}^2$, since $\hat{p}^2$ can only act in a subset of $D(\hat{p})$, namely the set of all functions $\hat{p}\,|\Psi\rangle \in D(\hat{p})$.

At last, it is worth pointing out that the relation (4.10), which was crucial to prove Ehrenfest's theorem, holds irrespective of the choice of the extension parameters $\lambda_\pm$, and therefore irrespective of whether one explicitly breaks parity or not, as pointed out in section 3.4. At first glance, the fact that the Ehrenfest theorem seems to be unbothered by a possible parity violation is rather counter-intuitive, but the most likely explanation for this issue is simply that position and parity behave in the same way under a parity transformation (i.e. they change their sign), so they react similarly when parity is broken.

[3] As one can easily verify, one could have also included a potential term $V(x)$ inside the interval without changing the validity of the theorem.

Chapter 5

Conclusions

This last chapter is supposed to quickly summarize the results from the previous parts of this thesis and present the main conclusions. Furthermore, some of the many open questions that have yet remained unanswered should be considered, giving an outlook on what could be done in subsequent research or on what has been done parallel to this work in other theses.

5.1 Summary and Conclusions

In the first half of this thesis, the standard treatment of a particle in a 1-d box with perfectly reflecting boundaries was generalized. This was done by finding and imposing the most general boundary conditions, the so-called Robin boundary conditions, which resulted from the only physically necessary requirement of probability conservation. They contain two real-valued parameters $\gamma_\pm$, one at each boundary, and they give rise to a 2-parameter family of self-adjoint extensions of the Hamiltonian, each of which has its own domain and describes its own physical situation. It was found that the self-adjointness of the Hamiltonian is what guarantees conservation of probability.
By solving the time-independent Schrödinger equation under different boundary conditions, one concluded that there were not only sinusoidal positive-energy eigenstates, but also linear or exponential solutions with zero or negative energy respectively, depending on the choice of the extension parameters $\gamma_\pm$. The solutions with large negative energies are interpretable as particles strongly localized at the boundaries.

Within this more general setting, the second part of this thesis then went forward to consider the standard momentum operator $-i\partial_x$. It was concluded that this operator is in general not even Hermitean and as such does not qualify to represent physical momentum as it does not provide one with a complete set of orthonormal eigenfunctions.
In order to retrieve a self-adjoint (and thus physical) momentum operator, one had to extend the Hilbert space. Instead of doing this in the infrared, the interval was discretized to find that one can construct a momentum operator $\hat{p} = \hat{p}_R + i\hat{p}_I$ on the lattice, which has a Hermitean component $\hat{p}_R$ containing two purely imaginary parameters $\lambda_\pm$ and which is given by a symmetrized forward-backward derivative over two lattice spacings. To find the analogue of $\hat{p}_R$ in the continuum, the Hilbert space had to be doubled, introducing a two-component wave function. As it turns out, the two parameters $\lambda_\pm$ are embedded in two boundary conditions that characterize the domain of the newly found self-adjoint operator $\hat{p}_R = -i\sigma_1\partial_x$ which proves itself as a sensible momentum operator.
To embed the Hamiltonian in this doubled Hilbert space, one necessarily has to deal with an ultraviolet-sensitivity in the energy spectrum, but the corresponding eigenstates are not necessary to give a description equivalent to the one obtained from the one-component formulation.

In the last part, the implications of the newly introduced operator $\hat{p}_R$ were analyzed to underline that it indeed gives an appropriate way to describe momentum. One of its most important properties is that it provides a quantized set of eigenvalues, fundamentally different from what one would expect if one were to extend the Hilbert space to cover the entire real axis. Although it is quite different from $-i\partial_x$ in this respect, it shows several similarities to the usual momentum description. The probability distribution of the new quantized momentum, in which one would be interested if one were to measure momentum in an experiment, is closely related to the one found in the usual treatment, given by the absolute value squared of the wave function's Fourier transform. Furthermore, an idealized momentum measurement would in both cases lead to the transfer of an infinite amount of energy to the particle. The only difference lies within how they do this: The operator $-i\partial_x$ does it in the infrared, whilst $\hat{p}_R$ does it in the ultraviolet.
Another striking similarity between the two operators is found when one considers their expectation values: The difference between the two expectation values is solely determined by the values of the wave function at the boundaries and thus by the extension parameters. In particular, the difference vanishes in the standard case with Dirichlet boundaries, meaning that $-i\partial_x$ as well as $\hat{p}_R$ have the same expectation value.
Irrespective of the extension parameters of $\hat{H}$ and $\hat{p}_R$, it was proved that the Ehrenfest theorem holds in the finite volume if one incorporates $\hat{p}_R$ as the physical momentum operator.

In conclusion, taking into account the subtle differences between Hermiticity and self-adjointness led to a much fuller, much more critical and much more interesting treatment of the seemingly simplest quantum mechanical problem there is, involving a completely new machinery to treat a system in a finite volume.

5.2 Outlook and Open Questions

Although many questions have been answered in the previous chapters, there is an even larger number of questions that are left unanswered. An issue to start with is treated in another Bachelor's thesis of this year [10]: The Heisenberg uncertainty relation. In order to provide a lower bound on the product of the momentum and position measuring uncertainties, one needs to be able, among other things, to calculate the expectation value of momentum. As was seen in this thesis, $\langle -i\partial_x \rangle$ is in general a complex quantity, and it is thus unclear how to relate it to real-valued measurements. Now that one has a refined concept for momentum, the question of how exactly it flows into the uncertainty relation automatically arises, and also whether $\hat{p}_I$ plays a role as well. As mentioned, these issues are discussed in [10].

The generalized treatment of the Hamiltonian led to circumstances where one finds energy eigenstates with zero or even negative energy. As these are energies lower than the minimum of the potential, this might at first seem contradictory and should be analyzed more carefully. This apparent contradiction, however, is closely tied to the boundary conditions (2.6). The states with negative energy are localized at the boundaries of the box, and they thus require $\gamma_\pm < \infty$. Such boundary conditions can physically be realized by a procedure given in [1]: When one adds a potential that has a value $-V_0 < 0$ in the region $[-L/2, -L/2 + \epsilon]$ and $[L/2 - \epsilon, L/2]$ for $\epsilon > 0$ and is zero otherwise to the usual potential of the box, this allows a bound state with negative energy. Appropriately taking the limit $\epsilon \to 0$ as well as $V_0 \to \infty$, one can produce the boundary conditions (2.6) with $\gamma_\pm < \infty$. As such, the parameters $\gamma_\pm$ characterize the strength of δ-function-like wells at the boundaries responsible for the desired boundary conditions. This also resolves the problem of the bound state energy being smaller than the potential minimum.

Another issue to push forward would be the Ehrenfest theorem. After having treated the case $\hat{A} = \hat{x}$, it might be interesting to consider the case $\hat{A} = \hat{p}_R$. In the infinite volume, the time-derivative of the expectation value of momentum is simply the expectation value of the force. In the context of the finite box, one could use this relation to define a force operator that satisfies this relation, aiming at a better understanding of the forces the boundaries exert on the particle.

The new concept for momentum has been introduced by investigating a 1-d box with two sharp boundaries. The next question is how this concept is applied to systems with, for example, only one boundary, like the half-line discussed in [8], or more physical examples in more dimensions, for which [8] provides several physical examples of confined quantum mechanical systems.

Although this self-adjoint momentum operator provides one, in theory, with a measurable quantity named momentum, it gives no hint on how this measurement could be performed in the laboratory. How closely related a measurement of $\hat{p}_R$ is to a measurement of $-i\partial_x$ is a question that is left to those who prefer to experience physics in a more hands-on fashion.

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Last but not least, my thanks also go to my family and friends who were patient with me whenever I drifted away from conversations when my attention was absorbed by thoughts on the new concepts and ideas with which I was confronted.

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Appendix A

Derivations

A.1 Quantization Condition

As eq. (2.13) is used quite frequently, a quick derivation shall be given here. Imposing the boundary conditions

$$\gamma_\pm \Psi(\pm L/2) \pm \partial_x \Psi(\pm L/2) = 0 \tag{A.1}$$

onto the general solution

$$\Psi(x) = A\exp(ikx) + B\exp(-ikx), \qquad k > 0 \tag{A.2}$$

leads to

$$\begin{aligned} &\gamma_- \left(A\exp\left(-\frac{ikL}{2}\right) + B\exp\left(\frac{ikL}{2}\right)\right) - ik\left(A\exp\left(-\frac{ikL}{2}\right) - B\exp\left(\frac{ikL}{2}\right)\right) = 0, \\ &\gamma_+ \left(A\exp\left(\frac{ikL}{2}\right) + B\exp\left(-\frac{ikL}{2}\right)\right) + ik\left(A\exp\left(\frac{ikL}{2}\right) - B\exp\left(-\frac{ikL}{2}\right)\right) = 0. \end{aligned} \tag{A.3}$$

Both equations can be rearranged such that they read

$$\begin{aligned} A(\gamma_- - ik) &= -B\exp(ikL)(ik + \gamma_-), \\ A(\gamma_+ + ik) &= B\exp(-ikL)(ik - \gamma_+). \end{aligned} \tag{A.4}$$

As $k > 0$ is assumed, one has $\gamma_\pm \pm ik \neq 0$. Furthermore, $A = 0$ would imply

$$(\gamma_- + ik)B\exp(ikL) = 0, \tag{A.5}$$

which would require $B = 0$. Then $\Psi(x)$ would not be normalizable, so one can assume $A \neq 0$, and similarly $B \neq 0$. This allows one to divide the equations in (A.4) to obtain

$$\frac{\gamma_- - ik}{\gamma_+ + ik} = \exp(2ikL)\frac{\gamma_- + ik}{\gamma_+ - ik} \quad \Longleftrightarrow \quad \exp(2ikL) = \frac{(\gamma_- - ik)(\gamma_+ - ik)}{(\gamma_- + ik)(\gamma_+ + ik)}. \tag{A.6}$$

A.2 Solution to $\hat{p}_R\phi_k(x) = k\phi_k(x)$

The goal of this appendix is to formally solve the eigenvalue problem

$$\langle x|\hat{p}_R|\phi_k\rangle = \begin{pmatrix} 0 & -i\partial_x \\ -i\partial_x & 0 \end{pmatrix} \begin{pmatrix} \phi_{k,e}(x) \\ \phi_{k,o}(x) \end{pmatrix} = -i\frac{d}{dx}\begin{pmatrix} \phi_{k,o}(x) \\ \phi_{k,e}(x) \end{pmatrix} = k\begin{pmatrix} \phi_{k,e}(x) \\ \phi_{k,o}(x) \end{pmatrix}. \tag{A.7}$$

For better readability, the index k is omitted from now on.
The above equation can be equivalently written as[1]

$$\frac{d}{dx}\begin{pmatrix}\phi_e(x)\\ \phi_o(x)\end{pmatrix} = \frac{d}{dx}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\phi_o(x)\\ \phi_e(x)\end{pmatrix} = ik\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\phi_e(x)\\ \phi_o(x)\end{pmatrix} \equiv ikM\begin{pmatrix}\phi_e(x)\\ \phi_o(x)\end{pmatrix}. \quad \text{(A.8)}$$

From linear algebra [12], one finds that this set of differential equations has the general solution

$$\begin{pmatrix}\phi_e(x)\\ \phi_o(x)\end{pmatrix} = \exp(ikMx)\begin{pmatrix}\phi_e(0)\\ \phi_o(0)\end{pmatrix} \equiv \exp(ikMx)\begin{pmatrix}\tilde{A}\\ \tilde{B}\end{pmatrix}. \quad \text{(A.9)}$$

In order to evaluate $\exp(ikMx)$, one should first diagonalize M. Its eigenvalues $m_{1,2}$ are easily found by solving the characteristic equation

$$\det(M - m\mathbb{1}) = m^2 - 1 \stackrel{!}{=} 0 \;\Rightarrow\; m_{1,2} = \pm 1. \quad \text{(A.10)}$$

The corresponding normalized eigenvectors are

$$v_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}, \qquad v_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}, \quad \text{(A.11)}$$

which yields the basis transformation matrix

$$S^{-1} = (v_1\ v_2) = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}, \qquad S = S^{-1}, \quad \text{(A.12)}$$

such that

$$D = SMS^{-1} = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \quad \text{(A.13)}$$

Having diagonalized M, one now obtains

$$\begin{aligned}\exp(ikMx) &= \sum_{n=0}^{\infty}\frac{(ikx)^n}{n!}M^n = \sum_{n=0}^{\infty}\frac{(ikx)^n}{n!}(S^{-1}DS)^n\\ &= S^{-1}\exp(ikDx)S = S^{-1}\begin{pmatrix}\exp(ikx) & 0\\ 0 & \exp(-ikx)\end{pmatrix}S\\ &= \frac{1}{2}\begin{pmatrix}\exp(ikx)+\exp(-ikx) & \exp(ikx)-\exp(-ikx)\\ \exp(ikx)-\exp(-ikx) & \exp(ikx)+\exp(-ikx)\end{pmatrix}\\ &\Rightarrow \begin{pmatrix}\phi_e(x)\\ \phi_o(x)\end{pmatrix} = \frac{1}{2}\begin{pmatrix}(\tilde{A}+\tilde{B})\exp(ikx)+(\tilde{A}-\tilde{B})\exp(-ikx)\\ (\tilde{A}+\tilde{B})\exp(ikx)-(\tilde{A}-\tilde{B})\exp(-ikx)\end{pmatrix}.\end{aligned} \quad \text{(A.14)}$$

Finally, after defining

$$A \equiv \frac{\tilde{A}+\tilde{B}}{2}, \qquad B \equiv \frac{\tilde{A}-\tilde{B}}{2}, \quad \text{(A.15)}$$

one retrieves the general solution

$$\begin{pmatrix}\phi_e(x)\\ \phi_o(x)\end{pmatrix} = \begin{pmatrix}A\exp(ikx)+B\exp(-ikx)\\ A\exp(ikx)-B\exp(-ikx)\end{pmatrix}. \quad \text{(A.16)}$$

A.3 Normalization of Momentum Eigenstates

After applying the boundary conditions (3.28) onto the general eigenstate in eq. (3.33), one is left with

$$\phi_k(x) = A\begin{pmatrix}\exp(ikL)+\sigma\exp(-ikL)\\ \exp(ikL)-\sigma\exp(-ikL)\end{pmatrix}, \qquad \sigma \equiv \exp(ikL)\frac{1-\lambda_+}{1+\lambda_+} \in S^1. \quad \text{(A.17)}$$

[1] As there is only one variable, x, one can safely replace partial with total derivatives.

The reason for $\sigma \in S^1$ is $\lambda_+ \in i\mathbb{R}$. In order to normalize $\phi_k(x)$, one applies the new inner product to obtain

$$\begin{aligned}\langle \phi_k | \phi_k \rangle &= |A|^2 \int_{-L/2}^{L/2} dx \begin{pmatrix} \exp(-ikL) + \sigma^* \exp(ikL) \\ \exp(-ikL) - \sigma^* \exp(ikL) \end{pmatrix}^T \begin{pmatrix} \exp(ikL) + \sigma \exp(-ikL) \\ \exp(ikL) - \sigma \exp(-ikL) \end{pmatrix} \\ &= |A|^2 \int_{-L/2}^{L/2} dx \, (2 + 2|\sigma|^2).\end{aligned} \tag{A.18}$$

As $\sigma \in S^1$, one has $|\sigma|^2 = 1$ and hence

$$1 \stackrel{!}{=} \langle \phi_k | \phi_k \rangle = |A|^2 \int_{-L/2}^{L/2} dx \, 4 = 4L|A|^2, \tag{A.19}$$

so up to an overall and thus negligible phase

$$A = \frac{1}{2\sqrt{L}}. \tag{A.20}$$

Appendix B

Lattice Treatment of the Hamiltonian

Although the treatment of the Hamiltonian on the interval was perfectly satisfactory, it is instructive to also treat it on the lattice, as it will lead to a better understanding of the two-component formulation. As soon as one has introduced the lattice given in (3.8), one should try to find the lattice analogue of the Hamiltonian. In the absence of a potential, this reduces to finding a discretized second derivative. A way to define a discretized second derivative is given by [13]

$$\Psi''(x_m) \equiv \frac{\frac{\Psi(x_m+a)-\Psi(x_m)}{a} - \frac{\Psi(x_m)-\Psi(x_m-a)}{a}}{a} \equiv \frac{\Psi_{x_{m+1}} - 2\Psi_{x_m} + \Psi_{x_{m-1}}}{a^2}. \tag{B.1}$$

Again, this works well for all lattice sites with $m \neq 1, N$. At the outmost sites, either the forward or the backward derivative within the second derivative is ill-defined. Motivated by the Robin boundary conditions (2.6), one can define the second derivates at these sites as

$$\begin{aligned} \Psi''(x_1) &\equiv \frac{\frac{\Psi(x_1+a)-\Psi(x_1)}{a} - \gamma_- \Psi(x_1)}{a}, \\ \Psi''(x_N) &\equiv \frac{-\gamma_+ \Psi(x_N) - \frac{\Psi(x_N)-\Psi(x_N-a)}{a}}{a}. \end{aligned} \tag{B.2}$$

With these definitions, the Hamiltonian $\hat{H} = -\frac{1}{2M}\,\partial_x^2$ can be represented as [2]

$$\hat{H} = -\frac{1}{2Ma^2} \begin{pmatrix} -a\gamma_- - 1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 & 0 \\ 0 & 1 & -2 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -2 & 1 & 0 \\ 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 & -a\gamma_+ - 1 \end{pmatrix}. \tag{B.3}$$

In order to solve the eigenvalue problem

$$\hat{H}\Psi_{l,x} = E_l \Psi_{l,x}, \tag{B.4}$$

a suitable ansatz comes from the continuum solution (2.12)

$$\Psi^+_{l,x} = A\exp(ilx) + B\exp(-ilx) \qquad \text{for all } n. \tag{B.5}$$

When one explicitly inserts this ansatz in (B.4), it is straightforward to find the corresponding energy eigenvalue[1]

$$E_l^+ = \frac{1}{2M}\left(\frac{2}{a}\sin\left(\frac{la}{2}\right)\right)^2, \tag{B.6}$$

as well the quantization condition

$$\exp(2il(L-a)) = \frac{(\gamma_+ + \frac{1}{a}[1-\exp(-ila)])(\gamma_- + \frac{1}{a}[1-\exp(-ila)])}{(\gamma_+ + \frac{1}{a}[1-\exp(ila)])(\gamma_- + \frac{1}{a}[1-\exp(ila)])}. \tag{B.7}$$

The superscript "+" has been included on purpose since this solution does not distinguish between even and odd lattice sites, and is thus similar to $\Psi^+(x)$ discussed in section 3.3. One should also notice that in the limit $a \to 0$, the quantization condition (B.7) turns into the expected condition (2.13) from the continuum.
Motivated by the solutions $\Psi^-(x)$ in the continuum case, one can also try the ansatz

$$\Psi^-_{l,x} = \begin{cases} A\exp(ilx) + B\exp(-ilx), & n \text{ even}, \\ -A\exp(ilx) - B\exp(-ilx), & n \text{ odd}. \end{cases} \tag{B.8}$$

As anticipated, this is also a solution to (B.4), but with energy

$$E_l^- = \frac{1}{2M}\left(\frac{2}{a}\cos\left(\frac{la}{2}\right)\right)^2. \tag{B.9}$$

and the quantization condition

$$\exp(2il(L-a)) = \frac{(\gamma_+ - \frac{1}{a}[1+\exp(-ila)])(\gamma_- - \frac{1}{a}[1+\exp(-ila)])}{(\gamma_+ - \frac{1}{a}[1+\exp(ila)])(\gamma_- - \frac{1}{a}[1+\exp(ila)])}. \tag{B.10}$$

Taking the limit $a \to 0$ gives

$$\begin{aligned} \lim_{a\to 0} E_l^+ &= \lim_{a\to 0}\frac{1}{2M}\left(\frac{2}{a}\sin\left(\frac{la}{2}\right)\right)^2 = \frac{l^2}{2M}, \\ \lim_{a\to 0} E_l^- &= \lim_{a\to 0}\frac{1}{2M}\left(\frac{2}{a}\cos\left(\frac{la}{2}\right)\right)^2 \to \infty, \end{aligned} \tag{B.11}$$

therefore the solutions $\Psi^-(x)$ indeed correspond to eigenstates with infinite energy.

[1] In order to obtain the energy eigenvalue, one should consider the equations that do not include $\gamma_\pm$, namely not the first and not the last of the matrix equation. To find the quantization condition, exactly these equations are required.

Erklärung

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