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Examples of Quasi-Exactly Solvability in Quantum Mechanics

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Abstract

A linear quantum mechanical system (Hamiltonian) is called exactly solvable if all its eigenfunctions and eigenvalues can be found explicitly. This means that for all its energy levels and corresponding wave functions, an explicit expression can be obtained and will give us the entire spectrum.

Such systems include the standard quadratic oscillator and several other examples, but very few.

In the late 1980s a new type of quantum mechanical systems has been discovered which are called quasi-exactly solvable. In such systems, it is possible to explicitly find a limited part of the spectrum, but not all of it, which means that there is a finite part of the energy spectrum, and related eigenfunctions that can be found exactly. Examples of such systems are quasi-exactly solvable potentials which usually depend on an integer parameter M . Usually for a given positive integer M , one can explicitly find the first M eigenfunctions and eigenvalues.

In this paper we give a short introduction to exactly solvable systems and quasi-exactly solvable systems. We give some important examples and an analysis of a particular quasi-exactly solvable system appearing in recent research. We introduce the framework of Schrödinger equations in quantum mechanics and study in details the case of the quantum harmonic oscillator. We also give a short introduction to the WKB approximation, which is a method one can use to obtain approximate information about quasi-exactly solvable systems.

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1 Introduction

In this section, we will go through the basic definitions and concepts of classical and quantum mechanics in order to understand the main ideas of quasi-exact solvability in quantum mechanics. For some notions and pre-requisites, we refer readers to the appendices.

1.1 Classical Mechanics

Classical mechanics is one of the oldest areas in physics and studies the motion of physical systems.

The earliest major progress in classical mechanics is Newtonian mechanics has been made by Isaac Newton in the 1670s and is now called Newtonian mechanics.

Isaac Newton was born in 1642 and made enormous contributions to many natural sciences, in the first place, to Newtonian mechanics and differential equations. One of his most important works is the book *Philosophiæ Naturalis Principia Mathematica* [5], which was published in 1687. In this treatise he formulated the *three universal laws of motions*; describing the relation of the forces acting on physical bodies and their resulting motions. These three laws laid the foundations of classical mechanics.

Further development of Newtonian mechanics has led to more general Hamiltonian mechanics developed mainly in the 19th century.

A *Hamiltonian system* is a dynamical system in a $2N$ -dimensional linear space with coordinates (\mathbf{q}, \mathbf{p}) which is completely determined by a scalar function $H(\mathbf{q}, \mathbf{p}, t)$, called its *Hamiltonian*.

The generalized coordinates momentum \mathbf{p} and position \mathbf{q} , where both \mathbf{p} and \mathbf{q} are vectors of dimension N , define the state of the system. The $2N$ -dimensional vector $\mathbf{r} = (\mathbf{q}, \mathbf{p})$ completely describes it.

Trajectories $(\mathbf{p}(t), \mathbf{q}(t))$ are uniquely determined by the system of the so-called *Hamilton-Jacobi equations* and their initial values, which are given by

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H(\mathbf{p}, \mathbf{q}, t)}{\partial \mathbf{q}} \quad \text{and} \quad \frac{d\mathbf{q}}{dt} = \frac{\partial H(\mathbf{p}, \mathbf{q}, t)}{\partial \mathbf{p}}. \quad (1.1)$$

In the special case where the Hamiltonian $H = H(\mathbf{p}, \mathbf{q})$ has no explicit time dependence, we can, by using the Hamilton-Jacobi equations, show that the value of the function $H(\mathbf{p}(t), \mathbf{q}(t))$ remains a constant independent of t . For more about how, see for instance [43].

By interpreting this constant with the energy, we can see that for time-independent systems the energy is preserved.

A simple example of a time-independent Hamiltonian system is the *harmonic oscillator*. Its phase space is 2-dimensional with coordinates $\mathbf{p} = p$ and $\mathbf{q} = x$, and its

Hamiltonian is given by

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2, \quad (1.2)$$

where p is the momentum, m is the mass of a particle, x is the position and k is the force constant, which is also known as the *spring constant* and is measured in Newtons per meter. Note that H is the total energy of the system, $\frac{p^2}{2m}$ is the potential energy and $\frac{1}{2}kx^2$ is the kinetic energy.

Since the Hamiltonian is independent of time, the total energy of the system is preserved.

1.1.1 The Harmonic Oscillator

The harmonic oscillator is one of the simplest systems in classical mechanics. It models small motions of a pendulum or a weight on a spring. When a weight attached to a spring is displaced from its equilibrium position, the spring reacts with a restoring force \vec{F} ,

$$\vec{F} = -k\vec{x}, \quad (1.3)$$

proportional to its displacement. Here k is a non-negative constant characterizing the constant of proportionality, often called the *spring constant*, and is measured in Newtons per meter. The spring constant is a measure of the stiffness of the spring and varies for different springs and materials. The greater the spring constant, the stiffer the spring, which makes it more difficult for it to stretch. The displacement \vec{x} is in the positive x -direction. The potential energy $\frac{1}{2}kx^2$ of the weight during the motion is interacting with its kinetic energy $\frac{1}{2}mv^2$. Therefore, the total energy E of the oscillating weight is the sum of its kinetic energy and its potential energy,

$$E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2. \quad (1.4)$$

In particular, at the equilibrium position of the spring, when $x = 0$, all of its potential energy has been converted into kinetic energy. Hence,

$$E = \frac{1}{2}mv^2.$$

Newton's second law for objects and systems with constant mass is given by

$$F = m\frac{d^2x}{dt^2}. \quad (1.5)$$

By substituting (1.3) into (1.5), we obtain

$$m\frac{d^2x}{dt^2} = -kx. \quad (1.6)$$

It is standard to remove the constant k from the Hamiltonian and replacing it with the classical oscillator frequency $\omega^2 = \frac{k}{m}$. We use this to rewrite (1.6) as

$$\frac{d^2x}{dt^2} + \omega^2x = 0. \quad (1.7)$$

From theory of ordinary differential equations, we know that (1.7) is a homogeneous linear differential equation with constant coefficients, so its solutions can be written as linear combinations of suitably chosen exponential functions, for example as $x(t) = Ce^{\lambda t}$. Differentiating and by inserting it into (1.7), we obtain the so-called characteristic polynomial $\lambda^2 + \omega^2 = 0$. The solutions for the constant λ are now given by

$$\lambda_{1,2} = \pm i\omega.$$

This means that $x_1(t) = C_1 e^{i\omega t}$ and $x_2(t) = C_2 e^{-i\omega t}$, with $C_1, C_2 \in \mathbb{C}$ solve the differential equation. The general solution is therefore given by

$$x(t) = C_1 e^{i\omega t} + C_2 e^{-i\omega t}. \quad (1.8)$$

By using Euler's formula $e^{i\phi} = \cos \phi + i \sin \phi$, we can express equation (1.8) in the real form as the following,

$$\operatorname{Re} x(t) = C_1 \cos(\omega t) + C_2 \sin(\omega t).$$

If $|C_1| = |C_2|$, the right-hand side is equal to $A \sin(\omega t + \phi)$. Then we have

$$x(t) = A \sin(\omega t + \phi), \quad (1.9)$$

where A denotes the amplitude of the motion and ϕ determines the starting point on the sine wave. Both A and ϕ can be determined from the initial conditions.

By inserting (1.9) together with its derivative into (1.4), and choosing $\phi = 0$, we obtain the total energy

$$\begin{aligned} E &= \frac{1}{2} A^2 (m\omega^2 (\cos \omega t)^2 + k(\sin \omega t)^2) \\ &= \frac{1}{2} A^2 \left(m \left(\frac{k}{m} \right) (\cos \omega t)^2 + k(\sin \omega t)^2 \right) = \frac{1}{2} k A^2. \end{aligned} \quad (1.10)$$

The total energy of the system is constant and independent of time.

We will return to the quantum analogue of the harmonic oscillator later.

1.1.2 Hamiltonian Systems and Symplectic Structure

A fundamental property of the Hamilton-Jacobi equations is that they preserve the so-called standard symplectic structure. In this section, we sketch how the Hamiltonian dynamical system fits in the context of symplectic geometry.

We start with some definitions.

Definition 1.1 (Differential Manifold). A differential manifold is a topological space which locally resembles real n -dimensional Euclidean space with a globally defined structure that allows differential calculus on the manifold.

Definition 1.2 (k -form). A k -form is an oriented density which can be integrated over a k -dimensional oriented manifold.

An example is the 1-form $f(x) dx$: if $a < b$, then the 1-form can be integrated over the interval $[a, b]$ as $\int_a^b f(x) dx$.

Another example is the 2-form, which can be integrated over an oriented surface.

Now we are ready to sketch.

Symplectic geometry studies differential manifolds which are equipped with a closed, non-degenerate 2-form that is defined on a smooth even-dimensional space. A $2N$ -dimensional symplectic geometry can be formed by taking pairs of directions

$$((x_1, x_2), (x_3, x_4), \dots, (x_{2N-1}, x_{2N}))$$

in a $2N$ -dimensional manifold along with a symplectic form

$$\omega = dx_1 \wedge dx_2 + dx_3 \wedge dx_4 + \dots + dx_{2N-1} \wedge dx_{2N}.$$

Let us give an example of a symplectic structure for the motion of a body in one dimension. In order to specify its trajectory, one requires both its position \mathbf{q} and its momentum \mathbf{p} . The symplectic form in this case is

$$\omega = d\mathbf{p} \wedge d\mathbf{q}.$$

For general $m \in \mathbb{N}$ we let $I = I_m$ and $0 = 0_m$ denote the $m \times m$ identity and zero matrix, respectively. The subscript will be omitted, whenever no confusion may arise. We let J be the real skew-symmetric $2N \times 2N$ matrix

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}.$$

We can, by taking $\vec{\mathbf{x}}$ to be the $2N$ -dimensional vector $\vec{\mathbf{x}} = \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}$ and $\mathbf{F}(\vec{\mathbf{x}})$ to be $\mathbf{F}(\vec{\mathbf{x}}, t) = J \cdot \frac{\partial H}{\partial \vec{\mathbf{x}}}$, with $\frac{\partial H}{\partial \vec{\mathbf{x}}} = \begin{bmatrix} \partial H / \partial \mathbf{p} \\ \partial H / \partial \mathbf{q} \end{bmatrix}$. We can now write the equations in (1.1) as

$$\frac{d\vec{\mathbf{x}}}{dt} = \mathbf{F}(\vec{\mathbf{x}}, t). \tag{1.11}$$

The J -matrix preserves the Hamiltonian structure.

1.2 Quantum Mechanics

In the end of the 19th century, important experiments and observations such as the black-body radiation and the correspondence between energy and frequency of the photoelectric effect were made. Such results could not be explained from the positions of classical mechanics. More exactly, the experiments with small particles such as electrons, contradicted the interpretation as bodies since they both have shown the characteristic features of particles as well as waves, and a new type of physics was needed to explain these phenomena. This was how quantum mechanics gradually arose; as a theory to explain such observations.

1.2.1 The Schrödinger Equation

In 1926, the Austrian physicist Erwin Schrödinger published a paper on wave mechanics called *Quantisierung als Eigenwertproblem* (Quantization as an Eigenvalue Problem) [6] and there presented what we now call the *Schrödinger equation*. In this paper, he gave a heuristic derivation of the wave equation for time-independent quantum systems and showed that one can obtain the correct predictions of the energy eigenvalues for a hydrogen-like atom. This marked the beginning of the creation of quantum mechanics.

In quantum mechanics, the *wave function*, denoted by $\Psi(x, t)$, is a complex-valued function which describes the quantum mechanical state of an elementary particle or a system of elementary particles. Its amplitude $|\Psi(x, t)|^2$ determines the probability density for the position or the momentum of the particle. As we already mentioned, light behaves as both a particle and a wave, which we call *wave-particle duality*. The photon is a particle with energy E , but has a frequency ν , which is the number of occurrences of a repeating event per unit of time, which is a wave attribute, and h is the Planck constant, where

$$E = h\nu. \tag{1.12}$$

The particle has a momentum p , but at the same time another wave attribute - a wavelength λ , which is given by

$$\lambda = \frac{h}{p}. \tag{1.13}$$

In 1924, French physicist Louis de Broglie proposed that the wave-particle duality was also valid for the matter particles such as electrons and neutrons, and concluded that (1.12) also holds for these particles.

We can rewrite (1.13) as

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \frac{2\pi}{\lambda} = \hbar k, \tag{1.14}$$

which in terms of the momentum fixes the wavelength, where $\hbar = \frac{h}{2\pi}$ and where k is the wave number.¹

We can also rewrite (1.12) as

$$E = \hbar\omega, \tag{1.15}$$

¹In quantum mechanics, it is convenient to use the wave number $k = \frac{2\pi}{\lambda}$ instead of the wavelength λ . A wave number is defined as the number of radians per unit distance, and $\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34} \text{ Js}$, where h is *Planck's constant*.

where $\omega = 2\pi\nu$ is the frequency of the wave and is measured in radians per second, which fixes the frequency of the wave ω in terms of the energy E of the particle.

The relations in (1.14) and (1.15) are called *de Broglie relations* and are valid for all particles. We can use these to derive the Schrödinger equation as follows.

The most basic wave function has the form,

$$\Psi(x, t) = Ae^{i\omega(t - \frac{x}{v})}, \quad (1.16)$$

where A is the amplitude of the oscillations, ω is the angular frequency, t is the time, x is the position and v is the velocity of the particle associated with this wave phenomenon.

By using (1.15), we can rewrite (1.16) as

$$\Psi(x, t) = Ae^{-i2\pi\nu(t - \frac{x}{v\lambda})} = Ae^{-i2\pi(\nu t - \frac{x}{\lambda})}, \quad (1.17)$$

where ν is the frequency of oscillations.

By inserting $\omega = 2\pi\nu$ into (1.15) we obtain $E = 2\pi\hbar\nu$. Solving for ν gives $\nu = \frac{E}{2\pi\hbar}$. We also decide to rewrite (1.13) as $\lambda = \frac{2\pi\hbar}{p}$. Now, we will use both of these relations and insert them into (1.17) to obtain

$$\Psi(x, t) = Ae^{-i2\pi(\frac{Et}{2\pi\hbar} - \frac{xp}{2\pi\hbar})} = Ae^{-\frac{i}{\hbar}(Et - xp)}, \quad (1.18)$$

which is a wave function associated with the motion of a free particle moving in the $+x$ direction with total energy E and momentum p .

From classical mechanics, momentum is defined as $p = mv$ so we can write the total energy as the following equation

$$E = \frac{1}{2}mv^2 + V(x) = \frac{p^2}{2m} + V(x), \quad (1.19)$$

where $V(x)$ is the potential energy.

If we would multiply both sides of equation (1.19) by the wave function, we obtain

$$E\Psi = \frac{p^2}{2m}\Psi + V(x)\Psi. \quad (1.20)$$

Differentiating (1.18) twice with respect to x , we obtain

$$\frac{\partial\Psi}{\partial x} = A\left(\frac{ip}{\hbar}\right)e^{-\frac{i}{\hbar}(Et - xp)} \quad (1.21)$$

$$\frac{\partial^2\Psi}{\partial x^2} = -A\left(\frac{p^2}{\hbar^2}\right)e^{-\frac{i}{\hbar}(Et - xp)} = \frac{p^2}{\hbar}\Psi. \quad (1.22)$$

Therefore, $p^2\Psi = -\hbar^2\frac{\partial^2\Psi}{\partial x^2}$.

If we now differentiate (1.18) with respect to t , we will obtain the time derivative,

$$\frac{\partial\Psi}{\partial t} = -A\frac{iE}{\hbar}e^{-\frac{i}{\hbar}(Et - xp)} = \frac{-iE}{\hbar}\Psi, \quad (1.23)$$

so $E\Psi = \frac{-\hbar}{i} \frac{\partial\Psi}{\partial t}$.

We use our results above and insert them into (1.20)

$$-\frac{\hbar}{i} \frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi. \quad (1.24)$$

Since Ψ depends on both x and t , we write (1.24) as

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right] \Psi(x, t), \quad (1.25)$$

which is the required Schrödinger equation.

By solving the Schrödinger equation (1.25) with a given potential, we obtain the wave function $\Psi(x, t)$ of the particle. Any solution to the Schrödinger equation with given initial data $\Psi(x, 0)$ is unique. As the wave function is time-dependent, it changes with time. The wave function is very useful for describing physical processes such as scattering or interference of particles.

1.2.2 The Time-Independent Schrödinger Equation and its Solutions

The time-independent Schrödinger equation relates in an interesting way to the time-dependent one. The time-independent Schrödinger equation only involves one independent variable x , and is therefore an ordinary differential equation instead of a partial differential equation, which the time-dependent Schrödinger equation is, but exactly how does one come up with it? With the requirement that H is time-independent, one can derive the time-independent Schrödinger equation by separating the wave function in a time-dependent and a space-dependent part,

$$\Psi(x, t) = f(t)\Psi(x). \quad (1.26)$$

We insert it into the time-dependent Schrödinger equation (1.25),

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

where

$$\begin{cases} \frac{\partial^2\Psi(x)f(t)}{\partial x^2} = f(t) \frac{\partial^2\Psi(x)}{\partial x^2} \\ \frac{\partial\Psi(x)f(t)}{\partial t} = \Psi(x) \frac{\partial f(t)}{\partial t}. \end{cases}$$

Thus, we rewrite the Schrödinger equation,

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

By dividing both sides by $f(t)\Psi(x)$, we have

$$\frac{1}{\Psi(x)} \left[-\frac{\hbar^2}{2m} \frac{\partial^2\Psi(x)}{\partial x^2} + V(x)\Psi(x) \right] = i\hbar \frac{1}{f(t)} \frac{df(t)}{dt}.$$

Since the right-hand side only depends on t , while the left-hand side is solely dependent on x , both of them must be equal to a constant. We call this constant E , with units of energy because the Hamiltonian operator H has units of energy. Then, we get

$$\frac{1}{\psi(x)} \left[-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) \right] = E$$

and

$$i\hbar \frac{1}{f(t)} \frac{\partial f(t)}{\partial t} = E,$$

where the first equation yields

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = H\psi(x), \quad (1.27)$$

and the second equation yields

$$i\hbar \frac{\partial f(t)}{\partial t} = Hf(t), \quad (1.28)$$

with the solution

$$f(t) = e^{-iEt/\hbar}.$$

The states $\psi(x, t) = e^{-iEt/\hbar}\psi(x)$ are called stationary, since the associated probability density functions $|\psi(x, t)|^2 = |\psi(x)|^2$ are time-independent.

For the space-dependent part, we obtain

$$H\psi = E\psi$$

accordingly. This equation is called the time-independent Schrödinger equation.

It follows that E must be an eigenvalue of the Hamiltonian $H := -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$. In other words,

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (1.29)$$

for some eigenvalue E and some eigenfunction $\psi \in \mathbb{C}$.

The relationship between the time-dependent and the time-independent equation can now be explained in the following way: Assume that E is an eigenvalue of the Hamiltonian with eigenfunction $\psi(x)$. Then we can observe that

$$i\hbar \frac{\partial}{\partial t} e^{-iEt}\psi(x) = i\hbar \cdot (-iEe^{-iEt}\psi(x)) = E\hbar e^{-iEt}\psi(x) = \hbar e^{-iEt} H\psi(x).$$

In other words, the function $\Psi(x, t) := e^{-iEt}\psi(x)$ solves the time-dependent Schrödinger equation. We summarize this information in the following lemma.

Lemma 1. *Assume that $\psi(x)$ solves the time-independent Schrödinger equation (1.29). Then the propagated function $\Psi(x, t) := e^{-iEt}\psi(x)$ is the unique solution to the time-dependent Schrödinger equation (1.27). Moreover, the derivative of the wave function is given by*

$$\frac{d}{dx} \Psi(x, t) = e^{-iEt} \frac{d}{dx} \psi(x).$$

We will now study the solutions to the time-independent Schrödinger equation (1.29). For a Hamiltonian H we are interested in finding its eigenfunctions ψ and its eigenvalues E , which are its corresponding energies. The possible energies of the time-independent Schrödinger equation may be either a discrete set, or a continuous set. For any given potential, there are many solutions. For convenience, we assume that the eigenfunctions and their energies can be enumerated by,

$$\begin{aligned} \psi_1(x), & E_1 \\ \psi_2(x), & E_2 \\ \vdots & \quad \quad \quad \vdots \end{aligned} \tag{1.30}$$

Let us assume that the eigenfunctions form a complete set of orthonormal functions (where every function can be expressed as a linear combination of some members of that set),

$$\int \psi_i^*(x)\psi_j(x) = \delta_{ij}, \tag{1.31}$$

where δ is the *Kronecker delta*, satisfying

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

If we now consider the time-independent Schrödinger equation in the following form,

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E - V(x))\psi, \tag{1.32}$$

then its solutions ψ will depend on the properties of the potential $V(x)$. It is difficult to make any general statements about the wave function, so we have to put restrictions on the potentials. Here, we will consider continuous as well as piece-wise continuous potentials. The potentials can also be unbounded and we will allow them to become $+\infty$ beyond certain points, which we will represent as thick barriers. Lastly, we will allow delta functions but we will not consider their powers nor their derivatives.

We seek to understand the general properties of the functions ψ and their behavior at points where $V(x)$ may have singularities. But we start by claiming that we must have a continuous wave function, because, if ψ is discontinuous, its derivative will contain the physical delta functions, also known as the Dirac delta function². Then, ψ'' on the left-hand side of equation (1.32) will contain derivatives of delta functions, which means that the right-hand side, too, has to contain derivatives of delta functions and then they would have to appear in the potential. This will contradict our earlier assumption that our potential would not contain derivatives of delta functions. So, our ψ must be continuous.

Now, we consider four possibilities regarding the potential $V(x)$:

- (1) $V(x)$ is continuous (and so is ψ). The continuity of ψ and (1.32) imply that ψ'' is also continuous. For that to be fulfilled, ψ' has to be continuous too.
- (2) $V(x)$ has finitely many discontinuities. Then ψ'' also has finitely many discontinuities. In this case, ψ' must be continuous with discontinuous derivative.

²See Appendix C.

(3) $V(x)$ contains delta functions. In this case, ψ'' also contains delta functions, and ψ' has a finite amount of discontinuities.

(4) $V(x)$ contains a thick barrier at point $x = a$ i.e., a potential that becomes infinite for $x > a$ and is finite to the left of $x = a$. Here, the wave function will vanish when $x \geq a$, and ψ' will be finite as $x \rightarrow a$, but vanish for $x > a$. So, ψ' is discontinuous at this barrier.

Now to summarize the cases above; in cases (1) and (2), ψ' is continuous, and in cases (3) and (4), it can have a finite discontinuity. That is, both ψ and ψ' are continuous unless the potential contains delta functions or thick barriers, where ψ' may have finite discontinuities.

We can explain the continuity of ψ and ψ' in the case of a potential with finitely many discontinuities using a different argument.

We start by integrating both sides of (1.32), from $a - \epsilon$ to $a + \epsilon$, and then we let $\epsilon \rightarrow 0$. We obtain the following,

$$\int_{a-\epsilon}^{a+\epsilon} dx \frac{d}{dx} \left(\frac{d\psi}{dx} \right) = -\frac{2m}{\hbar^2} \int_{a-\epsilon}^{a+\epsilon} dx (E - V(x))\psi(x), \quad (1.33)$$

where the left-hand side integrand can be written as $\frac{d\psi}{dx}|_{a+\epsilon} - \frac{d\psi}{dx}|_{a-\epsilon}$.

Note that the potential $V(x)$ in (1.33) shows us that there exists bounded particles. Therefore, we will have boundary conditions, which we will try to find.

The discontinuity of ψ' at $x = a$ is, by definition, the limit as $\epsilon \rightarrow 0$, so the left-hand side can be written as

$$\lim_{\epsilon \rightarrow 0} \left(\frac{d\psi}{dx} \Big|_{a+\epsilon} - \frac{d\psi}{dx} \Big|_{a-\epsilon} \right) = \Delta_a \left(\frac{d\psi}{dx} \right). \quad (1.34)$$

We can now write

$$\Delta_a \left(\frac{d\psi}{dx} \right) = \lim_{\epsilon \rightarrow 0} \frac{2m}{\hbar^2} \int_{a-\epsilon}^{a+\epsilon} dx (V(x) - E)\psi(x). \quad (1.35)$$

Here, the potential V is not infinite around $x = a$ but discontinuous. ψ , too, is finite. E is assumed to be finite. Since the integrand remains finite, and the range of the integral becomes vanishingly small about $x = a$, the integral goes to 0. Therefore, we have

$$\Delta_a \left(\frac{d\psi}{dx} \right) = 0. \quad (1.36)$$

In this way, we obtained one of our boundary conditions: there is no discontinuity in ψ' .

We will now obtain the second boundary condition: the continuity of ψ .

We use (1.33) and apply the range from $x_0 < a$ to x . We obtain

$$\frac{d\psi(x)}{dx} = \frac{d\psi}{dx} \Big|_{x_0} - \frac{2m}{\hbar} \int_{x_0}^x (E - V(x')) dx' \quad (1.37)$$

and note that the integral is a bounded function of x . Now, we integrate (1.37) from $a - \epsilon$ to $a + \epsilon$,

$$\psi(a + \epsilon) - \psi(a - \epsilon) = 2\epsilon \left. \frac{d\psi}{dx} \right|_{x_0} - \frac{2m}{\hbar} \int_{a-\epsilon}^{a+\epsilon} dx \int_{x_0}^x dx' (E - V(x')). \quad (1.38)$$

By letting $\epsilon \rightarrow 0$, the first term on the right-hand side vanishes and the second term goes to 0, since the second integral is a bounded function of x . Finally, we have $\Delta_a \psi = 0$, which shows that the wave function is continuous at $x = a$, which is our second boundary condition.

1.2.3 The Quantum Harmonic Oscillator

In quantum mechanics, to describe the total energy (i.e. both the kinetic and the potential energy) of a system we can use the Hamiltonian H . In the case of the quantum harmonic oscillator, the Hamiltonian is given by

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2, \quad (1.39)$$

where m is the mass of the particle, $\hat{p} = -i\hbar \frac{\partial}{\partial x}$ is the momentum operator, $\omega = \sqrt{\frac{k}{m}}$ is the angular frequency of the oscillator and $\hat{x} = i\hbar \frac{\partial}{\partial p}$ is the position operator which is given by x . The first term in the right-hand side represents the kinetic energy of the particle and the second term represents its potential energy.

The time-independent Schrödinger equation is then

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \right] \psi(x) = E\psi(x). \quad (1.40)$$

The *spectrum* of the Hamiltonian, also known as the *energy spectrum* or set of *energy eigenvalues* provides us with the information, for instance the frequency, the mass and the energy, about possible solutions of the time-independent equation. In a physical setting it may be obtained by measuring the total energy of the system.

We want to find the spectrum of the quantum harmonic oscillator, but first we notice that the right-hand side of equation (1.39) is an expression of a characteristic length scale a , such that $\frac{\hbar^2}{2m} \frac{1}{a^2} = \frac{1}{2}m\omega^2 a^2$ where $a^2 = \frac{\hbar}{m\omega}$. Now, we will find the spectrum. We start by multiplying equation (1.32) by $(\frac{2}{\hbar\omega})$. We will then get

$$-\frac{\hbar}{m\omega} \frac{d^2\psi}{dx^2} + \frac{m\omega}{\hbar} x^2 \psi = \frac{2E}{\hbar\omega} \psi, \quad (1.41)$$

We introduce the dimensionless constant $\mathcal{E} := \frac{2E}{\hbar\omega}$ and we continue by writing $x = au$, where u is a new variable but without units. This gives us $\frac{d}{dx} = \frac{1}{a} \frac{d}{du}$ and $\frac{d^2}{dx^2} = \frac{1}{a^2} \frac{d^2}{du^2}$. By inserting these derivatives as well as the above expression for a^2 into (1.41), we obtain

$$-\frac{d^2\psi}{du^2} + u^2\psi = \mathcal{E}\psi. \quad (1.42)$$

We want to apply asymptotic analysis to gain insight into what will happen. We notice that

$$\lim_{u \rightarrow \infty} (u^2 - \mathcal{E}) \approx u^2.$$

In (1.42), we can see that $u^2\psi$ will be much larger than $\mathcal{E}\psi$ regardless what ψ is, since we are working with some fixed energy. So, the equation we will try to solve, as $u \rightarrow \infty$, is $\psi'' = u^2\psi$. We try $\psi(u) = \psi e^{\alpha u^2/2}$, where α is a number, and we find $\frac{\partial\psi}{\partial u} = \alpha u\psi$ and $\frac{\partial^2\psi}{\partial u^2} = (\alpha + \alpha^2 u^2)\psi \approx \alpha^2 u^2\psi$. We compare this with the differential equation in (1.42). We see that we need $\alpha^2 = 1$, which gives us $\alpha = \pm 1$. Since this is a second order differential equation, it should have two independent solutions. So for $u \rightarrow \infty$, we have $\psi(u) = \psi_A e^{u^2/2} + \psi_B e^{-u^2/2}$.

The solution with coefficient A will not yield an energy eigenfunction, since it diverges as $u \rightarrow \infty$, so we use the following ansatz,

$$\psi(u) = s(u)e^{-u^2/2}. \quad (1.43)$$

Finally, plugging (1.43) into (1.42) and simplifying, we find a second-order linear differential equation for $s(u)$ given by

$$\frac{d^2s}{du^2} - 2u\frac{ds}{du} + (\mathcal{E} - 1)s = 0. \quad (1.44)$$

If we assume that $s(u)$ is a polynomial of degree j , giving

$$s(u) = u^j + \alpha_1 u^{j-1} + \alpha_2 u^{j-2} + \dots,$$

then the first term in equation (1.44) is a polynomial of degree $j - 2$ and each of the other two terms are of degree j . So in order for the equation to make sense, the coefficients of u^j and u^{j-1} have to vanish. We start by calculating the coefficient of u^j :

$$-2j + \mathcal{E} - 1 = 0 \quad \Rightarrow \quad \mathcal{E} = 2j + 1.$$

From this, we know that a polynomial solution $s(u)$ of degree j requires $\mathcal{E} = 2j + 1$. We continue by calculating the coefficient of u^{j-1} :

$$(-2(j-1) + \mathcal{E} - 1)\alpha_1 = 0.$$

This is satisfied when $\alpha_1 = 0$. Thus, the polynomial is of the following form,

$$s(u) = u^j + \alpha_2 u^{j-2} + \dots$$

Since the harmonic oscillator is even, the states have to be either even or odd, and since the exponential in (1.43) is even, $\psi(u)$ will be either even or odd, depending on what $s(u)$ is.

If we now assume that $s(u)$ is analytical and is a polynomial of degree k , we can use the power series expansion which is a method used in for instance ordinary differential equations,

$$s(u) = \sum_{k=0}^{\infty} a_k u^k. \quad (1.45)$$

We select from each term the contribution to the coefficient of w^j and plug it into the differential equation. This yields

$$\sum_{j=0}^{\infty} ((j+1)(j+2)a_{j+2} - (2j+1-\mathcal{E})a_j)w^j = 0, \quad (1.46)$$

which means that

$$a_{j+2} = \frac{2j+1-\mathcal{E}}{(j+1)(j+2)}a_j. \quad (1.47)$$

In order to find all of the coefficients, we need to specify both a_0 and a_1 . Let us suppose that there exists an n such that when $j = n$, the numerator of (1.47) will be equal to 0, giving $\mathcal{E} = 2n + 1$. Note that all of the subsequent terms satisfy $a_j = 0$. From before, we also know that $\mathcal{E} := \frac{2E}{\hbar\omega}$, therefore, under the assumptions we made, the energy eigenvalues for a quantum harmonic oscillator are given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad (n = 0, 1, 2, \dots). \quad (1.48)$$

Figure 1 below shows the energy eigenvalues for the first three energy levels for a quantum harmonic oscillator. The parabola represents the potential $V(x)$.

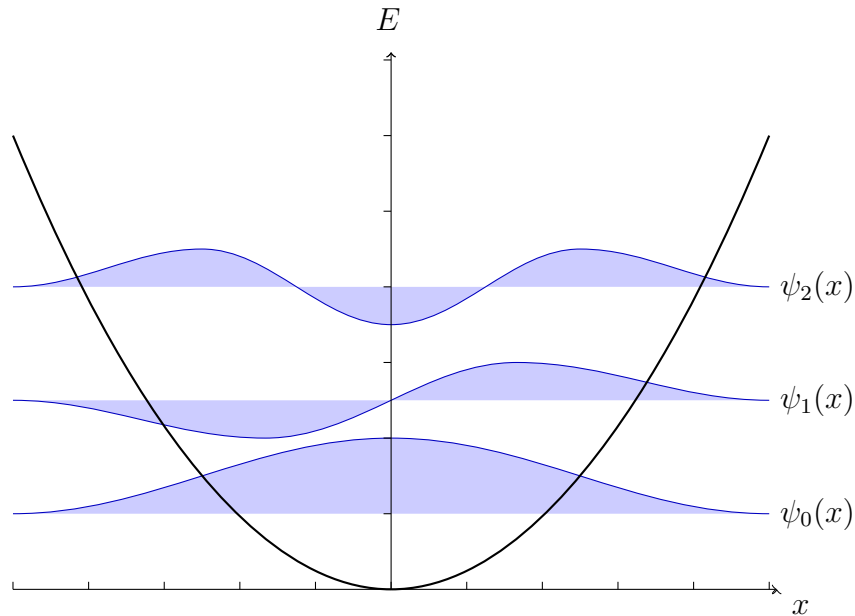


Figure 1. Wave function representations for the first three energy eigenvalues.

2 Potentials

In this section we will provide examples of both exactly solvable potentials and quasi-exactly solvable potentials.

Finding such potentials is still an active area of research in physics.

2.1 Exactly Solvable Potentials

As we mentioned above, exactly solvable potentials are potentials which can be solved analytically exactly; that is all their wave functions and all the energy levels from the ground state up to arbitrary excited states can be calculated in a finite number of algebraic steps.

There are several known exactly solvable potentials besides the quadratic oscillator. Table 1 describes a few of them; the first column contains the name of the potential, the second column presents its equation, and the last column contains the description of the equation.

The Coulomb Potential [29]	$V_E = \frac{1}{4\pi\epsilon_0} \frac{Q}{r}$	The Coulomb Potential V_E describes the electric potential energy from a point charge Q , with a distance r from another charge, where ϵ_0 is the permittivity of vacuum.
The Morse Potential [30]	$V'(r) = D_e(1 - e^{-a(r-r_e)})^2$	The Morse Potential is a model for the potential energy of a diatomic molecule, where r is the distance between atoms, D_e is the dissociation energy, a is the width of the potential and r_e is the equilibrium bond distance.
The Rosen-Morse Potential [31]	$V_{tRM}^{(a,b,\lambda)}(\chi) = \frac{a(a-\lambda)}{\sin^2 \lambda \chi} - 2b \cot \lambda \chi$	The Rosen-Morse Potential is a trigonometric potential, where $\lambda \chi \in [0, \pi]$ rescales the parameter of the angle, while $\chi = \frac{r}{R}$, where r is the relative distance, and R is a matching length parameter.
The Quartic Potential [37]	$V(x) = ax^2 + bx^4, \quad a, b \in \mathbb{R}_{>0}$	

The Pöschl-Teller Potential [9]	$V(x) = \frac{\hbar^2 \alpha^2}{8\pi^2 m} \left[\frac{\nu(\nu-1)}{\sin^2 \alpha(r-r_0)} + \frac{\mu(\mu-1)}{\cos^2 \alpha(r-r_0)} \right]$	The symmetric Pöschl-Teller Potential is one of the potentials for which the Schrödinger equation is analytically solvable. We have that m is the mass of the oscillator, α is a reciprocal length, ν and μ are two numbers greater than one, and $0 \leq \alpha(r - r_0) \leq \frac{\pi}{2}$.
The Woods-Saxon Potential [32]	$V(r) = -\frac{V_0}{1 + \exp\left(\frac{r-R}{a}\right)}$	The Woods-Saxon Potential is a mean field potential which is used to approximately describe the forces applied on each nucleon inside the atomic nucleus, where V_0 is the depth of the potential well, r is the distance from the center of the nucleus, A is the atomic mass number, $R = r_0 A^{1/3}$ is the nuclear radius where $r_0 = 1.25$ fm. By transforming this potential into a hypergeometric differential equation, you can solve the Schrödinger equation analytically.

Table 1: Examples of exactly solvable potentials.

2.2 Quasi-Exactly Solvable Potentials

As mentioned above, in the late 1980s a new type of quantum mechanical systems was discovered, which are called quasi-exactly solvable.

Unlike exactly solvable potentials, where the whole spectrum can be found explicitly, for quasi-exactly solvable potentials only a limited part of the energy spectrum can explicitly be found. Table 2 presents a few of them; the first column contains the name of the potential, the second column presents its equation, and the last column contains the description of the equation.

The Anharmonic Oscillator Potential [19], [21]	$V(x) = x^6 + 2bx^4 + (b^2 - (4m + 2p + 3))x^2, \quad p \in \{0, 1\}$	The one-dimensional sextic anharmonic oscillator is frequently used to approximate various situations in quantum mechanics.
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The Quartic Potential [18]	$V(x) = -x^4 + 2iax^3 + (a^2 - 2b)x^2 + 2i(ab - J)x, \quad J \in \mathbb{N}, a, b \in \mathbb{R}$	Based on the assumption that the Hamiltonian is non-Hermitian. We can find exactly the first J eigenvalues and eigenfunctions. The lowest J eigenvalues are the roots of a polynomial of degree J . Its spectrum is real, discrete and bounded below.
The Inverse Quartic Power Potential [10]	$V(r) = \frac{a}{r} + \frac{b}{r^2} + \frac{c}{r^3} + \frac{d}{r^4}, \quad d > 0$	It determines analytic properties of the scattering amplitude in the case of a singular potential. This form of anharmonicity is useful in physical applications.
The Inverse Sextic Power Potential [10]	$V(r) = \frac{e}{r^4} + \frac{d}{r^6}, \quad d > 0$	This is the case of a non-relativistic quantum mechanics problem of scattering by the singular potential $\frac{d}{r^{2+2n}} + \frac{e}{r^{2+n}}$, where $n = 2$. It is used in atomic, molecular and nuclear physics.
The Inverse Octic Power Potential [10]	$V(r) = \frac{a}{r} + \frac{b}{r^2} + \frac{c}{r^3} + \frac{d}{r^4} + \frac{e}{r^5} + \frac{f}{r^6} + \frac{g}{r^7} + \frac{h}{r^8}, \quad h > 0$	This potential is an extension of the inverse quartic and the inverse sextic power potentials.
The Inverse Decatic Power Potential [10]	$V(r) = \frac{a}{r^4} + \frac{b}{r^6} + \frac{c}{r^8} + \frac{d}{r^{10}}, \quad d > 0$	
The Third-Order Hyperbolic Potential [11]	$V_{a,b,c,d}(x) = a \tanh(x) + b \tanh^2(x) + c \tanh^3(x) + d, \quad a, b, c, d \in \mathbb{R}$	One considers the stationary Schrödinger equation ³ for a non-solvable, hyperbolic potential of the third order. A nonsolvable third-order hyperbolic potential becomes quasi-exactly solvable after the introduction of a hyperbolic effective mass step.
The Manning Potential [12], [13]	$V(x) = \frac{\nu_1}{\cosh^2(x)} + \frac{\nu_2}{1+g \cosh^2(x)} + \frac{\nu_3}{(1+g \cosh^2(x))^2}, \quad g \gg 1$	The one-dimensional potential becomes the Manning potential, where $V(x) = \nu_4 \operatorname{sech}^2(x) + \nu_5 \operatorname{sech}^4(x)$ for $\nu_4 = \nu_1 + \frac{\nu_2}{g}$, $\nu_5 = \frac{\nu_3}{g^2}$. The one-dimensional Manning potential is generally used in molecular systems.

Table 2: The first column contains the name of the potential, the second column presents its equation, and the last column contains the description of the equation.

⁴ $\frac{1}{2m(x)}\Psi''(x) - \frac{m'}{2m^2(x)}\Psi'(x) + (E - V(x))\Psi(x) = 0$ with the potential V and the effective mass m , which we take to be a smooth step function $m(x) = 1 + \tanh(x)$.

2.3 The Quartic Potential

In classical mechanics, the low-energy motion in a potential $V(x)$, having its minimum at the origin, can be approximated by the harmonic potential αx^2 , where $\alpha = \frac{1}{2}V''(0)$. To describe this quantum motion, we have to consider the anharmonic corrections to the harmonic term. The common model of this type is *the quartic anharmonic oscillator* with the Hamiltonian

$$H = -\frac{\partial^2}{\partial x^2} + \alpha x^2 + \beta x^4, \quad (2.1)$$

where the harmonic term is αx^2 and the anharmonic term is βx^4 .

To find out the closeness of (2.1) to the harmonic oscillator, we first observe the lowest energy level for the harmonic oscillator ($H := -\frac{\partial^2}{\partial x^2} + \alpha x^2$), which is given by the following wave function

$$\psi(x) = \exp\left\{-\frac{\sqrt{\alpha}x^2}{2}\right\}.$$

This implies that the probability to find a particle when coordinate x is not 0 is in the following domain,

$$x^2 \lesssim \frac{1}{\sqrt{\alpha}}.$$

When we compare the harmonic term with the anharmonic term within the above mentioned domain, we obtain two essentially different cases:

- i) $\frac{\beta}{\alpha^{3/2}} \ll 1$
- ii) $\frac{\beta}{\alpha^{3/2}} \gtrsim 1$

In case (i), we can see that the harmonic term is large in comparison with the anharmonic term, which one can consider as a small correction. For low excitations, the harmonic oscillator and (2.1) are quite similar. The perturbative approach⁴ can be used to account for the small quantitative difference.

In case (ii), the anharmonic term has at least the same order as the harmonic term. When we compare the physics of this system with the physics of the harmonic oscillator, we can draw the conclusion that this cannot be studied using the same approach as in case (i).

On the other hand, when $\alpha = 0$, the wave function $\psi(x) = \exp\left\{-\frac{\sqrt{\alpha}x^2}{2}\right\}$ equals to 1 and its derivative $\psi'(x)$ equals to 0. This means that we can not solve the associated Schrödinger equation.

⁴See Appendix B.

2.4 The Quasi-Exactly Solvable Sextic Oscillator

One can show that under the assumption that the Hamiltonian is Hermitian⁵, the one-dimensional quasi-exactly solvable polynomial potential of lowest possible degree must be sextic. Non-Hermitian Hamiltonians though, allow for new types of quasi-exactly solvable theories.

As many physicists were working towards understanding the quartic anharmonic oscillator, other polynomial models like the sextic did not get as much attention. The one-dimensional quasi-exactly sextic oscillator is now frequently used to approximate situations in quantum mechanics. The quasi-exactly solvable potential was the first example of its kind in quantum mechanics and was discovered in 1978 by physicists V. Singh, K. Datta and S. N. Biswas [21]. The potential is given by

$$V(x) = x^6 + 2bx^4 + (b^2 - (4m + 2p + 3))x^2, \quad p \in \{0, 1\}, \quad (2.2)$$

where $m \in \mathbb{N}$ is fixed and $b \in \mathbb{C}$ is arbitrarily chosen. It was proven by physicists A. V. Turbiner and A. G. Ushveridze [22] that the value of b is independent on the amount of eigenvalues for the Schrödinger equation. Therefore, the Schrödinger equation

$$H = -\frac{d^2}{dx^2} + V(x) = \lambda y \quad (2.3)$$

with the boundary conditions

$$y(\pm\infty) = 0$$

on \mathbb{R} has $m + 1$ explicitly calculable eigenfunctions. These eigenfunctions are of the form

$$\phi(x) = Q(x) \exp \left\{ -\frac{x^4}{4} - \frac{bx^2}{2} \right\}, \quad (2.4)$$

where $Q(x)$ is either an even polynomial of degree $2m$ when $p = 0$ or an odd polynomial of degree $2m + 1$ when $p = 1$, or

$$\phi(x) = \exp \left\{ -\frac{x^4}{4} - \frac{bx^2}{4} \right\} \sum_{n=0}^{\infty} \left(-\frac{1}{4} \right)^n \frac{P_n(E)}{n! \Gamma[n + \frac{1}{2}]} x^{2n}.$$

In our case, we are only interested in even solutions, so $\phi(x)$ has to fulfil

$$P_n(E) = \left(E - \frac{(4n-3)b}{2} \right) P_{n-1}(E) + 16(n-1)(n-J-2) \left(n - \frac{3}{2} \right) P_{n-2}(E),$$

where J is a non-negative integer. The initial conditions are given by $P_{-1}(E) = 0$ and $P_0(E) = 1$. By choosing a particular value of J , we obtain a particular solution of our problem. The odd solutions can be treated analogy. Γ is the gamma function, which by definition is a function with the property $\Gamma(n) = (n-1)!$ for each $n \in \mathbb{N}$.

The quasi-exactly solvable problems, as mentioned in the introduction, only have a finite quantity of eigenfunctions which can be found explicitly, while the rest can be found by numerical methods. This means that both the eigenfunctions and the eigenvalues that we will be able to find, can be found through an algebraic procedure, which we soon will explain, while other solutions remain unknown. The

⁵See Appendix A.

eigenvalues we *can* find will form the so-called *algebraic part* of the total spectrum of H . The procedure to explicitly describe the algebraic part of the spectrum is purely algebraic. If an eigenfunction $\phi(x)$ of the form (2.4) has an eigenvalue λ , we can, by differentiating (2.4) and comparing it to the potential (2.2), show that its polynomial factor $Q(x)$ satisfies the following differential equation,

$$-Q''(x) + 2(x^3 + bx)Q'(x) - ((4m + 2p)x^2 - b)Q(x) = \lambda Q(x). \quad (2.5)$$

We define the following differential operator $\delta := -\frac{d^2}{dx^2} + 2(x^3 + bx)\frac{d}{dx} - ((4m + 2p)x^2 - b)$, which we can see occurs on the left-hand side of (2.5). This differential operator will preserve the $(m + 1)$ -dimensional linear space W_{ev} of all even polynomials of degree $\leq 2m$ for when $p = 0$, and preserves the $(m + 1)$ -dimensional linear space W_{odd} of all odd polynomials of degree $\leq 2m + 1$. We can therefore state that the algebraic part of the spectrum H is the spectrum of the operator δ restricted to W_{ev} for $p = 0$, or to W_{odd} for $p = 1$. We can explicitly calculate the action of δ by fixing the monomial basis respectively for each linear space; $(1, x^2, x^4, \dots, x^{2m})$ in W_{ev} , and $(x, x^3, x^5, \dots, x^{2m+1})$ in W_{odd} .

By setting $x^2 = t$ for $p = 0$ we can rewrite equation (2.5) in the form

$$-4t \frac{d^2 Q(t)}{dt^2} + (4t^2 + 4bt - 2) \frac{dQ(t)}{dt} - (4mt - b)Q(t) = \lambda Q(t). \quad (2.6)$$

If we restrict equation (2.6) to W_{ev} for $p = 0$, we can calculate the $(m + 1) \times (m + 1)$ -matrix $M_m(b)$. The case for when $p = 1$ can be solved in a similar way.

For $Q(t) = \mathbf{1}$ in (2.6), we get: $-4mt + b = \lambda$.

For $Q(t) = t$, we get: $4t^2 + 4bt - 2 - (4mt - b)t = \lambda t$
 $\Rightarrow t^2(4 - 4m) + t(5b) - 2 = \lambda t$.

For $Q(t) = t^2$, we get: $-4t \cdot 2 + (4t^2 + 4bt - 2) \cdot 2t - (4mt - b)t^2 = \lambda t^2$
 $\Rightarrow t^3(8 - 4m) + t^2(9b) + t(-12) = \lambda t^2$.

For $Q(t) = t^3$, we get: $-4t \cdot 6t + (4t^2 + 4bt - 2) \cdot 3t^2 - (4mt - b)t^3 = \lambda t^3$
 $\Rightarrow t^4(12 - 4m) + t^3(13b) + t^2(-30) = \lambda t^3$.

\vdots

We insert our values into our matrix where every row element follows the elements in our basis $(1, t, t^2, \dots, t^n)$,

$$M_m(b) = \begin{pmatrix} b & -4m & 0 & 0 & 0 & \dots \\ -2 & 5b & 4 - 4m & 0 & 0 & \dots \\ 0 & -12 & 9b & 8 - 4m & 0 & \dots \\ 0 & 0 & -30 & 13b & 12 - 4m & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}.$$

Figure 2 below shows the first four eigenfunctions of the $M_m(b)$ -matrix. The rows of the matrix are represented as curves: the red curve represents $Q(t) = 1$, the blue curve represents $Q(t) = t$, the green curve represents $Q(t) = t^2$ and the yellow curve represents $Q(t) = t^3$.

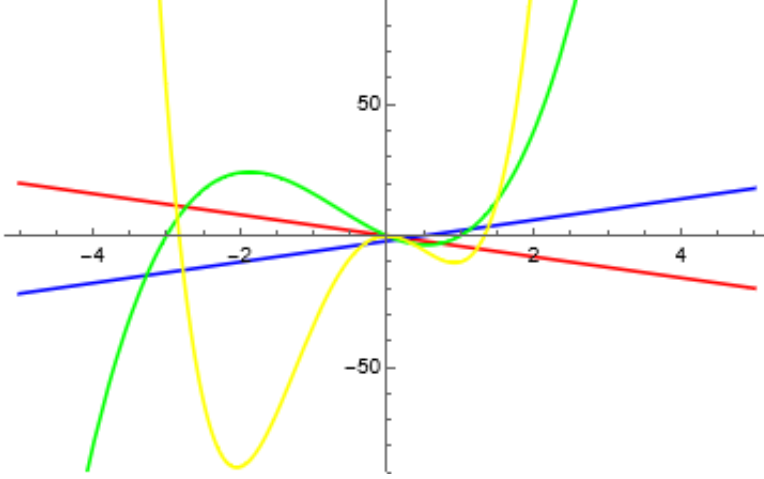


Figure 2. The first four eigenfunctions of the $M_m(b)$ -matrix.

We can compare this with the results obtained in [19] by B. Shapiro and M. Tater, where the characteristic polynomials of principal submatrices $\Delta_m^{(i)}$, $i = 1, \dots, m + 1$ were used. The determinant of the i th principal submatrix of $\lambda I_{m+1} - M_m(b)$, where I_{m+1} is the identity matrix of size $m + 1$. The characteristic polynomials will have to be the same as in [19],

$$\Delta_m^{(i)} = (\lambda - (4i - 3)b)\Delta_m^{(i-1)} - 4(2i - 2)(2i - 3) \times (m + 2 - i)\Delta_m^{(i-2)}, \quad (2.7)$$

where $i = 1, \dots, m + 1$, with the initial conditions $\Delta_m^{(-1)} = 0$ and $\Delta_m^{(0)} = 1$. Using the *Gräffe-Lobachevskii method*, a root-finding algorithm for polynomials which we will omit to show, it is possible to calculate the density of the asymptotic root distribution. In [17] by B. Shapiro and M. Tater, it was proven that the maximal absolute value of the roots of $D_m(\lambda, b) := \Delta_m^{(m+1)}(\lambda, b)$ grows as $\frac{16m^{3/2}}{3\sqrt{3}}$ so the density ρ is given by the following integral,

$$\rho = \frac{C}{\pi} \int_0^1 \frac{d\tau}{\sqrt{64\tau(\tau - 1)^2 - C^2x^2}}, \quad (2.8)$$

where $x \in [-C, C]$ and $C = \frac{16}{3\sqrt{3}}$.

By scaling $\tilde{b} = bm^{1/2}$ and $\tilde{\lambda} = \frac{\lambda}{m^{3/2}}$ in matrix $M_m(b)$, we obtain the matrix $\tilde{M}_m(b)$,

$$\tilde{M}_m(b) = \begin{pmatrix} \frac{b}{m} & \frac{-4}{m^{3/2}} & 0 & 0 & 0 & \dots \\ \frac{-2}{m^{3/2}} & \frac{5b}{m} & \frac{4-4m}{m^{3/2}} & 0 & 0 & \dots \\ 0 & \frac{-12}{m^{3/2}} & \frac{9b}{m} & \frac{8-4m}{m^{3/2}} & 0 & \dots \\ 0 & 0 & \frac{-30}{m^{3/2}} & \frac{13b}{m} & \frac{12-4m}{m^{3/2}} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}.$$

By studying degree m polynomial solutions in (2.6) with respect to the new variables $\tilde{\lambda}$ and \tilde{b} , is

$$-4t \frac{d^2 Q(t)}{dt^2} + (4t^2 + 4\tilde{b}t - 2) \frac{dQ(t)}{dt} - (4mt - \tilde{b})Q(t) = \tilde{\lambda} m^{3/2} Q(t) \quad (2.9)$$

obtained. The characteristic polynomials $\tilde{\Delta}_m^{(i)}(\tilde{\lambda}, \tilde{b})$ of the principal submatrices of $\tilde{M}_m(b)$ satisfy the following 3-term recurrence

$$\tilde{\Delta}_m^{(i)} = \left(\tilde{\lambda} - \frac{4i-3}{m} \tilde{b} \right) \tilde{\Delta}_m^{(i-1)} - \frac{4(2i-2)(2i-3)(m+2-i)}{m^3} \tilde{\Delta}_m^{(i-2)}, \quad (2.10)$$

where the initial values are $\Delta_m^{(-1)} = 0$ and $\Delta_m^{(0)} = 1$. For any given \tilde{b} , we can study the asymptotic root-counting measure $\mu_{\tilde{b}}$ of the polynomial sequence $\{\tilde{D}_m(\tilde{\lambda}, \tilde{b})\}$, where $\tilde{D}_m(\tilde{\lambda}, \tilde{b}) := \tilde{\Delta}_m^{(m+1)}(\tilde{\lambda}, \tilde{b})$. With results from [42] by A. B. J. Kuijlaars and W. van Assche, we can calculate the Cauchy transform of the asymptotic root-counting measure $\mu_{\tilde{b}}$ outside a bounded domain in \mathbb{C} by averaging the Cauchy transform in a 1-parameter family. That is, by letting $\frac{i}{m} \rightarrow \tau$, where $\tau \in [0, 1]$, we can consider the 1-parameter family of 3-term recurrence relations and rewrite (2.10) as follows

$$\Delta_\tau^{(i)} = (\tilde{\lambda} - 4\tau\tilde{b})\Delta_\tau^{(i-1)} - 4(2\tau)^2(1-\tau)\Delta_\tau^{(i-2)}, \quad \tau \in [0, 1], \quad (2.11)$$

where its characteristic equation is given by

$$\psi^2 = (\tilde{\lambda} - 4\tau\tilde{b})\psi - 16\tau^2(1-\tau). \quad (2.12)$$

The values of $\tilde{\lambda}$ in (2.12) are the points where it has a double root with respect to ψ . These are determined by

$$(\tilde{\lambda} - 4\tau\tilde{b})^2 = 64\tau^2(1-\tau), \quad (2.13)$$

or

$$\tilde{\lambda}_{1,2}(\tau) = 4\tau\tilde{b} \pm 8\sqrt{\tau^2(1-\tau)}, \quad \tau \in [0, 1]. \quad (2.14)$$

For when τ runs over the interval $[0, 1]$, the Cauchy transform of $\mu_{\tilde{b}}$ is given by the following formula

$$C_{\tilde{b}}(z) = \int_0^1 \frac{d\tau}{\sqrt{(z - 4\tau\tilde{b})^2 - 64\tau^2(1-\tau)}}. \quad (2.15)$$

The polynomial sequence $\{\tilde{D}_m(\tilde{\lambda}, \tilde{b})\}$ is therefore given by (2.14) and (2.15). With this polynomial sequence, we can find all of the explicitly calculable eigenfunctions of the spectrum of (2.3).

3 The WKB Approximation

The WKB approximation is named after G. Wentzel, H. A. Kramers and L. N. Brillouin.

By using the WKB approximation, one can obtain approximate information about the asymptotical development of an oscillator where one do not need to find everything explicitly. This technique is usual for high frequencies, while its validity deteriorates at low frequencies. More about this can be found in for instance [39].

The method is based on the development of the Schrödinger equation in terms of powers of \hbar . This gives the Hamilton-Jacobi equation of classical mechanics of the 0th order. The first order is the WKB approximation. We will only consider the process in one dimension.

We consider the one-dimensional motion of a particle in a potential $V(x)$. We can for the Schrödinger equation create an ansatz

$$\psi(x) = \exp \left\{ \frac{i}{\hbar} S(x) \right\},$$

where $S(x)$ is a complex function. We assume that $\psi \neq 0$. The time-independent Schrödinger equation $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) = (E - V(x))\psi(x)$ can be written in terms of the local momentum squared,

$$-\hbar \frac{\partial^2}{\partial x^2} \psi = p^2(x)\psi.$$

We insert the ansatz in the time-independent Schrödinger equation above and obtain

$$-\hbar^2 \frac{d^2}{dx^2} \exp \left\{ \frac{i}{\hbar} S(x) \right\} = p^2(x) \exp \left\{ \frac{i}{\hbar} S(x) \right\}, \quad (3.1)$$

We differentiate the left-hand side and obtain

$$-\hbar^2 \frac{d^2}{dx^2} \left(\exp \left\{ \frac{i}{\hbar} S(x) \right\} \right) = -\hbar^2 \frac{d}{dx} \left(\frac{i}{\hbar} S'(x) \exp \left\{ \frac{i}{\hbar} S(x) \right\} \right) = -\hbar^2 \left(\frac{iS''}{\hbar} - \frac{(S')^2}{\hbar^2} \right) \exp \left\{ \frac{i}{\hbar} S(x) \right\}.$$

Plugging this back into (3.1), we obtain

$$-\hbar^2 \left(\frac{iS''}{\hbar} - \frac{(S')^2}{\hbar^2} \right) = p^2(x).$$

We can rewrite this,

$$(S'(x))^2 - i\hbar S''(x) = p^2(x), \quad (3.2)$$

which is our obtained final form.

If we now consider $S(x) = S_0 + \hbar S_1 + \hbar^2 S_2 + \dots$ an expansion in \hbar and insert this expansion in (3.2), we get

$$(S'_0 + \hbar S'_1 + \hbar^2 S'_2 + \dots)^2 - i\hbar(S''_0 + \hbar S''_1 + \hbar^2 S''_2 + \dots) - p^2(x) = 0.$$

We see that the left-hand side is a power series expansion in \hbar . We neglect all terms of order \hbar^2 and higher and we get

$$(S'_0)^2 - p^2(x) + \hbar(2S'_0 S'_1 - iS''_0) = 0,$$

which gives us two equations; one for the coefficient of \hbar^0 and another for the coefficient of \hbar . We start with the first equation for the coefficient of \hbar^0 ,

$$(S'_0)^2 - p^2(x) = 0. \quad (3.3)$$

Solving the differential equation of an eigenfunction of energy E

$$E = \frac{1}{2m}(S''_0) + V(x),$$

we obtain

$$S_0(x) = \pm \int_{x_0}^x \sqrt{2m(E - V(x'))} dx' = \int_{x_0}^x p(x') dx'. \quad (3.4)$$

Using this, we can solve equation (3.3),

$$(S'_0) = \pm p(x) \quad \Rightarrow \quad S_0(x) = \pm \int_{x_0}^x p(x') dx'. \quad (3.5)$$

The second equation for the coefficient of \hbar gives us

$$2S'_0 S'_1 - iS''_0 = 0, \quad (3.6)$$

which we will found to be imaginary,

$$S'_1 = \frac{i}{2} \frac{S''_0}{S'_0} = \frac{i}{2} \frac{(\pm p'(x))}{2(\pm p(x))} = \frac{i}{2} \frac{p'}{p}, \quad (3.7)$$

with solution

$$iS_1(x) = -\frac{1}{2} \ln p(x) + C'. \quad (3.8)$$

Using the obtained results for S_0 and S_1 , we have the following approximate solution,

$$\begin{aligned} \psi(x) &= \exp \left\{ \frac{i}{\hbar} (S_0 + \hbar S_1) \right\} \\ &= \exp \left\{ \pm \frac{i}{\hbar} \int_{x_0}^x p(x') dx' \right\} \exp \left\{ -\frac{1}{2} \log p(x) + C' \right\}. \end{aligned} \quad (3.9)$$

Accordingly, the general solution to the Schrödinger equation up to the terms of order \hbar^2 is given by,

$$\psi(x) = \frac{C}{p(x)^{1/2}} \exp \left\{ \pm \frac{i}{\hbar} \int_{x_0}^x p(x') dx' \right\}, \quad (3.10)$$

where C is a constant. When $p(x) \rightarrow 0$, this solution breaks down. Practically, this happens when a particle stops and turns due to the potential. These points are called *classical turning points*.

3.1 The Quantum Harmonic Oscillator

In this section we will use the WKB approximation to obtain the eigenvalues of the quantum harmonic oscillator.

The classical turning points $\pm A$ for when the kinetic energy equals to 0, that is when

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} = 0,$$

then the energy E can be written as

$$E = V(x) = \frac{1}{2}m\omega^2 x^2.$$

This is giving us

$$\pm A = \pm \sqrt{\frac{2E}{m\omega^2}}.$$

By inserting these obtained values for $x > A$ into (3.10), we get

$$\psi(x) = C \frac{1}{p(x)^{1/2}} \exp \left\{ - \int_A^x p(x) dx \right\}. \quad (3.11)$$

Using the connection formulas⁶ we obtain the following wave function for $0 < x < A$,

$$\psi(x) = 2C \frac{1}{p(x)^{1/2}} \cos \left\{ \int_x^A p(x) dx - \frac{\pi}{4} \right\}. \quad (3.12)$$

We use the initial condition $\psi(0) = 0$, which gives us

$$\int_0^A p(x) dx - \frac{\pi}{4} = \frac{\pi}{2}(2n + 1). \quad (3.13)$$

Finally, inserting the values using the equation $p(x) = \frac{1}{\hbar} \sqrt{2m(E - V(x))}$, we obtain

$$p(x) = \frac{1}{\hbar} \sqrt{2m \left(E - \frac{1}{2}m\omega^2 x^2 \right)} = \left(\frac{m\omega A}{\hbar} \right) \sqrt{1 - \left(\frac{x}{A} \right)^2}. \quad (3.14)$$

Integrating (3.14) from 0 to A , setting $\left(\frac{x}{A} \right)^2 = \rho^2$, we obtain

$$\int_0^A p(x) dx = \frac{m\omega A^2}{\hbar} \int_0^1 \sqrt{1 - \rho^2} d\rho = \frac{m\omega^2 A^2}{\hbar} \cdot \frac{\pi}{4} = \frac{E\pi}{2\hbar\omega}. \quad (3.15)$$

Solving for E using (3.14) and (3.10), we find the eigenvalues,

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right), \quad (n = 0, 1, 2, \dots), \quad (3.16)$$

which is the same result we got in equation (1.48), making the WKB approximation to the energy levels of the quantum harmonic oscillator exact.

⁶For further reading about the connection formulas, see [40].

Appendices

A Abstract Functional Analysis

Here we go deeper into the Hilbert space and spectral theory of hermitian operators.

The state of a physical system in quantum mechanics is represented by a vector belonging to a complex vector space. To represent this, we use the *Dirac "bra-ket" notation*. The Dirac "bra-ket" notation is generally used to represent linear algebra but is mostly used in quantum mechanics. The physical state is then represented by a symbol, $|\rangle$, which is known as a state vector *ket*, or a wave function. In linear algebra, this expression refers to the column vector of a function. Furthermore, the set of all possible wave functions, which describe a given physical system, forms a complex vector space \mathcal{H} . This vector space is known as the *Hilbert space* of the system and may be either infinite- or finite-dimensional. Another presentation of a Hilbert space is a function space called *Lebesgue space* denoted by $L^2(X)$, where X is a measure space. More about this comes later in this chapter.

Hilbert spaces inherit important properties of general vector spaces:

1. A **linear combination** $|\Psi\rangle$ of two (or more) vectors $|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_n\rangle$ is also a vector of the system and is written on the following form

$$|\Psi\rangle = c_1 |\psi_1\rangle + c_2 |\psi_2\rangle + \dots + c_n |\psi_n\rangle = \sum_{i=1}^n c_i |\psi_i\rangle,$$

where $c_1, c_2, \dots, c_n \in \mathbb{C}$.

2. **Linearity**. If a physical state of a system is given by a vector $|\Psi\rangle$, then the vector $c|\Psi\rangle$, for $c \in \mathbb{C}$ and non-zero, will also represent the same system.

However, from linear algebra, we are aware of the existence of the row vector. The quantity $\langle\Psi|$ represents the *complex conjugates* of the corresponding vector $|\Psi\rangle$, and is known as *bra*. These vectors are elements of the vector space \mathcal{H}^* , also known as the *dual space* of the Hilbert space \mathcal{H} . Then, if a vector that represents the physical space is given by $|\Psi\rangle = c_1 |\psi_1\rangle + c_2 |\psi_2\rangle$, the corresponding vector space spanned by the *bra* vector is given by

$$\langle\Psi| = c_1^* \langle\psi_1| + c_2^* \langle\psi_2|.$$

For each *ket* vector in \mathcal{H} , there will exist an associated *bra* vector in \mathcal{H}^* .

A.1 Inner Product and Hilbert Spaces

If we let $|\psi\rangle$ and $|\phi\rangle$ be any two wave functions in Hilbert space \mathcal{H} , we can, by definition, use the *inner product*, $\langle\psi|\phi\rangle$. In quantum mechanics, this inner product is an analog of the scalar product in vector spaces, where the inner product of two vectors is a scalar, albeit in this situation a complex number. The value of the inner product is the *probability amplitude* for the state ϕ to collapse into ψ (in other words, it describes the overlap of ϕ onto ψ).

The inner product has the following properties,

- i) **Distributivity and associativity** $\langle \psi | \{c_1 | \phi_1 \rangle + c_2 | \phi_2 \rangle \} = c_1 \langle \psi | \phi_1 \rangle + c_2 \langle \psi | \phi_2 \rangle$
- ii) **Complex conjugate** $\langle \psi | \phi \rangle = \langle \phi | \psi \rangle^*$
- iii) **Positive definiteness** $\langle \psi | \psi \rangle \geq 0$. $\langle \psi | \psi \rangle = 0$ implies that the wave function $|\psi\rangle = 0$ is the null element of the Hilbert space (which is given by the functions that are zero almost everywhere).
- iv) **Orthogonality** Given two wave functions $|\psi\rangle$ and $|\phi\rangle$, they are said to be orthogonal if $\langle \psi | \phi \rangle = 0$.

We summarize this information in the following definition,

Definition A.1 (Hilbert Space). A Hilbert space \mathcal{H} is a complex vector space equipped with an inner product.

All vectors in the Hilbert space have a finite norm so they can be normalized to unity.

A.2 The Normalization Condition

We interpret the equation $|\psi(x)|^2 = \psi^*(x)\psi(x)$ as defining a probability distribution for finding a particle at some position x . The sum of probabilities taken over all possible positions x should be 1. We ensure that this is the case by *normalizing* a wave function ψ (we multiply it by a constant). Therefore, we integrate the probability distribution over the whole space,

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1, \quad (\text{A.1})$$

or

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1. \quad (\text{A.2})$$

A.3 Lebesgue Spaces

Lebesgue spaces, or the L^p -spaces are defined using p -norm (or l_p -norm). On a measure space (X, M, μ) , where X is a set, M is a σ -algebra of subsets of X , and μ is a *countably additive measure* on M , we can informally define an L^2 -function as a function $f : X \rightarrow \mathbb{R}$,

$$|f|^2 = \int_X |f|^2 d\mu,$$

with respect to the measure μ exists and is finite.

The p -norm, for $p \geq 1$, $p \in \mathbb{R}$ of vector $\mathbf{x} = (x_1, \dots, x_n)$ is given by

$$\|\mathbf{x}\|_p := \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}, \quad (\text{A.3})$$

and for $p = 2$ we get the *Euclidean norm*, which is the only Hilbert space among the Lebesgue spaces.

The collection of L^2 -functions on a measure space X is denoted by $L^2(X)$.

L^2 -functions are important in quantum mechanics, where probabilities of wave functions are given by equation (A.2). Here, L^2 -functions occur because of the requirement that the quantities remain finite.

A.4 Hermitian Operators in \mathcal{H}

Definition A.2 (Hermitian Operator). A bounded linear operator A in a Hilbert space \mathcal{H} is called *Hermitian* if

$$\langle Ax, y \rangle = \langle x, Ay \rangle \tag{A.4}$$

holds for all $x, y \in \mathcal{H}$.

Hermitian operators have two important properties that form the basis of quantum mechanics; the eigenvalues of a Hermitian operator are real and the eigenfunctions of a Hermitian operator are orthogonal to each other (or can be made orthogonal by taking linear combinations of them). Proofs of these claims can be found in other literature, for instance in [33] or [34].

For the time-independent Schrödinger equation, $H\psi = E\psi$, the physical quantities must be Hermitian. Since each physical quantity of the system can be measured, the eigenvalues which are being used to obtain them, must be real. In order for the eigenvalues to be real, the corresponding operators must be Hermitian.

Theorem A.1 (Spectral Theorem). *Let V be a finite-dimensional inner product space over \mathbb{F} and $T : V \rightarrow V$ is a Hermitian linear transformation. Then V has an orthonormal basis eigenvectors of T , which tells us that T is diagonalizable.*

The set of eigenvalues of T is called the *spectrum* of T .

B Perturbation Theory

Perturbation theory is a useful approach in quantum mechanics for describing a real complicated quantum system in terms of a simpler one.

Finding exact solutions to the Schrödinger equation for Hamiltonians can be difficult; if the problem cannot be solved exactly, perturbation theory can be applied by adding a small term to the exactly solvable problem.

The approach begins with a system that already has a known mathematical solution and then adding an additional "perturbing" Hamiltonian that represents a weak disturbance to the system. As long as this disturbance is kept small in comparison to the size of the quantities themselves, the energy levels and eigenstates associated with the perturbed system can by the means of perturbation theory be expressed as small "corrections" to those of the simple system.

We can calculate them using approximated methods (for example with *asymptotic series*; which we will omit in this thesis). As a result, the complicated system can be studied using knowledge of the simpler system; so it is describing a complicated unsolved system using a simple, solvable system.

The Hamiltonians, such as the quantum harmonic oscillator for which we have exact solutions, are too idealized to describe most systems. Perturbation theory allows one to apply known solutions to a range of more complicated systems. Although the expressions produced by perturbation theory are not exact, they can lead to accurate results.

However in some cases the perturbation theory can be an invalid approach to take. This occurs for instance when the system we want to describe cannot be described by a small perturbation imposed on some simple system.

C The Dirac Delta Function

The Dirac delta function was introduced by physicist Paul Dirac as a tool often used in probability theory. The Kronecker delta function is the discrete analog of the Dirac delta function.

Definition C.1 (The Dirac Delta Function). The Dirac delta function is defined by

$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0, \end{cases}$$

with

$$\int_{x_1}^{x_2} dx \delta(x) = 1$$

if $0 \in [x_1, x_2]$ and 0 otherwise.

An important property of the Dirac delta function is

$$\int dx f(x)\delta(x) = f(0) \tag{C.1}$$

for any function $f(x)$. We know this, since $\delta(x)$ vanishes everywhere except for when $x = 0$, so the importance of the values the function $f(x)$ takes, except for when $x = 0$, is low. Therefore we can write also write $f(x)\delta(x) = f(0)\delta(x)$. Furthermore, since $f(0)$ is independent of x , we can pull this outside the integral, and then we obtain the right-hand side in equation (C.1).

Equation (C.1) can also be generalized and have the form

$$\int dt f(x)\delta(x - x_0) = f(x_0).$$

Since the Dirac delta function is too singular, it is not a function, but a distribution and can be used only inside integrals. As long as it is known that the Dirac delta function will be integrated, we can use it as if it were a function.

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