Mathematical foundations of the eigenvalue problem in quantum mechanics

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Abstract

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The mathematical foundations of the quantum theory are recapitulated up to the formulation of the time-independent eigenvalue problem. The work follows closely to that of John von Neumann in his book the mathematical foundations of quantum mechanics. The requirements set for the Hilbert space and the ensuing theorems are summarized in a prompt manner. The greatest effort is used up in addressing the geometry of Hilbert space. With the theory thus far developed, an overlook into the proper formulation of the eigenvalue problem is stated. The work finishes with an example of the eigenvalue problem in an infinitely deep potential well. The example points out the need of proper understanding of the development of the quantum theory.

Keywords: Mathematical foundations, time-independent, eigenvalue problem, quantum mechanics

Tiivistelmä

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Kvanttimekaniikan ajasta riippumattoman ominaisarvo ongelman matemaattiset perusteet
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Työssä tarkastellaan kvanttiteorian ominaisarvo-ongelman matemaattisia perusteita asettamalla vaatimuksia Hilbertin avaruudelle. Työ seuraa läheisesti John von Neumannin käsittelyä kirjassa ”Mathematical Foundations of Quantum Mechanics”. Vaatimukset Hilbert avaruudelle, sekä niistä seuraavat teoreemat, on yhteenvedetty lyhyesti. Aiheen käsittelyssä keskitytään Hilbert-avaruuden geometriaan, johon ominaisarvo-ongelman muodostaminen pohjautuu. Lopuksi käsitellään esimerkkiä äärettömän syvästä potentiaalikuopasta, jonka kautta nähdään tarve kvanttiteorian määritelmien ja teoreemien korrektille ymmärtämiselle.

Avainsanat: Matemaattiset perusteet, ajasta riippumaton, ominaisarvo ongelma, kvanttimekaniikka

Foreword

In writing this work as my bachelor's thesis, I am not trying to invent the quantum theory anew. And it is my impression that it is not required from me. Therefore the treatment as given here follows closely to that of John von Neumann in his book the mathematical foundations of quantum mechanics.

I took my first course in quantum mechanics in the fall 2015 and the simplicity of the theory, that describes phenomenon which are all but intuitive, made an impression on me. The title that now stands on the front page of this thesis was by no means the first thing that I wished to write my thesis on. It has changed quite many times along this journey but I am still extremely satisfied with it.

The underlying motivation was to learn in detail the mathematical foundations on which the quantum theory stands upon. Only after that I hoped to summarize the essential requirements and theorems therein. Therefore, the beginning of this work is rather abstract. However, after that it is possible to offer an example why the presented mathematical rigour is needed in quantum mechanics.

There is much more to the quantum theory as what is presented in this work. For this work, the eigenvalue problem was the natural moment at which to stop the review. Up to that point, I still hope that this work might serve as a comprehensive summary of the mathematical foundations to any other third year physics student.

In Jyväskylä, 3.6.2016

Topi Löytäinen

Contents

1 Introduction

The great success of the quantum theory can hardly be denied by anyone in the scientific community. A student of physics is inevitably encountered by quantum mechanics at some point in his studies. Therefore the aim of this work is to give a short summary of the mathematical foundations of quantum mechanics. As the quantum theory is relatively large, the scope will be limited to the development of the eigenvalue problem.

This work will follow closely to the work of John von Neumann in his book the mathematical foundations of quantum mechanics. The work given by Neumann consists roughly of introductory considerations, development of the mathematical machinery needed for a detailed inspection and some general considerations on measurements and the problems included in it. This work will focus on the first two chapters of Neumann's book.

At the beginning of the 20th century great efforts were made to escort the quantum theory into a unified body capable of explaining physical problems with mathematical plainness. Two different approaches accomplished the same end. One commenced by Heisenberg and developed by the likes of Born, Jordan and Dirac and the other, the so-called ''wave mechanics'', developed by Schrödinger. These two theories were proved to be the same in a mathematical sense by Schrödinger in the year 1926. This unified structure, the ''transformation theory'', became the basis of quantum mechanics as we know it today [1, p.5]. The ideas related to these two theories and their correspondence are discussed.

The development of a pragmatic quantum theory requires a wide variety of different areas of mathematics including geometry, analysis, linear algebra and statistics. In this work we shall put our effort into defining an entity called the Hilbert space with some certain mathematical properties. As the nature of this thesis is more of a literature summary, the focus of this work will be on the narration of the necessary requirements of the Hilbert space and the mathematical theorems thereby acquired.

The work ends with a general statement on how the eigenvalue problem $\mathrm{H}\psi = \lambda\psi$

should be stated with the help of a family of projections $E(\lambda)$. As a final chapter before the conclusions, an example is taken from the eigenvalue problem of an infinitely deep potential well. This example follows closely to that of reference [4] but takes a different form of the solutions to $\mathrm{H}\psi = \lambda\psi$ and a different wave function as the objects of scrutiny. The results are in agreement with [4].

When the reader is in doubt what the particular mathematics or physics term means, he is encouraged to check the glossary of terms in the appendix. The terms are in alphabetical order to make the referencing as effortless as possible. Furthermore, all proofs, definitions and postulates that are given in chapters 2 and 3, are addressed in greater detail in [1].

2 Preliminary considerations

The year 1925 witnessed the birth of the first complete system of quantum theory called the Heisenberg-Born-Jordan ''matrix mechanics''. Schrödinger accomplished the same ends by developing the so-called ''wave mechanics''. And in the year 1926 he proved that the two theories are in fact equivalent. With the help of Born's statistical interpretation, Dirac and Jordan united the two theories in to the ''transformation theory'' [1, p.5]

Both theories begin by proposing a classical mechanical problem which is characterized by the Hamiltonian function $H(q_1,...,q_k,p_1,...,p_k)$. Here $q_1,...,q_k$ symbolize the values of k coordinates and $p_1,...,p_k$ the conjugate momenta of the $q_1,...,q_k$ coordinates. After this, the task is to find out as much as possible about the behaviour of the system with the help of the Hamiltonian. These properties include the possible energy levels, stationary states, transition probabilities et cetera[1, p.6-8].

In the matrix mechanics we seek a system of k matrices $Q_1,...,Q_k,P_1,...,P_k$ which satisfy the well known commutation rules of quantum mechanics. Then, by joining these with the classical mechanical Hamiltonian function, we get the matrix $W = H(Q_1,...,Q_k,P_1,...,P_k)$ which must become a diagonal matrix. It follows then that the allowed energy levels of the system are the diagonal elements $w_1,w_2,...$ of the matrix W. Furthermore, the elements $q^{(1)}_{mn},...,q^{(k)}_{mn}$ of the matrices $Q_1,...,Q_k$ determine, in a certain way, the transition probabilities and hence the radiation emitted[1, p.8-9]. The fundamental problem of this method is then in solving the eigenvalue equation:

$$\sum_{\nu} h_{\mu\nu} x_{\nu} = \lambda x_{\mu} \tag{1}$$

where λ determines the desired w_μ, x_μ is some vector of the configuration space and $h_{\mu\nu}$ the elements of the matrix $\overline{H}$ [1, p.21]. Where in turn $\overline{H}$ is used to find the diagonal matrix W [1, p.17-18].

In the wave mechanics, we first form the same Hamiltonian $H(q_1,...,q_k,p_1,...,p_k)$, take an arbitrary function $\Psi(q_1,...,q_k)$ from the configuration space of $(q_1,...,q_k)$ and then form the differential equation [1, p.11]:

$$\mathrm{H}\left(\mathrm{q}_1,...,\mathrm{q}_k,-i\hbar\frac{\partial}{\partial \mathrm{q}_1},...,-i\hbar\frac{\partial}{\partial \mathrm{q}_k}\right)\Psi(\mathrm{q}_1,...,\mathrm{q}_k)=\lambda\Psi(\mathrm{q}_1,...,\mathrm{q}_k). \tag{2}$$

Schrödinger proved that equation 2 has a character of an eigenvalue problem. Particularly it is required that the eigenfunction $\Psi(\mathrm{q}_1,...,\mathrm{q}_k)$ vanishes at the boundaries of the configuration space and that it is regular. In this sense the values of λ in equation 2 are the allowed energy levels [1, p.13].

Even though this work is about the time-independent eigenvalue problem, it should be briefly pointed out, for purposes of completeness, that if the system varies in time, it does it so according to the differential equation [1, p.14]:

$$\mathrm{H}\left(\mathrm{q}_1,...,\mathrm{q}_k,-i\hbar\frac{\partial}{\partial \mathrm{q}_1},...,-i\hbar\frac{\partial}{\partial \mathrm{q}_k}\right)\Psi(\mathrm{q}_1,...,\mathrm{q}_k;t)=i\hbar\frac{\partial}{\partial \mathrm{t}}\Psi(\mathrm{q}_1,...,\mathrm{q}_k;t). \tag{3}$$

Moreover the time-dependence of Ψ can be derived from equations 2 and 3 to be of the following form [1, p.16]:

$$\Psi=\Psi(\mathrm{q}_1,...,\mathrm{q}_k;t)=\sum_{\mathrm{n}=1}^{\infty}e^{\frac{-i\lambda_\mathrm{n}(t-t_0)}{\hbar}}\mathrm{a}_\mathrm{n}\Psi_\mathrm{n}(\mathrm{q}_1,...,\mathrm{q}_k). \tag{4}$$

However, from here onwards we shall consider the wave functions of equation 2 which are independent of time [1, p.15].

These are the two theories that Dirac and Jordan proved to be equal. We can see that the two theories differ considerably in what branch of mathematics quantum mechanical problems are to be solved. It should not then come as a surprise that, in order to set a mathematical relation between them, one is faced with some serious mathematical difficulties. Nevertheless, it has been proved that the two theories must always yield alike results [1, p.31].

In order to sketch the outlines of this proof we need to define few concepts. Take the discrete space of index values Z = (1,2,...) and the continuous state space Ω of a mechanical system. Here Ω is k-dimensional and k is the number of degrees of freedom. In Z, functions are the sequences $x_1,x_2,...$ and in Ω functions are the wave functions $\psi(\mathrm{q}_1,...,\mathrm{q}_k)$ [1, p.28]. We wish to establish a relation between certain functions of these two spaces. From both Z and Ω we only accept functions with finite

$$\sum_\nu |\mathrm{x}_\nu|^2 \text{ or } \underbrace{\int ... \int}_{\Omega} |\Psi(\mathrm{q}_1,...,\mathrm{q}_k)|^2 \mathrm{dq}_1...\mathrm{dq}_k$$

respectively and we also call the totality of such functions F_Z and F_Ω respectively. The reader can now see where the term function space originates from. It can then be proven that F_Z and F_Ω are isomorphic [1, p.29]. It should be emphasized that in this way there is no direct relation between the spaces Z and Ω. But that is not what we need. We are only looking for functions that have a finite sum of squares or a finite integral of the square. And isomorphism between F_Z and F_Ω means in this context, that they have the same desired abstract mathematical properties in different forms. And therefore, as it has been stated, it follows that they must always give same results[1, p.31].

The structure F_Z is generally known as Hilbert space [1, p.33]. In order to develop a unified theory out of these two, we shall continue to investigate properties common to both F_Z and F_Ω. The mathematical structure which we thereby achieve is called the abstract Hilbert space[1, p.33]. Therefore, in the following chapter we shall report the requirements we set for the abstract Hilbert space and that the properties that ensue must belong both to F_Z as well as F_Ω.

3 Abstract Hilbert space

3.1 Defining the Hilbert space

In defining an abstract Hilbert space in this context, we need to keep in mind the concepts that are needed in quantum mechanics. Furthermore these concepts need to have the same meaning both in F_Z and in F_Ω. As for the concepts, we need the scalar product, the addition and subtraction of two elements of the Hilbert space and the inner product of two elements [1, p.34]. Before we continue with this, let us state the notation explicitly.

Points of Hilbert space will be denoted by f,g, . . . ,ϕ,ψ, . . . , complex numbers by a,b, . . . , x,y, . . . and positive integers by k,l,m, . . . ,μ,ν, ... Furthermore the Hilbert space shall be denoted by $\Re_n$ or $\Re_\infty$ and when there is no need to distinguish whether the space is finite or infinite dimensional, it shall be denoted by $\Re$ [1, p.35]. It should then be understood merely as space. We can now state our first two requirements for the space:

Requirement A: $\Re$ is a linear space [1, p.36].

Requirement B: A Hermitian inner product is defined in $\Re$ [1, p.38].

Basically these two guarantee that vector algebra works the way that we have been accustomed to it. That is, addition is both commutative and associative and multiplication is distributive and associative. Furthermore, we have the null element and the identity element at our disposal. From this it naturally follows that linear vector calculus can also be used [1, p.37]. Moreover, the inner product is also of great importance since it allows us to define length in the space $\Re$ [1, p.39].

It should be noted that while all of this is very similar to the treatment done in the formation of a two dimensional Euclidean space, it is not the same. We are in progress of defining generally the properties of an Euclidean space for the spaces F_Z and F_Ω. In the last section we already stated the final result: F_Z and F_Ω are isomorphic. Now we are building the theory from down to up, aiming at this result. For the purpose of doing this correctly in a mathematical way, a certain level of abstraction has to be preserved. So for now, the points f,g, . . . ,ϕ,ψ, . . . should merely be regarded as mathematical abstractions called points.

From the requirements it then follows that addition $f+g$, the scalar product af [1, p.36] and the Hermitian inner product (f,g) are all defined [1, p.38]. With these at our disposal we can make the following three definitions:

Definition 1: The magnitude of an element $f \in \Re$ is $||f|| = \sqrt{(f,f)}$ and the distance between f and g is $||f-g||$ [1, p.39].

Definition 2: Elements $f_1,...,f_k \in \Re$ are linearly independent if it follows from $a_1 f_1 + ... + a_k f_k = 0$ that $a_1 = ... = a_k = 0$ [1, p.37].

Definition 3: A subset $\mathbb{M}$ of $\Re$ is called a linear manifold if it contains all the linear combinations $a_1 f_1 + ... a_k f_k$ of any $k(=1,2,...)$ of its elements $f_1,...,f_k$. Taking any arbitrary subset $\mathbb{A}$ of $\Re$, it then follows that a linear combination containing it, is called the linear manifold spanned by $\mathbb{A}$. It is denoted by $\{\mathbb{A}\}$ [1, p.38].

It follows then that the magnitude has all the properties of distance. It can especially be proven that Cauchy's inequality holds [1, p.40]. Furthermore, it follows that the magnitude has the property of being positive definite [1, p.42]. Moreover, the algebraic vector operations $af, f+g, (f,g)$ of all $f,g \in \Re$ are all continuous in all variables [1, p.44].

Requirements **A** and **B** do not allow us to differentiate between $\Re_n$ and $\Re_\infty$. As the concept of dimensions is related to the amount of linearly independent vectors, we need take a new requirement **C**. There are two different versions of this which we separate to $\mathbf{C}^{(n)}$ and to $\mathbf{C}^{(\infty)}$ [1, p.45].
Requirement $\mathbf{C}^{(n)}$: There are exactly n linearly independent vectors. That is, it is possible to specify n such vectors, but not $n+1$ [1, p.45].
Requirement $\mathbf{C}^{(\infty)}$: There are arbitrarily many independent vectors [1, p.45].

It should be noted that **C** is not essentially a new requirement since if **A** and **B** hold then either $\mathbf{C}^{(n)}$ or $\mathbf{C}^{(\infty)}$ holds. It then follows without further assumptions that $\Re$ with $\mathbf{C}^{(n)}$ has all the properties of a n-dimensional, complex Euclidean space. However, in order to guarantee the identity between $\Re$ and the infinite dimensional Hilbert space $\Re_\infty$ we need two additional requirements for the space to fulfil [1, p.45].

Requirement D: $\Re$ is complete [1, p.46].

Requirement E: $\Re$ is separable [1, p.46].

It should be noted that for a n-dimensional space, that is $\Re_n$, we require **A**, **B** and $\mathbf{C}^{(n)}$ and from these requirements **D** and **E** will follow. Whereas for infinite dimensional space we have to take all five [1, p.45]. Effectively these requirements allow us to define the geometry of the Hilbert space [1, p.46]. And that is what we shall consider in the next chapter.

3.2 The geometry of Hilbert space

The point of the first part of this chapter is to give an idea to the reader how $\mathrm{F_Z}$ and F_Ω come to satisfy the conditions **A**-**E**. This being said, we begin the exploration of the geometry of the Hilbert space with the following two definitions:

Definition 4: Two units f,g of $\Re$ are orthogonal if $(f,g) = 0$. Two linear manifolds $\mathbb{M}_1, \mathbb{M}_2$ are orthogonal if each element of $\mathbb{M}_1$ is orthogonal to each element of $\mathbb{M}_2$. A set $\mathbb{D}$ is called an orthonormal set if for all $f,g \in \mathbb{D}$, $(f,g) = \delta_{fg}$. Where δ_{fg} is the Kronecker delta function. Moreover, $\mathbb{D}$ is complete if it is not a subset of any other set that contains extra elements [1, p.46-47].

Definition 5: A linear manifold which is also closed is called a closed linear manifold. If $\mathbb{A}$ is any set in $\Re$, and we add to $\{\mathbb{A}\}$ all its limit points, we obtain a closed linear manifold which contains $\mathbb{A}$. We call it the closed linear manifold spanned by $\mathbb{A}$ and denote it by $[\mathbb{A}]$ [1, p.47-48].

The property of orthonormality can hardly be stressed too much in geometry. For this reason definitions 4 and 5 are of crucial importance. Furthermore, almost every theorem, that is about to follow, has something to do with orthonormal sets. It should also be pointed out that definition 5 is important only in $\Re_\infty$ because in $\Re_n$ all linear manifolds are of the type described by it [1, p.47]. With these we may present our first two theorems:

Theorem 1: In $\Re_n$ every orthonormal set has $\leq n$ elements, and is complete if and only if it has n elements [1, p.48].

Theorem 2: In $\Re$ each orthonormal set is finite or countably infinite set. If the set is complete then it is also infinite [1, p.49].

The first theorem for $\Re_n$ furnishes us with a relatively simple check of completeness; property which will be exploited later on. However, for $\Re_\infty$, the infinite amount of elements is not sufficient for its completeness [1, p.50]. In order to achieve this, we need to acquire few more results. Since by definition completeness of a set is closely related to convergence, the required completeness property is achieved by addressing the convergence criterion through the postulate $\mathbf{C}^{(\infty)}$. Then the following theorems hold generally:

Theorem 3: Let $\phi_1,\phi_2...$ be an orthonormal set. Then all series of infinitely many terms, such as $\sum_\nu (f,\phi_\nu)\overline{(g,\phi_\nu)}$, are absolutely convergent. Especially if $f = g$ then $\sum_\nu |(f,\phi_\nu)|^2 \leq |f|^2$ [1, p.51].

Theorem 4: Let $\phi_1,\phi_2...$ be an infinite orthonormal set. Then the series $\sum_{\nu=1}^{\infty} x_\nu \phi_\nu$ converges if and only if $\sum_{\nu=1}^{\infty} |x_\nu|^2$ does. It then follows, assuming convergence, that for $f = \sum_\nu x_\nu \phi_\nu$, it holds that $(f,\phi_\nu) = x_\nu$ [1, p.52-53].

Theorem 5: Let $\phi_1,\phi_2...$ be an orthonormal set and f an arbitrary vector. Then for $x_\nu = (f,\phi_\nu)$ and $(\nu = 1,2,...)$ the sum $f' = \sum_\nu x_\nu \phi_\nu$ is always convergent if the series is infinite. Also, the expression $f - f'$ is orthogonal to $\phi_1,\phi_2,...$ [1, p.53].

Theorem 3 effectively establishes an idea of convergence and thus serves as a stepping stone for theorem 4. Theorem 5 in itself is not useful to us, but as it is used in the proof of the following theorem, it is given for purposes of completeness. Therefore, the general criteria of completeness, for both finite or infinite dimensional space, is given by the following theorem [1, p.54]:

Theorem 6: Let $\phi_1,\phi_2...$ be an orthonormal set. Each one of the following conditions is necessary and sufficient for completeness:

1. The closed linear manifold $[\phi_1,\phi_2...]$ spanned by $\phi_1,\phi_2...$ is equal to $\Re$.
2. $f = \sum_\nu x_\nu \phi_\nu$, where $x_\nu = (f,\phi_\nu)$ is always true.
3. $(f,g) = \sum_\nu (f,\phi_\nu)\overline{(g,\phi_\nu)}$ is always true [1, p.54].

In addition to completeness, we would like to be able to come up with a method how to orthonormalize a given set. In linear algebra this is known as the Gram-Schmidt procedure [2, p.79-80]. And as linear manifolds are merely some sets with properties as given in definition 3, we would like to extend this notion of orthonormality to them. This is because it is almost always convenient to choose an orthonormal basis for our calculations [2, p.79]. With this, we can give the last two theorems of the geometry of the Hilbert space.

Theorem 7: Both in infinite and finite dimensional space, to each set f_1,f_2,..., there corresponds an orthonormal set ϕ_1,ϕ_2,... which spans the same linear manifold as the former set [1, p.55]

Theorem 8: Corresponding to each closed linear manifold $\mathbb{M}$ there is an orthonormal set which spans the same $\mathbb{M}$ as a closed linear manifold [1, p.56].

With theorem 8 we have arrived to the point where we can address how $\Re$ can be shown to be identical with $\Re_n$ or $\Re_\infty$, depending whether $\mathbf{C}^{(n)}$ or $\mathbf{C}^{(\infty)}$ holds [1, p.58]. It suffices to show that $\Re$ allows a one to one mapping on the set of all $\{x_1,...,x_k\}$ or $\{x_1,x_2,...\}$ respectively, in such a way that

1. $af \leftrightarrow \{ax_1,ax_2,...\}$ follows from $f \leftrightarrow \{x_1,x_2,...\}$
2. $f + g \leftrightarrow \{x_1 + y_1,x_2 + y_2\}$ follows from $f \leftrightarrow \{x_1,x_2,...\}$ and $g \leftrightarrow \{y_1,y_2,...\}$
3. $(f,g) = \sum_{\nu=1}^{n \text{ or } \infty} x_\nu \overline{y}_\nu$ follows from $f \leftrightarrow \{x_1,x_2,...\}$ and $g \leftrightarrow \{y_1,y_2,...\}$ [1, p.58-59]

Needles to say that such a mapping can be defined and a reader more interested in the details of the proof is encouraged to see reference [1] for further details.

We have now come far enough to address the problem whether the requirements **A**-**E** hold in $\mathrm{F_Z}$ and $\mathrm{F_\Omega}$. However, as the exact proof of how they come to hold in $\mathrm{F_Z}$ and $\mathrm{F_\Omega}$ is not necessary for the understanding of the coming text [1, p.59], we shall only recite here the essential points. For $\mathrm{F_Z}$ this follows from the fact that an $\Re$ with **A**-**E** must be identical in all properties with $\Re_\infty$ [1, p.58-59]. It should also be pointed out that requirements **D** and **E** follow from **A**-$\mathbf{C}^{(n)}$ but not from **A**-$\mathbf{C}^{(\infty)}$ [1, p.45,59]. Which means that for an infinite dimensional space requirements **D** and **E** have to be stated explicitly.

Before considering $\mathrm{F_\Omega}$, it should be noted that in the k-dimensional space q_1,...,q_k, where $\mathrm{F_\Omega}$ is defined, the dimensions q_1,...,q_k are allowed to vary from minus infinity to plus infinity [1, p.60]. With this in mind the validity of the requirements **A**-**E** in $\mathrm{F_\Omega}$ can be checked one by one. For this we rely on the Lebesgue measure and the thus defined Lebesgue integral [1, 3, p.59-61]. For **A** we must show that if f,g belong to $\mathrm{F_\Omega}$ then af and $f \pm g$ also belong to it [1, p.60]. For **B** we define the inner-product (f,g) as $\int_\Omega f\overline{g}$ [1, p.61]. For **C** it can be shown that $\mathbf{C}^\infty$ holds [1, p.62]. For **D** it can be shown that for a sequence f_1,f_2,... that satisfies the Cauchy convergence criterion, there exists a limit f that belongs to F_Ω. Furthermore f is also the limit of a subsequence $f_{n_1}, f_{n_2}, \ldots$ of $f_1, f_2, \ldots$ [1, p.62-64] And finally for **E** we are capable of specifying a function sequence $f_1, f_2, \ldots$ that is everywhere dense in F_Ω which is exactly what was required [1, p.64-69].

Taken $\Re$ which satisfies **A**-**E**, we can also answer the question as to what is the condition for a subset $\mathbb{M}$ of $\Re$, so that $\mathbb{M}$ satisfies the same requirements. The condition is that $\mathbb{M}$ must be a closed linear manifold [1, p.69-70].

With the above we have shown several theorems of orthonormal sets within $\Re$ and established an understanding of the underlying concepts proving the isomorphism between F_Z and F_Ω. Now we may go further into the geometric analysis of Hilbert space [1, p.73]. Effectively this means discussion on the various projection theorems of Hilbert space.

We now wish introduce new notation which allows us to discuss the topic more effectively. Taken any arbitrary sets $\mathbb{A}$,$\mathbb{B}$,... of $\Re$, the set that results from their combination, whether a linear manifold or a closed linear manifold, is denoted by $\{\mathbb{A}, \mathbb{B}, \ldots\}$ or $[\mathbb{A}, \mathbb{B}, \ldots]$ respectively. The same notation holds for arbitrary elements too. Moreover, if in particular $\mathbb{M}$,$\Re$ are closed linear manifolds then we designate the closed linear manifold $[\mathbb{M}, \Re, \ldots]$ by $\mathbb{M} + \Re + \ldots$ [1, p.73]. Furthermore, taken a subset $\mathbb{M}$ of $\Re$, we denote the totality of elements of $\Re$ which are orthogonal to all elements of $\mathbb{M}$ by $\Re - \mathbb{M}$. It follows that the set $\Re - \mathbb{M}$ is a closed linear manifold and we call it as the closed linear manifold complementary to $\mathbb{M}$ [1, p.73-74]. With this we get the following theorem:

Theorem 9: Let $\mathbb{M}$ be a closed linear manifold. Then each f of $\Re$ can be resolved in one and only one way into two components, $f = g + h$ where g is from $\mathbb{M}$ and h from $\Re - \mathbb{M}$ [1, p.74].

We call g the projection of f in $\mathbb{M}$ and h the normal from f onto $\mathbb{M}$. Since g is acquired from f through an operation, that is the act of checking what part of it lies in the manifold $\mathbb{M}$, we introduce the notation $\mathrm{P}_\mathbb{M} f$ for g [1, p.74]. From this it follows that the projection has the properties mentioned in theorem 10. As the concept of an operator is needed, let us specify it explicitly in definition 6.

Definition 6: An operator R is a function defined in a subset of $\Re$ with values from $\Re$. That is, a relation which establishes a correspondence between certain elements $f \in \Re$ and elements $\mathrm{R}f \in \Re$ [1, p.87].

Theorem 10: The operator $P_{\mathbb{M}}$ has the following properties:

1. $P_{\mathbb{M}}(a_1 f_1 + ... + a_k f_k) = P_{\mathbb{M}} a_1 f_1 + ... + P_{\mathbb{M}} a_k f_k$.

2. $(P_{\mathbb{M}} f, g) = (f, P_{\mathbb{M}} g)$

3. $P_{\mathbb{M}}(P_{\mathbb{M}} g) = P_{\mathbb{M}} g$ [1, p.75].

It can be noted that the manifold $\mathbb{M}$ can be characterized as the set of all solutions to the equation $P_{\mathbb{M}} f = f$. Furthermore the first property defines the so-called linear operators and the second the so-called Hermitian operators [1, p.75-76]. As the projection $P_{\mathbb{M}}$ is related to the manifold $\mathbb{M}$ in question, we would like to characterize such operators independently of the manifold in question [1, p.77]. Thus we give the following theorem:

Theorem 11: An operator E that is defined everywhere, is a projection if and only if it has the properties: $(\mathrm{E}f,g)=(f,\mathrm{E}g)$ and $\mathrm{E}^2=\mathrm{E}$. If these properties are satisfied, it also follows that 1-E is also a projection [1, p.77,79].

We can then ask ourselves how the magnitude of the element f is affected by the operation of projection. We recall the notation introduced in definition 1 for the magnitude of an element. It can then be especially shown that $||\mathrm{E}f||^2=(\mathrm{E}f,f)$ and $||\mathrm{E}f|| \leq ||f||$ is always true. Furthermore, E is continuous as can be seen from $||\mathrm{E}f\text{-}\mathrm{E}g||=||\mathrm{E}(f-g)|| \leq ||f-g||$ [1, p.79].

Let us consider two operators R,S. Then by R±S, aR and RS we understand the operators that are defined by $(\mathrm{R}\pm\mathrm{S})f=\mathrm{R}f\pm\ \mathrm{S}f$, $(\mathrm{aR})f=\mathrm{a}-\mathrm{R}f$, $(\mathrm{RS})f=\mathrm{R}(\mathrm{S}f)$, respectively. Moreover, we use the notation $\mathrm{R}^0=1$, $\mathrm{R}^1=\mathrm{R}$, $\mathrm{RR}=\mathrm{R}^2$ and so on. Furthermore, $\mathrm{R}^l\mathrm{R}^m=\mathrm{R}^{l+m}$ is also true [1, p.80]. The rules of calculation for different projections are also of interest to us and it can be shown that all elementary calculations are generally valid for the exception of commutation [1, p.80]. Therefore we give the following theorem:

Theorem 12: Let E,F be projections of the closed linear manifolds $\mathbb{M},\Re$. Then EF is also a projection if and only if E and F commute. Also, EF belongs to the closed linear manifold $\mathbb{B}$ which consists of the elements common to $\mathbb{M},\Re$. The operator E+F is a projection if and only if EF=0 or FE=0. Thus all of $\mathbb{M}$ is orthogonal to all of $\Re$. It then follows that E+F belongs to $\mathbb{M}+\Re$ and especially in this case it equals to $\mathbb{M}+\Re$. Moreover, the operator E-F is a projection if and only if EF=F or if FE=F [1, p.80-81].

Now we may also ask, how does the property of magnitude, carry over for projections. It can be shown that it works in the most sensible way. That is, the statement E$\leq$F is equivalent to the general validity of $||\mathrm{E}f|| \leq ||\mathrm{F}f||$ [1, p.83]. Further properties of magnitude of the projection operators can be given with the following two theorems.

Theorem 13: Let $\mathrm{E}_1,...,\mathrm{E}_k$ be projections. Then $\mathrm{E}_1 + ... + \mathrm{E}_k$ is a projection if and only if all $\mathrm{E}_l,\mathrm{E}_m$, where $l,m = 1,...,k$ and $l \neq m$, are all mutually orthogonal. Another necessary and sufficient condition is that for all f, the condition $||\mathrm{E}_1 f||^2 + ... + ||\mathrm{E}_k f||^2 \leq ||f||^2$ holds. Furthermore, $\mathrm{E}_1 + ... + \mathrm{E}_k$ is the projection of $\mathbb{M}_1 + ... + \mathbb{M}_k$ where we note that $\mathrm{E}_1 = \mathrm{P}_{\mathbb{M}_1},...,\mathrm{E}_k = \mathrm{P}_{\mathbb{M}_k}$ [1, p.84].

Theorem 14: Let $\mathrm{E}_1,\mathrm{E}_2,...$ be an increasing or decreasing sequence of projections. That is either $\mathrm{E}_1 \leq \mathrm{E}_2 \leq ...$ or $\mathrm{E}_1 \geq \mathrm{E}_2 \geq ...$ respectively. These converge to a projection E in the sense that for all f, $\mathrm{E}_n f \rightarrow \mathrm{E}f$. Furthermore, it holds that $\mathrm{E}_n \leq \mathrm{E}$ or $\mathrm{E}_n \geq \mathrm{E}$ respectively [1, p.85].

We can now conclude our geometry oriented study of the functional spaces. In the next chapter we shall narrate through some of the different operators of the spaces $\mathrm{F}_\mathrm{Z},\mathrm{F}_\Omega$. Before this, it should be noted that we have already stated a great deal about operators in the space $\mathfrak{R}$. Theorems 1 through 9 were considered purely in order to establish rigorously the concept and the properties of a closed linear manifold. This was then further developed as a study of projection operators.

Yet, before we continue to linear operators, it should be stated that, in the simplest of terms an operator can be described as an instruction to do something to the function that follows after [2, p.16]. Moreover, in function spaces operators behave as linear transformations, provided that they carry all functions to other functions within the space and in such a manner that it satisfies the linearity condition [2, p.97]. And as $\mathrm{F}_\mathrm{Z},\mathrm{F}_\Omega$ are both just the kind, we have spend considerable effort into getting ourselves to this point.

3.3 Linear operators in Hilbert space

The focus of this chapter will be on the linear operators of the Hilbert space. We have already stated the definition of an operator in the preceding section. In addition to that definition, we shall consider relations which are linear. However, let us first consider properties of operators in general.

If the domain of an operator R encompasses the entire $\Re$, it is said to be defined everywhere. However, it is not necessary that the range of R is contained in the domain of R. This is to say that $\mathrm{R}^2 f$ is not necessarily defined even if $\mathrm{R}f$ is [1, p.87]. It should also be noted that R$\pm$S is defined only in the intersection of the domains of R and S [1, p.88].

The inverse R^{-1} of the operator R is defined if $\mathrm{R}g = f$ has a solution g and this g is then the inverses value. It is also required that $\mathrm{R}f$ takes on each of its values only once [1, p.88-89]. The operator laws of calculation given after theorem 11 hold here too. However, we can further extend these properties. Taken R,S which have inverses, then RS has an inverse too which is $(\mathrm{RS})^{-1}=\mathrm{S}^{-1}\mathrm{R}^{-1}$. Moreover for a non-zero constant a, it holds that $(a\mathrm{R})^{-1}=\frac{1}{a}\mathrm{R}^{-1}$. Finally we can set the same power notation for the inverses: $\mathrm{R}^{-1}\mathrm{R}^{-1}=\mathrm{R}^{-2}$, $\mathrm{R}^{-1}\mathrm{R}^{-1}\mathrm{R}^{-1}=\mathrm{R}^{-3}$ and so on [1, p.89].

From here onwards, we shall only consider operators that are linear and whose domains are everywhere dense [1, p.89]. Because of this we need the following definition:

Definition 7: An operator A is said to be linear if its domain is a linear manifold and if $\mathrm{A}(a_1 f_1 + ... + a_k f_k) = a_1 \mathrm{A} f_1 + ... + a_k \mathrm{A} f_k$ holds [1, p.89].

It should be noted that in quantum mechanics we must abandon the requirement that operators should be defined everywhere. Instead a sufficient substitute is acquired by requiring that the domain of an operator is everywhere dense [1, p.90]. For example let us consider a one dimensional configuration space in Schrödinger's wave mechanics. So we have $\mathrm{q} \in\ ]-\infty,\infty[$ and for the wave functions $\psi(\mathrm{q})$ square integrability holds:

$$\int_{-\infty}^{\infty} |\psi(\mathrm{q})|^2 \, \mathrm{dq} < \infty. \tag{5}$$

And as it has been said multiple times, these type of functions form the Hilbert space [1, p.90]. Now considering the position operator q, which is a linear operator, we notice that its domain is not the entire Hilbert space [1, p.90]. This is because the value of the integral

$$\int_{-\infty}^{\infty} |\mathrm{q}\psi(\mathrm{q})|^2 \, \mathrm{dq} = \int_{-\infty}^{\infty} \mathrm{q}^2|\psi(\mathrm{q})|^2 \, \mathrm{dq}$$

can be infinite even if equation 5 holds [1, p.90]. If this happens then the position operator q has carried the wave function ψ(q) out of the Hilbert space; that is qψ(q) is not part of the Hilbert space [1, p.90].

Definition 8: Two operators A,A* are said to be adjoint if they have the same domain, and if in this domain both (Af,g)=(f,A*g) and (A*f,g)=(f,Ag) hold [1, p.91-92].

It should be stressed that the requirement of equal domains in definition 8 is an important one. The consequences of negligent treatment of domains shall be elaborated more in detail in Chapter 4.

Without getting stuck on the properties of an adjoint operator, it can be shown that in the Schrödinger wave mechanics, assuming a k-dimensional configuration space, the equations $(q_l)^* = q_l$ and $\left(-i\hbar\frac{\partial}{\partial q_l}\right)^* = -i\hbar\frac{\partial}{\partial q_l}$ hold for the position and momentum operators; where $1 \leq l \leq k$ [1, p.92-93]. Furthermore, in the matrix theory, for any linear operator A, that is characterized by the matrix $\mathrm{a}_{\mu\nu}$, it can be seen that the adjoint A*, is the complex-conjugate-transposed matrix $\bar{\mathrm{a}}_{\nu\mu}$ [1, p.95-96]. We further define:

Definition 9: The operator A is called self-adjoint if A*=A [2, p.83]. It is also said definite if it is always true that (Af,f) ≥ 0. The operator U is said to be unitary if UU*=U*U=1 [1, p.96].

Again it should be emphasized that from the condition A*=A it follows that the operators have the same domain. Furthermore, all unitary operators are continuous, which is not always the case for self-adjoint operators. For example the position and momentum operators q and $-i\hbar\frac{\partial}{\partial q}$ are both discontinuous [1, p.97-98]. Moreover, we know that all projections are self-adjoint, and as it was stated above, both the position and momentum operators are self-adjoint [1, p.98].

For operators, just as for numerical functions in analysis, the property of continuity is of elementary importance [1, p.99]. For this reason we wish to state the subsequent theorem.

Theorem 15: A linear operator R is everywhere continuous if it is continuous at the point $f = 0$. A necessary and sufficient condition for this property is the existence of a constant C for which the inequality $||\mathrm{R}f|| \leq \mathrm{C}||f||$ holds in general. It follows that this condition is equivalent to the general validity of the inequality $|(\mathrm{R}f,g)| \leq \mathrm{C}||f||\ ||g||$. Moreover, for a self-adjoint R this is required only for $f = g$; that is, the inequalities $-\mathrm{C}||f||^2 \leq (\mathrm{R}f,f) \leq C||f||^2$ must hold [1, p.99].

It would be to our advantage, if we could somehow limit the inner product of two elements, where the other is operated on by some operator R, in a similar manner to that of the Cauchy's inequality. In practice this is achieved with theorem 16.

Theorem 16: If R is self-adjoint and definite, then $|\overline{(\mathrm{R}f,g)}| \leq \sqrt{(\mathrm{R}f,f)(\mathrm{R}g,g)}$. From $(\mathrm{R}f,f)$=0, it then follows that $\mathrm{R}f$=0 [1, p.101].

3.4 The Eigenvalue problem

With the mathematical machinery thus far developed, we can now formulate equations 1 and 2 in a unified manner. In essence, from both of the equations, we are trying to find all the non-zero solutions ϕ of

$$\mathrm{H}\phi = \lambda\phi \tag{6}$$

where H is the Hamiltonian described in chapter two and in particular it is a self-adjoint operator, ϕ is an element of the Hilbert space and λ a real number [1, p.102-103]. From the solutions we require that they span $\Re_\infty$ as a closed linear manifold [1, p.105]. In the matrix theory, that is in the space $\mathrm{F_Z}$, it is required that a matrix $\mathrm{S} = \{\mathrm{s}_{\mu\nu}\}$ can be formed from the solution ϕ of the equation 6 such that it possesses an inverse S^{-1} [1, p.103]. On the other hand, in the wave theory, that is in the space F_Ω, it is required that each wave function $\phi(\mathrm{q}_1,...,\mathrm{q}_f)$, which does not have to be a solution of equation 6, can be developed in a series of the solution ϕ such that

$$\phi(\mathrm{q}_1,...,\mathrm{q}_f) = \sum_{n=1}^{\infty} c_n\phi_n(\mathrm{q}_1,...,\mathrm{q}_f)$$

where ϕ_1,ϕ_2,... may even belong to different λ [1, p.103]. One of the properties of the solutions to the equation 6 is that they are all orthogonal to each other. This can be seen from the inner-product of two solutions that belong to different λ_1,λ_2

$$\lambda_1(\phi_1,\phi_2) = (\lambda_1\phi_1,\phi_2) = (\mathrm{H}\phi_1,\phi_2) = (\phi_1,\mathrm{H}\phi_2) = (\phi_1,\lambda_2\phi_2) = \lambda_2(\phi_1,\phi_2)$$

where you should start reading the equation from the term $(\mathrm{H}\phi_1,\phi_2)$. And as $\lambda_1(\phi_1,\phi_2) = \lambda_2(\phi_1,\phi_2)$ but $\lambda_1 \neq \lambda_2$ it must follow that $(\phi_1,\phi_2) = 0$ [1, p.104]. We could have also used the Gram-Schmidt procedure to achieve an orthonormal set. Furthermore from theorem 2 it follows that we can write both the eigenvalues λ and the solutions ϕ_1,ϕ_2 as a sequence which may or may not terminate [1, p.104-105].

It then follows that the solutions to equation 6 form a closed linear manifold, but only if we assume that H is continuous and everywhere defined [1, p.105]. Then by theorem 7 there must exist another set ψ_1,ψ_2,... that spans the same closed linear manifold as the solutions themselves. And as it was required at the beginning of the chapter, these solutions must span the whole $\Re_\infty$. From this it follows that the set ψ_1,ψ_2,... must also do this and because of theorem 6, the set ψ_1,ψ_2,... is also complete [1, p.105-106].

Therefore in quantum mechanics the solution to the eigenvalue problem requires finding a sufficient number of solutions ψ and λ to equation 6 such that an orthonormal set can be formed from them [1, p.106]. However, this is not always possible. In the wave theory for a certain subset of the solutions to equation 6 there exists no finite value for the integral of the square of the absolute value [1, p.106].

The requirement that a complete orthonormal set can be formed from the solutions of equation 6 comes from the well known algebraic fact that in $\Re_n$ the solutions of

$$\sum_{\nu=1}^{n} \mathrm{h}_{\mu\nu}\mathrm{x}_\nu = \lambda \mathrm{x}_\mu \quad (\mu = 1,...,n)$$

form a complete orthonormal set [1, p.107]. See the correspondence to equation 1. The transition to the limit $n \to \infty$ does not come without complications. Essentially we have to formulate the eigenvalue problem anew in $\Re_n$ and then transition ourselves to the limit $n \to \infty$ such that we have the desired completeness property of the solutions in $\Re_\infty$ [1, p.107]. The property that we require is that we can diagonalize the matrix form of H. This formulation is carried out in detail in reference [1] but the result is as follows: For the operator H, we seek a family of projections E(λ) where $-\infty < \lambda < \infty$. For E($\lambda$) we require the properties:

P$_1$: For $\lambda \to -\infty$, $\mathrm{E}(\lambda)f \to 0$ and for $\lambda \to \infty$, $\mathrm{E}(\lambda)f \to f$. Moreover for $\lambda \to \lambda_\mathrm{o}$, $\lambda \geq \lambda_\mathrm{o}$, $\mathrm{E}(\lambda)f \to \mathrm{E}(\lambda_\mathrm{o})f$ [1, p.118]

P$_2$: From $\lambda' \leq \lambda$" it follows that $\mathrm{E}(\lambda') \leq \mathrm{E}(\lambda")$ [1, p.118]

P$_3$: The integral

$$\int_{-\infty}^{\infty} \lambda^2 \mathrm{d}(||\mathrm{E}(\lambda)f||^2)$$

determines the domain of H. The integral may be convergent or divergent. However Hf is defined only if the integral is convergent. It follows that

$$(Hf,g) = \int_{-\infty}^{\infty} \lambda d(E(\lambda)f,g)$$

and whenever the former integral is finite the latter integral is absolutely convergent [1, p.118].

A family of projections $E(\lambda)$ with the properties $\mathbf{P}_1$ and $\mathbf{P}_2$ is known as the resolution of identity. Furthermore, a resolution of identity with a relation $\mathbf{P}_3$ to H is said to belong to H [1, p.119] It should be noted that properties $\mathbf{P}_1$ and $\mathbf{P}_2$ make no reference to the operator H [1, p.119]. Furthermore, in $\mathbf{P}_3$ we have used Stieltjes concept of the integral.

Now the eigenvalue problem in $\mathfrak{R}_\infty$ changes to the question that, does there always exist, for the operator H, resolutions of the identity belonging to H? If so, how many? The answer we would like to have, is that there always exists precisely one [1, p.119]. In addition to this we have to ascertain that, if the resolution of the identity $E(\lambda)$ belongs to a self-adjoint operator A, when is the equation

$$A\phi = \lambda\phi$$

solvable? We exclude the uninteresting $\phi = 0$ solution. Carrying out the inspection we can deduce that the equation is solvable only at the discontinuities of $E(\lambda)$ and the solutions ϕ form a closed linear manifold [1, p.120-123]. Furthermore the discontinuities of $E(\lambda)$ are known as the discrete spectrum of A [1, p.124].

In the context of this text it is difficult to emphasize the importance of the above theorem enough. However, it should be explicitly stated that the above theorem applies to all self-adjoint operators and it has been given the name spectral theorem [5, p.87-88,97]. The significance follows from its applicability to the position and momentum operators. The reader is encouraged to see references [1] and [5] for a more detailed explanation.

There is a great deal more that should be considered about the solvability of the eigenvalue problem in order to achieve mathematical rigour. However, for our purposes the development has been carried far enough. As the self-adjointness property of the operator in the eigenvalue problem is of importance, we shall briefly consider an example for the Hamiltonian.

4 Self-adjoint Hamiltonian operator

Before we continue onwards it is a good idea to recall definitions 8 and 9. In particular the requirement that for an adjoint operator the domains must be the same. Moreover for a self-adjoint operator it follows that the formal expression of the adjoint is the same. With this in mind let us turn our attention towards the example of an infinite square well in one dimension. The reason why we choose such a simplified example, is, that it is somewhat the standard problem of quantum mechanics [4] and that it serves as an accessible test case for other systems [2, p.25].

We shall first consider the expectation value of energy to familiarize the reader with the calculations. Then we shall consider the expectation value of the square of the energy first as $\langle E^2 \rangle = \langle \mathrm{H}\psi, \mathrm{H}\psi \rangle$ and then as $\langle E^2 \rangle = \langle \psi, \mathrm{H}^2\psi \rangle$. We will show that this leads to a contradiction if the proper domain of H is not considered.

Should the reader feel like some calculations are not clear, he is encouraged to check reference B for clarification. In this example we shall adopt the Schrödinger wave mechanics approach as the means of analysis. The particle in the system in question is restricted by a potential of the form:

$$V(x) = \begin{cases} \infty & |x| \geq \frac{L}{2} \\ 0 & |x| < \frac{L}{2}, \end{cases}$$

where L is the width of the well [4]. Outside this well the probability of finding the particle in question is zero [2, p.25]. This means that we can analyse the situation only within the interval $|x| < \frac{L}{2}$. In this interval the Hamiltonian takes on the form [2, p.25]

$$\mathrm{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2},$$

and the domain $D(\mathrm{H})$ of the Hamiltonian is:

$$D(\mathrm{H}) = \Big\{\phi,\ \mathrm{H}\phi \in \mathrm{F}_\Omega\Big(-\frac{L}{2},\frac{L}{2}\Big),\ \phi\Big(\pm\frac{L}{2}\Big) = 0\Big\}. \tag{7}$$

It should be noted that F_Ω is not the commonly used notation for a Hilbert space where functions are square integrable. Usually it is noted by L_2 or $\mathcal{L}^2$ where the number 2 indicates that functions are square-integrable [2, 4, p.101]. However, since in this work we have been talking about the functional spaces as F_{Z} and F_{Ω}, we hang on to that notation. In any case, the eigenvalue problem that we are trying to solve is the time-independent Schrödinger equation [2, p.25]:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi.$$

This equation can be solved to have the following normalized eigenfunctions:

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\cos\left(\frac{(n+1)\pi}{L}x\right) & \text{when } n \text{ is even} \\ \sqrt{\frac{2}{L}}\sin\left(\frac{(n+1)\pi}{L}x\right) & \text{when } n \text{ is odd.} \end{cases} \tag{8}$$

It should be noted that presenting the solutions in this form $n \in \mathbb{N}$ and that zero is included in $\mathbb{N}$. The benefit of giving the solutions in this form is that a particular eigenfunction has the same parity as the running number n. Moreover, the energy levels can be calculated to be:

$$E_n = \frac{\pi^2\hbar^2}{2mL^2}(n+1)^2. \tag{9}$$

Now let us consider this situation in a similar manner as set in references [4] and [2]. For our example let us choose the state $n = 1$ from equation 8 to define the initial normalized wave function:

$$\psi(x) = \begin{cases} \sqrt{\frac{105}{2L^5}}x\left(L - \frac{4}{L}x^2\right) & |x| \leq \frac{L}{2} \\ 0 & |x| \geq \frac{L}{2}. \end{cases} \tag{10}$$

This function fulfils all the requirements that we set for the domain of functions for the Hamiltonian in equation 7. It should be noted that at the beginning of chapter 3.4 we set the requirement that in wave mechanics, we must be able to present all wave functions in the form of equation 11. The reader is encouraged to revisit the result given in theorem 4. In more familiar terms this follows from the completeness of the solutions 8 that the initial function 10 can be expressed as a linear combination of them [2, 4, p.27-28]:

$$\psi(x) = \sum_{n=1,3,5,\dots}^{\infty} c_n\psi_n(x), \ c_n = (\psi_n,\psi) = \frac{24\sqrt{105}(-1)^{\frac{n-1}{2}+1}}{\pi^3(n+1)^3}, \tag{11}$$

where the index n is now all odd numbers. We shall need the value of $\mathrm{H}\psi$ later on so let us calculate it here:

$$\widetilde{\psi} = \mathrm{H}\psi = \frac{\hbar^2}{m}\sqrt{\frac{7560}{L^7}}x. \tag{12}$$

With all these preliminary calculations done, we can turn our attention towards the different energy values that the system can acquire. The mean energy can be calculated in a similar manner as set in the calculation of reference [4] and in [2, p.30]:

$$\langle E\rangle = \sum_{n=1,3,5,\dots}^{\infty} |c_n|^2 E_n = \frac{30240\hbar^2}{\pi^4 m L^2} \sum_{n=1,3,5,\dots}^{\infty} \frac{1}{(n+1)^4} = \frac{21\hbar^2}{mL^2}. \tag{13}$$

The energy can also be calculated by using the Hamiltonian in a manner described in [2, p.22-23] and in [4]:

$$\langle E\rangle = (\psi,\mathrm{H}\psi) = (\psi,\widetilde{\psi}) = \frac{21\hbar^2}{mL^2}. \tag{14}$$

It can be seen from equations 13 and 14 that it does not matter in which way the mean energy is calculated. Furthermore we can compare our result with the energy E_1. Calculating this from equation 9 we can see that:

$$\langle E\rangle = \frac{21}{2\pi^2} E_1. \tag{15}$$

So the mean energy of a particle in the state defined by equation 10 is just slightly more than the energy of a particle in the state ψ_1. This sounds like a reasonable result. Let us now continue to calculate $\langle E^2\rangle$ using the same two methods as above. First we get:

$$\langle E^2\rangle = \langle H\psi, H\psi\rangle = \sum_{n=1,3,5,\dots}^{\infty} |c_n|^2 E_n^2 = \frac{15120\hbar^4}{\pi^2 m^2 L^4} \sum_{n=1,3,5,\dots}^{\infty} \frac{1}{(n+1)^2} = \frac{630\hbar^4}{m^2 L^4}. \tag{16}$$

Again the reader is reminded that the sum contains only odd integers. But using the Hamiltonian in the manner as described in [2, p.23] and [4]:

$$\langle E^2\rangle = (\psi,\mathrm{H}^2\psi) = (\psi,\mathrm{H}\widetilde{\psi}) = (\psi,0) = 0. \tag{17}$$

We can see that the values of equations 16 and 17 differ even though they are supposed to be the same value of interest. So where did our calculations go wrong? Let us recall the example given just after definition 7. There we questioned the square-integrability of the expression:

$$\int_{-\infty}^{\infty} \mathrm{q}^2 |\psi(\mathrm{q})|^2 \,\mathrm{dq}. \tag{18}$$

Here, on the other hand, the expression resulting in the value of equation 17 surely is integrable. However, we also known that it must be wrong. The problem lies in the fact that we operated with the Hamiltonian to a function which is not part of it's domain. That is, the expression of equation 12 does not fulfil the boundary conditions as set in equation 7 and thus $\tilde{\psi}$ is not in the domain of H. From this it follows that $\langle \mathrm{H}\psi, \mathrm{H}\psi\rangle \neq \langle \psi, \mathrm{H}^2\psi$ and the contradiction arises.

The aim of this example was to point out the importance one should pay to mathematical rigour. It is important to keep in mind the defined domain of the operator that we are working with. As it is pointed out in reference [4] the value of $\langle E^2\rangle$ should be calculated in the following manner.

Recognizing $|(\psi_n,\psi)|^2$ as the probability that the system is in particular eigenstate with energy E_n [2, 4, p.106] and the fact that eigenvalues must be real, as pointed out at the beginning of chapter 3.4, we get the expression:

$$\begin{aligned}\langle E^2\rangle &= \langle \mathrm{H}\psi, \mathrm{H}\psi\rangle = \sum_{n=1,3,5,\ldots}^{\infty} E_n^2|(\psi_n,\psi)|^2 = \sum_{n=1,3,5,\ldots}^{\infty} E_n^2(\psi,\psi_n)(\psi_n,\psi)\\ \langle E^2\rangle &= \sum_{n=1,3,5,\ldots}^{\infty} (\psi,\mathrm{H}\psi_n)(\mathrm{H}\psi_n,\psi).\end{aligned} \tag{19}$$

Now we can use the self-adjointedness property of H in accordance with definitions 8 and 9 and the result presented in reference [4]:

$$\langle E^2\rangle = \sum_{n=1,3,5,\ldots}^{\infty} (\mathrm{H}\psi,\psi_n)(\psi_n,\mathrm{H}\psi) = \sum_{n=1,3,5,\ldots}^{\infty} (\widetilde{\psi},\psi_n)(\psi_n,\widetilde{\psi}) = (\widetilde{\psi},\widetilde{\psi}) = \frac{630\hbar^4}{m^2L^4}, \tag{20}$$

which is what we got as a result in equation 16 for $\langle E^2\rangle$. If the reader finds the transition from the sum to the expression $(\widetilde{\psi},\widetilde{\psi})$ unfamiliar, he is encouraged to revisit theorems 3 and 6.

5 Conclusions

We set out to write this work with the intention of summarizing the essential mathematical machinery that is needed for a rigorous treatment of the quantum theory. In particular, our aim was to outline the theory up to the point of the time-independent eigenvalue problem as it is presented in reference [1]. And in order to do full justice to the title of this work, we chose a simple example to point out the importance of fully appreciating the exact definitions of the operator theory.

It must be said that the first part of this work is rather abstract and does not offer much to a reader that has no experience with the quantum theory. However, our aim was to write this to a person, that has had the first contact with the quantum theory, and wishes to see a summary of the treatment, that has to be carried out, in order to properly develop the quantum theory. It is my experience that some of the mathematical niceties, as someone might call them, are overlooked in the most basic courses of quantum theory. That was the motivation behind this work.

I believe that into an extent this work functions as an adequate summary of the mathematical foundations of the quantum theory. Moreover, the example we took in chapter 4 highlights the necessity of being aware of the exact definitions in order to develop a functioning theory. The exact calculations are not necessary for the understanding of this work, but they do offer a deeper insight to the problem at hand. Therefore they are included in reference B.

On the basis of this text, a more detailed description of the spectral theory could be pursued. This could be supported with examples for the position and momentum operators. However, taking that into consideration goes beyond the scope of this work. In conclusion, I would still like to claim that this thesis has fulfilled its original purpose.

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A Glossary of terms

The terms and concepts explained here appear in alphabetical order. If the term in question is defined within the main text, it will not appear here. Since there are multiple terms taken from the source [3] the referencing is done, for purposes of practicality, in the manner that the term between the square brackets is the search word one should use in the provided site.

Associative property: A property that a certain calculation or an operation possesses. That is, for an operation $\oplus$, the following holds: $(a \oplus b) \oplus c = a \oplus (b \oplus c)$ [1, p.36].

Boundedness: A function $F(f) \in \Re$ or in any subset of $\Re$, is said to be bounded if for all f it holds that $||F(f)|| < C$ or $|F(f)| < C$ where $C \in \mathbb{R}$ [1, p.43].

Cauchy-convergence criterion: For a sequence $f_1,f_2,...$ there exists an $N = N(\epsilon)$, for each $\epsilon > 0$, such that $||f_m - f_n|| < \epsilon$ for all $m,n > N$ [1, p.46].

Cauchy's inequality: For $f,g \in \Re$ it holds that $|(f,g)| \leq ||f|| \cdot ||g||$. It follows that for the equality to hold, f,g must be identical except for a constant complex factor [1, 3, p.40-41,Cauchy's Inequality].

Closed set: A set $\mathbb{A} \in \Re$ is said to be closed if it contains all its limit points [1, p.44].

Commutation rules of quantum mechanics: For the coordinates and momentum: $[\mathrm{Q}_m,\mathrm{Q}_n] = 0, [\mathrm{P}_m,\mathrm{P}_n] = 0$ respectively. And for the coordinate momentum pair: $[\mathrm{P}_m,\mathrm{Q}_n] = -i\hbar\delta_{mn}$, where δ_{mn} is the Kronecker delta function [1, p.9].

Commutative property: For an operation $\oplus$, the following holds: $a \oplus b = b \oplus a$ [1, p.36].

Completeness of $\Re$: $\Re$ is said to be complete if a sequence $f_1,f_2,... \in \Re$ satisfies the Cauchy convergence criterion and thus is convergent [1, p.46].

Continuity: A function $F(f) \in \Re$ is continuous at the point $f_0 \in \Re$, if for each $\epsilon > 0$ there exists a $\delta > 0$, such that from $||f - f_0|| < \delta$ it follows that $||F(f) - F(f_0)|| < \epsilon$ or $|F(f) - F(f_0)| < \epsilon$ [1, p.43].

Convergence: A sequence $f_1,f_2,...$ is said to converge to f, or to have the limit f, if the numbers $||f_1 - f||,||f_2 - f||,...$ converge to zero [1, p.43].

Countably infinite: Any given set is said to be countably infinite if one can arrange the set to one-to-one correspondence with the natural numbers [3, Countably Infinite].

Diagonal matrix: A matrix H is said to be diagonal, if all elements outside the main diagonal are zero. Illustration below [2, p.90]:

$$\mathrm{H}_{m,m} = \begin{pmatrix} \mathrm{h}_{1,1} & 0 & \cdots & 0 \\ 0 & h_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathrm{h}_{m,m} \end{pmatrix}$$

Distributive property: For an operation $\oplus$, the following holds: $(a+b)\oplus c = a\oplus c + b\oplus c$ and $c\oplus(a+b) = c\oplus a + c\oplus b$ [1, p.36].

Domain: For an operator R, the domain is the class of the f for which Rf is defined [1, p.87].

Everywhere dense set: A set $\mathbb{A} \in \Re$ is said to be everywhere dense if its limit points encompass all $\Re$ [1, p.44].

Hermitian inner product: The inner product (f,g) has the following properties: $(f' + f'',g) = (f',g) + (f'',g)$, $(af,g) = a(f,g)$, $(f,g) = \overline{(g,f)}$ and $(f,f) \geq 0$. The equality in the last property is achieved if and only if $f = 0$ [1, p.38-39].

Intersection: The intersection of two sets A and B is the set of elements common to both A and B [3, Intersection].

Isometry: Isometry is a length preserving mapping between two mathematical structures [1, p.30].

Isomorphism: An isomorphism between two algebraic structures means that it is possible to set up a one-to-one correspondence between them that is linear and isometric [1, p.30].

Kronecker's delta funtion: A function which looks at two given index entities and assigns value 0 if they differ. If they are the same, then the function assigns the value 1. This can be seen below [2, p.27]:

$$\delta_{m,n} = \begin{cases} 1, \text{ for } m = n \\ 0, \text{ for } m \neq n \end{cases}$$

Lebesgue integral: This type of integral covers a wider class of functions than the Riemann integral. It is defined by using the Lebesgue measure of a set and it uses the Lebesgue sum $S_n = \sum_i \eta_i \mu(E_i)$. Here η_i is the value of the function on the subinterval i and $\mu(E_i)$ is the Lebesgue measure of the set E_i of points for which values are approximately η_i [3, Lebesgue Integral].

Lebesgue measure: An extension of classical notions of length and area to more complicated sets. For example, given an open set $S \equiv \sum_k (a_k,b_k)$ containing disjoint intervals, the Lebesgue measure μ_L of the set S, is defined as $\mu_L(S) \equiv \sum_k (b_k - a_k)$ [3, Lebesgue Measure].

Limit point: A point is a limit point of a set $\mathbb{A} \in \Re$, if it is a limit of a sequence from $\mathbb{A}$ [1, p.43-44].

Linearity condition: A transformation $\hat{T}$ is linear if the following equation holds for any vectors $|\alpha\rangle$, $|\beta\rangle$ and scalars a,b:

$$\hat{T}(a\,|\alpha\rangle + b\,|\beta\rangle) = a(\hat{T}\,|\alpha\rangle) + b(\hat{T}\,|\beta\rangle)$$

Where we used the bra-ket notation for vectors [2, p.80].

Linear manifold: For a set that contains f_1,...,f_k, it follows that $a_1 f_1 + ... + a_k f_k$ is also contained in it where a_1,...,a_k are any arbitrary constants [1, p.89]. See also the definition of a linear space below.

Linear space: For units f and g of the space, addition $f+g$ and scalar multiplication af, where $a \in \mathbb{C}$, is defined. That is if f and g belong to the space, so does $f + g$ and af. Furthermore, the space has a null element [1, p.36].

Operator: An operator R is a function defined in a subset of $\Re$ with values from $\Re$. That is, a correspondence which designates to certain $f \in \Re$ certain R$f \in \Re$ [1, p.75].

Positive definitiveness: A function F is said to be positive definitive, if the matrix $\{F(x_i x_j^{-1})\}$ is Hermitian and all its eigenvalues are non-negative [3, Positive Definite Function].

Range: The range of an operator R is the mapping of the operators domain mediated by R [1, p.87].

Regular function: A function is called regular if and only if it is analytic and single-valued throughout a region [3, Regular Function]

Separable $\Re$: $\Re$ is called separable if there exists a sequence f_1,f_2,... $\in \Re$ which is everywhere dense in $\Re$ [1, p.46].

Single valued function: For each point in the domain of the function, the function has a unique value in the range [3, Single-valued function]

Stieltjes integral: For a subdivision v_0,v_1,...,v_k of the interval [a,b]

$$a \leq v_0 < v_1 < ... < v_k \leq b$$

we form the sum

$$\sum_{n=1}^{k} f(v_n)(g(v_n) - g(v_{n-1}))$$

If this sum converges always as the subdivisions v_0,v_1,...,v_k are made smaller and smaller, then the integral

$$\int_a^b f(x)\mathrm{d}g(x)$$

exists and it is defined to be equal to this limit. For $g(x) = x$ this is equivalent to the Riemann integral [1, p.112].

B Calculations

Let us calculate the wave function defined by ψ_1 that will satisfy the boundary conditions of our system. Because we choose to inspect the sine function, which is an odd function, the initial wave function has to be of the form $\psi(x) = Ax(B - Cx^2)$. One requirement is that the function will be zero at the edges of the potential. This means that $(B - Cx^2) = 0$ must hold when $x = \pm\frac{L}{2}$. From this we can deduce that $B = L$ with $C = \frac{4}{L}$ works. From the normalization requirement we have:

$$1 = \int_{-L/2}^{L/2} |\psi(x)|^2 \mathrm{d}x = |A|^2 \int_{-L/2}^{L/2} x^2 \Big(L - \frac{4}{L}x^2\Big)^2 \, \mathrm{d}x. \tag{21}$$

This polynomial is fairly simple to integrate and by inserting the limits to the integrated function we get:

$$1 = |A|^2 L^5 \frac{2}{105} \rightarrow A = \pm\sqrt{\frac{105}{2L^5}}. \tag{22}$$

The final form of the wave function defined by ψ_1 is $\psi = \sqrt{\frac{105}{2L^5}} x\Big(L - \frac{4}{L}x^2\Big)$. Let us next calculate the coefficients c_n:

$$c_n = (\psi_n,\psi) = \int_{-L/2}^{L/2} \sqrt{\frac{2}{L}} \sin(\frac{(n+1)\pi}{L}x) \sqrt{\frac{105}{2L^5}} x(L - \frac{4}{L}x^2) \, \mathrm{d}x. \tag{23}$$

Integrating this with Maxima gives us:

$$c_n = \frac{2\sqrt{105}\left((2\pi^2 n^2 + 4\pi^2 n + 2\pi^2 - 24)\sin\left(\frac{\pi n + \pi}{2}\right) + (12\pi n + 12\pi)\cos\left(\frac{\pi n+\pi}{2}\right)\right)}{\pi^4 n^4 + 4\pi^4 n^3 + 6\pi^4 n^2 + 4\pi^4 n + \pi^4}$$

This monstrosity gives us the desired c_n. However, we can simplify it quite a lot since we are only interested in the odd integers. So let us examine the trigonometric functions more in detail. Their argument is of the form $(n+1)\pi/2$ where the index n is all the positive odd integers. From this it follows that the argument is always some multiple of pi; that is π,2π,3π,4π,... Therefore sine has a value zero all the time whereas for cosine the values are -1,1,-1,1,... It then follows that the cosine function can be expressed as $(-1)^{\frac{n-1}{2}+1}$. Therefore the above expression for c_n can be simplified to:

$$c_n = \frac{2\sqrt{105}(12\pi n + 12\pi)(-1)^{\frac{n-1}{2}+1}}{\pi^4(n^4 + 4n^3 + 6n^2 + 4n + 1)} \tag{24}$$

The expression for n in the denominator can be factorized to get:

$$c_n = \frac{2\sqrt{105}12\pi(n+1)(-1)^{\frac{n-1}{2}+1}}{\pi^4(n+1)^4} \tag{25}$$

which further simplifies to:

$$c_n = \frac{24\sqrt{105}(-1)^{\frac{n-1}{2}+1}}{\pi^3(n+1)^3} \tag{26}$$

Next, let us investigate the expression $\widetilde{\psi} = \mathrm{H}\psi$:

$$\mathrm{H}\psi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[\sqrt{\frac{105}{2L^5}}x\Big(L - \frac{4}{L}x^2\Big)\right] = -\frac{\hbar^2}{2m}\left[-\sqrt{\frac{105}{2L^5}}\frac{24}{L}x\right] = \frac{12\hbar^2}{m}\sqrt{\frac{105}{2L^7}}x. \tag{27}$$

And the final form is acquired by taking the 12 inside the square root:

$$\widetilde{\psi} = \mathrm{H}\psi = \frac{\hbar^2}{m}\sqrt{\frac{7560}{L^7}}x. \tag{28}$$

As stated in the main text the mean energy can be calculated by using the equation:

$$\langle E \rangle = \sum_{n=1,3,5,\dots}^{\infty} |c_n|^2 E_n. \tag{29}$$

It should be stressed that here the summing index goes over only the odd numbers. Continuing by inserting equation 26 and

$$E_n = \frac{\pi^2\hbar^2}{2mL^2}(n+1)^2 \tag{30}$$

into equation 29, we get:

$$\langle E \rangle = \sum_{n=1,3,5,\dots}^{\infty} \frac{60480}{\pi^6(n+1)^6}\frac{\pi^2\hbar^2(n+1)^2}{2mL^2} = \frac{30240\hbar^2}{\pi^4 mL^2}\sum_{n=1,3,5,\dots}^{\infty}\frac{1}{(n+1)^4}. \tag{31}$$

Now we notice that this form of the sum resembles a lot of the well known Riemann zeta function. The only difference is that the index runs through only all the positive odd integers; not all positive integers. However, this can be compensated with a change of the index. We notice that the term $n+1$ is always an even number. So we apply the change $n + 1 = 2k$ where the index k is allowed to have any positive integer value. With this we acquire for the mean energy the expression:

$$\langle E \rangle = \frac{30240\hbar^2}{\pi^4 m L^2} \sum_{k=1}^{\infty} \frac{1}{(2k)^4} = \frac{1890\hbar^2}{\pi^4 m L^2} \sum_{k=1}^{\infty} \frac{1}{k^4}. \tag{32}$$

Now using the well known result for the Riemann zeta function:

$$\zeta(4) = \sum_{k=1}^{\infty} \frac{1}{k^4} = \frac{\pi^4}{90}. \tag{33}$$

Substituting this value we get:

$$\langle E \rangle = \frac{1890\hbar^2}{\pi^4 m L^2} \frac{\pi^4}{90} = \frac{21\hbar^2}{mL^2}. \tag{34}$$

And a quick dimension analysis with $\hbar = [\text{Js}], m = [\text{kg}]$ and $L = [\text{m}]$ shows that:

$$\langle E \rangle = \left[\frac{(\text{Js})^2}{\text{kgm}^2} \right] = [\text{J}] \tag{35}$$

as it should be. Continuing with the mean energy, but this time calculating the value by using the Hamiltonian:

$$\langle E \rangle = (\psi, \text{H}\psi) = (\psi, \widetilde{\psi}) = \int_{-L/2}^{L/2} \sqrt{\frac{105}{2L^5}} x \left(L - \frac{4}{L} x^2 \right) \frac{\hbar^2}{m} \sqrt{\frac{7560}{L^7}} x \, \mathrm{d}x. \tag{36}$$

By taking the constants out and simplifying the expression we get:

$$\langle E \rangle = \frac{630}{L^6} \frac{\hbar^2}{m} \int_{-L/2}^{L/2} x^2 \left(L - \frac{4}{L} x^2 \right) \mathrm{d}x = \frac{630}{L^6} \frac{\hbar^2}{m} \left[\frac{L}{3} x^3 - \frac{4}{5L} x^5 \right]_{-L/2}^{L/2} \tag{37}$$

and by substituting the limits we acquire the result:

$$\langle E \rangle = \frac{21\hbar^2}{mL^2} \tag{38}$$

Continuing with the calculation of $\langle E^2 \rangle$:

$$\begin{aligned} \langle E^2 \rangle &= \sum_{n=1,3,5,\ldots}^{\infty} |c_n|^2 E_n^2 = \sum_{n=1,3,5,\ldots}^{\infty} \frac{60480}{\pi^6 (n+1)^6} \frac{\pi^4 \hbar^4 (n+1)^4}{4m^2 L^4} \\ \langle E^2 \rangle &= \frac{15120\hbar^4}{\pi^2 m^2 L^4} \sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{(n+1)^2} \end{aligned} \tag{39}$$

Applying the same trick $n + 1 = 2k$ for the index as before we get:

$$\langle E^2 \rangle = \frac{3780\hbar^4}{\pi^2 m^2 L^4} \sum_{k=1}^{\infty} \frac{1}{(k)^2}. \tag{40}$$

And by using the result known for the zeta function:

$$\zeta(2) = \sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6} \tag{41}$$

we get for $\langle E^2 \rangle$ the expression:

$$\langle E^2 \rangle = \frac{3780\hbar^4}{\pi^2 m^2 L^4} \frac{\pi^2}{6} = \frac{630\hbar^4}{m^2 L^4}. \tag{42}$$

Now let us calculate this using the Hamiltonian. For this we need to figure out the value of $\mathrm{H}\widetilde{\psi}$. Recalling equation 28 we get:

$$\mathrm{H}\widetilde{\psi} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \left[\frac{\hbar^2}{m} \sqrt{\frac{7560}{L^7}} x \right] = 0 \tag{43}$$

and therefore for the integral we have

$$\langle E^2 \rangle = (\psi, \mathrm{H}^2 \psi) = \int_{-L/2}^{L/2} \sqrt{\frac{105}{2L^5}} x \left(L - \frac{4}{L} x^2 \right) 0 \ \mathrm{d}x = 0. \tag{44}$$

Let us calculate $\langle E^2 \rangle$ in the ''proper'' manner. As stated in the main text, the value of $\langle E^2 \rangle$ can be calculated from the expression:

$$\langle E^2 \rangle = \sum_{n=1,3,5,\dots}^{\infty} E_n^2 |(\psi_n, \psi)|^2 \tag{45}$$

where we can use the well known result $|z|^2 = z^* z$ and distribute the E_n inside the inner products to get:

$$\begin{aligned} \langle E^2 \rangle &= \sum_{n=1,3,5,\dots}^{\infty} E_n^2 (\psi, \psi_n)(\psi_n, \psi) = \sum_{n=1,3,5,\dots}^{\infty} (\psi, E_n \psi_n)(E_n \psi_n, \psi) \\ \langle E^2 \rangle &= \sum_{n=1,3,5,\dots}^{\infty} (\psi, \mathrm{H}\psi_n)(\mathrm{H}\psi_n, \psi). \end{aligned} \tag{46}$$

Now because both ψ_n and ψ are in the domain of H we can use the symmetry property to get:

$$\langle E^2 \rangle = \sum_{n=1,3,5,\dots}^{\infty} (\mathrm{H}\psi, \psi_n)(\psi_n, \mathrm{H}\psi) = \sum_{n=1,3,5,\dots}^{\infty} (\widetilde{\psi}, \psi_n)(\psi_n, \widetilde{\psi}). \tag{47}$$

In the main text we used the result:

$$\sum_{n=1,3,5,\dots}^{\infty} (\widetilde{\psi}, \psi_n)(\psi_n, \widetilde{\psi}) = (\widetilde{\psi}, \widetilde{\psi}). \tag{48}$$

In agreement with reference [4]. The value of $(\widetilde{\psi},\widetilde{\psi})$ can be calculated from the integral:

$$(\widetilde{\psi},\widetilde{\psi}) = \int_{-L/2}^{L/2} \frac{\hbar^2}{m}\sqrt{\frac{7560}{L^7}}x\frac{\hbar^2}{m}\sqrt{\frac{7560}{L^7}}x \, \mathrm{d}x = \frac{\hbar^4}{m^2}\frac{7560}{L^7}\int_{-L/2}^{L/2} x^2 \, \mathrm{d}x. \tag{49}$$

And by integrating and substituting the limits we get as before:

$$\langle E^2 \rangle = (\widetilde{\psi},\widetilde{\psi}) = \frac{630\hbar^4}{m^2 L^4}. \tag{50}$$

One might also be curious as how to calculate the sum of equation 48. We shall show it explicitly here. Since both ψ_n and $\widetilde{\psi}$ are real it follows that $(\widetilde{\psi},\psi_n) = (\psi_n,\widetilde{\psi})$. Therefore equation 48 simplifies to:

$$\sum_{n=1,3,5,\ldots}^{\infty} (\widetilde{\psi},\psi_n)(\psi_n,\widetilde{\psi}) = \sum_{n=1,3,5,\ldots}^{\infty} (\widetilde{\psi},\psi_n)^2 \tag{51}$$

where $\widetilde{\psi}$ is as defined in equation 28 and the full expression for ψ_n has to be carried over from the main text:

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\cos\left(\frac{(n+1)\pi}{L}x\right) & \text{when } n \text{ is even} \\ \sqrt{\frac{2}{L}}\sin\left(\frac{(n+1)\pi}{L}x\right) & \text{when } n \text{ is odd.} \end{cases} \tag{52}$$

So we are faced with the trouble that ψ_n fluctuates between sine and cosine. Let us investigate the inner product more in detail. The expression $(\widetilde{\psi},\psi_n)$ can be calculated from the integral:

$$(\widetilde{\psi},\psi_n) = \int_{-L/2}^{L/2} \widetilde{\psi}(x)\psi_n(x) \, \mathrm{d}x. \tag{53}$$

However, we notice from equation 28 that $\widetilde{\psi}$ is an odd function and that cosine is an even function. Since the integration limits are symmetrical we can conclude that all the inner products between $\widetilde{\psi}$ and cosine are zero. And since sine is an odd function we can expect to find a finite value between $\widetilde{\psi}$ and it. Therefore it suffices only to consider the value of the integrals:

$$\int_{-L/2}^{L/2} \frac{\hbar^2}{m}\sqrt{\frac{7560}{L^7}}x\sqrt{\frac{2}{L}}\sin\left(\frac{(n+1)\pi}{L}x\right) \, \mathrm{d}x. \tag{54}$$

Before we begin, let us state the full expression to which we are trying to find a value to:

$$\langle E^2 \rangle = \sum_{n=1,3,5,\ldots}^{\infty} \left[\int_{-L/2}^{L/2} \frac{\hbar^2}{m}\sqrt{\frac{7560}{L^7}}x\sqrt{\frac{2}{L}}\sin\left(\frac{(n+1)\pi}{L}x\right) \, \mathrm{d}x \right]^2. \tag{55}$$

The constants in equation 55 can be taken out of the integral, raised to the power of two and then taken out of the sum:

$$\langle E^2 \rangle = \frac{\hbar^4}{m^2}\frac{15120}{L^8}\sum_{n=1,3,5,\ldots}^{\infty}\left[\int\limits_{-L/2}^{L/2} x\sin\left(\frac{(n+1)\pi}{L}x\right)\,\mathrm{d}x\right]^2. \tag{56}$$

Integrating this yields:

$$\langle E^2 \rangle = \frac{\hbar^4}{m^2}\frac{15120}{L^8}\sum_{n=1,3,5,\ldots}^{\infty}\left[\frac{2L^2\Big(\sin\left(\frac{\pi(n+1)}{2}\right) - \pi(n+1)\cos\left(\frac{\pi(n+1)}{2}\right)\Big)}{2\pi^2(n+1)^2}\right]^2. \tag{57}$$

For this expression we can do the same treatment as we did for the expression of c_n. Therefore the equation simplifies down to:

$$\langle E^2 \rangle = \frac{\hbar^4}{m^2}\frac{15120}{L^8}\sum_{n=1,3,5,\ldots}^{\infty}\left[\frac{-L^2(-1)^{\frac{n-1}{2}+1}}{\pi(n+1)}\right]^2. \tag{58}$$

Raising this expression to the second power and taking the constants out of the sum we get:

$$\langle E^2 \rangle = \frac{15120\hbar^4}{\pi^2 m^2 L^4}\sum_{n=1,3,5,\ldots}^{\infty}\frac{1}{(n+1)^2}. \tag{59}$$

We can already see that this is the result we arrived at in the calculation of equation 39. So by identical treatment as before we arrive at the result:

$$\langle E^2 \rangle = \frac{630\hbar^4}{m^2 L^4}. \tag{60}$$

This completes our examination of the calculations.