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On Quantum Mechanical Scattering Theory And Its Connection To Unitary Matrices

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Abstract

The principle of probability conservation in quantum mechanics is studied by an analysis of scattering amplitudes limited to one and three dimensional cases. In particular we show that scattering matrices are represented by unitary matrices.

Keywords:

quantum mechanical scattering, probability conservation, unitary matrix.

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Contents

1. Introduction and background of study

In our everyday life we are used to objects which are concrete for us. We can see them, feel them and understand approximately how they will behave, they are deterministic. Our intuition about behavior of macroscopic objects is based on experience and was beautifully mathematically explained by **Isaac Newton** in his *Philosophiæ Naturalis Principia Mathematica*. Although Newtonian mechanics was a success in dealing with large or macroscopic objects it was shorthanded when several experiments in the beginning of 1900's, like the photoelectric effect and the Compton effect, showed that microscopic objects behave much differently from the theoretical predictions given by Newtonian mechanics. In an attempt to solve the difficulty **L. de Broglie** proposed in 1923 that a *moving* object has wave as well as particle characteristics **[1]**. The main idea evolved from quantization of light; the energy E of a photon is given by $E = hf$, where f is the frequency of the light and h is Planck's constant. The momentum p of a photon could then be calculated as $p = hf/c = h/\lambda$, where c is the speed of light and λ is the wavelength. If implementing this idea to a moving object we can calculate de Broglie wavelength as $\lambda=h/p$. This means than every moving object, regardless of size, is characterized like a matter wave!

Attempts to construct a theoretical framework which incorporate the results of experimental evidence of quantization and wave-particle duality were elaborated by mid 1920's. Two main quantum mechanical theories emerged. The first one called matrix mechanics **[2]** which obeyed a non commutative algebra and the second one called wave mechanics following ideas about matter waves **[3]**.[1] Though, the matrix mechanics and wave mechanics were proved equivalent by E. Schrödinger **[4]**, both theories are forms of a general formulation of quantum mechanics developed by Paul Dirac in 1930 **[5]**. An important element in quantum mechanical theory presented by all **[3][4][5]** is the presence of randomness. Randomness and models of random phenomena are objects of probability theory. In particular we are interested in describing physical experiments that can be repeated and where future outcomes cannot be predicted. Especially in the early development of quantum mechanics many of the performed experiments which showed nature of randomness had its roots in scattering theory. Scattering phenomena is also an important branch in physics where much of what we know about atoms and nuclear physics comes from. There is also a good deal of modern technical application which is provided by our knowledge of scattering phenomena. Such applications are electron microscope **[20]**, scanning tunneling microscope **[21]** and many areas in x-ray scattering. Although randomness is not new and has been actively performed in form of games of chance for thousands of years, a mathematically well presented treatment of the theory of probability only emerged in the early 1930s, formulated by A.N. Kolmogorov **[6]**. The fact of close connection between the probability theory and quantum mechanical theory gives us an idea to evaluate this connection and try to understand how it can be described mathematically.

In this paper we will examine some ***basic concepts*** from the ***theory of quantum mechanics*** and its ***connection*** to the ***probability theory***. To be more specific we will show that the ***principle of conservation of probability*** in quantum mechanical ***scattering theory*** give rise to ***unitary scattering matrices***. To achieve a less abstract view of the theory, we will apply the quantum mechanics to some basic problems in scattering theory.

[1] There is actually an exciting story by Felix Bloch [**17**] behind how the wave mechanics emerged in the early days of quantum theory. Especially the well known Schrödinger equation could equally be called Debye's equation if Peter Debye (1884-1966) had done some simple calculations to show wave properties of moving matter.

We now continue in section 2 to define the basic terms, notations and present some results in connection with unitary matrices. In section 3 important notations and principles from quantum mechanics will be presented. Implementation of the theory from both sections 2 and 3 will be used as tools when dealing with scattering theory in section 4. We present our conclusions in section 5.

2. Unitary and Hermitian matrices and operators

The mathematical language of quantum mechanics is based on linear algebra which is supposedly the reader is somewhat familiar with. Let us therefore concentrate in this section on building up a mathematical framework which will be used later when dealing with quantum scattering problem.

Definition 2.1 The ***inner product*** on a vector space $\mathcal{V}$,[2] is a function that associates a complex number $\langle \boldsymbol{a}|\boldsymbol{b}\rangle$ to each pair of vectors in $\mathcal{V}$, such that the following axioms are satisfied for all vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ in $\mathcal{V}$ and all complex scalars γ and δ with their complex conjugate $\gamma^*$and δ^*:

1. $\langle \boldsymbol{a}|\boldsymbol{b}\rangle = \langle \boldsymbol{b}|\boldsymbol{a}\rangle^*$
2. $\langle \boldsymbol{a}|(\gamma|\boldsymbol{b}\rangle + \delta|\boldsymbol{c}\rangle) = \gamma^*\langle \boldsymbol{a}|\boldsymbol{b}\rangle + \delta^*\langle \boldsymbol{a}|\boldsymbol{c}\rangle$
3. $\langle \boldsymbol{a}|\boldsymbol{a}\rangle \geq 0 \;\; and \;\; \langle \boldsymbol{a}|\boldsymbol{a}\rangle = 0 \;\; if\ and\ only\ if\ \boldsymbol{a} = 0$

We will be using an inner product on $\mathbb{C}^n$, which can be checked to satisfy Definition 2.1, defined by:

$$\langle \boldsymbol{a}|\boldsymbol{b}\rangle = \sum_i^n a_i^* b_i.$$

In **vector notation** in $\mathbb{C}^n$ the inner product can be written as $\bar{\boldsymbol{a}}^{\boldsymbol{T}}\boldsymbol{b}$ if we define $\boldsymbol{a} = (a_1\ a_2 \ldots a_n)^T$ and $\boldsymbol{b} = (b_1\ b_2 \ldots b_n)^T$.

The vectors we will encounter in quantum mechanical scattering theory are functions. We need therefore to introduce the inner product on the vector space of functions.

Definition 2.2 Let f and g be two complex-valued functions in the vector space of all continuous functions on the class interval [*a*,*b*], then the inner product can be defined as:

$$\langle f|g\rangle = \int_a^b f^*(x)g(x)dx.$$

Definition 2.3 A complete inner product space, commonly denoted as $\mathcal{H}$, is called ***Hilbert space***.[3]

In section 3 we will see that not all complex-valued functions in [*a*,*b*] can represent a possible quantum mechanical "state". We therefore need to define a set called $L_2(a,b)$ which constitute a collection of *square integrable functions*.

Definition 2.4 The collection of all square integrable functions f on a complex continuous interval [*a*,*b*] such that:

[2] Though the interpretation of a vector space is generally known one may consult appendix A3 for a detailed definition.

[3] See appendix A3 for a detailed definition of a completeness.

$$\|f\|^2 = \langle f|f\rangle = \int_a^b f^*(x)f(x)dx = \int_a^b |f(x)|^2 dx < \infty\,,$$

is called by $L_2(a,b)$ (*Lebesgue square integrable vector space)*.

Now, if two functions f and g are both in $L_2(a,b)$ space their inner product is limited which can be proven by Schwarz inequality on integrals:

$$\left|\int_a^b f^*(x)g(x)dx\right| \leq \sqrt{\int_a^b |f(x)|^2 dx}\sqrt{\int_a^b |g(x)|^2 dx} < \infty.$$

One can show by Riesz-Fischer theorem that the space $L_2(a,b)$ is complete and therefore is an example of Hilbert space.

A linear transformation T from a vector space $\mathcal{H}$ to itself is defined by ordinary rules of matrix multiplication as:

$$T(|k_1\boldsymbol{\beta}_1\rangle + |k_2\boldsymbol{\beta}_2\rangle) = |k_1 T\boldsymbol{\beta}_1\rangle + |k_2 T\boldsymbol{\beta}_2\rangle \quad \text{for all } \boldsymbol{\beta}_1, \boldsymbol{\beta}_2 \in \mathcal{H} \quad \text{and} \quad k_1, k_2 \in \mathbb{C}.$$

Here the analogy to often used notation of vector transformation is:

$$|\boldsymbol{\beta}\rangle = T|\boldsymbol{\alpha}\rangle \rightarrow \vec{\boldsymbol{b}} = \boldsymbol{T}\vec{\boldsymbol{a}}.$$

A linear transformation from a finite dimensional vector space, such as $\mathbb{C}^n$, to itself can be described by a square matrix. In quantum mechanics we will be using a infinite dimensional vector space $L_2(a,b)$. Linear transformations from $L_2(a,b)$ to itself are often called operators[4] which correspond to certain observables such speed or position of an object.

We will need several definitions to be able to deal with different linear transformations.

Definition 2.5 If A is a complex matrix, then the conjugate transpose of A, denoted by A^*, is defined by: $A^* = \overline{A^T}$.

Definition 2.6 For a (bounded) operator $T : \mathcal{H} \rightarrow \mathcal{H}$, the adjoint $T^* : \mathcal{H} \rightarrow \mathcal{H}$ is defined by the equation:

$$\langle T\boldsymbol{x}|\boldsymbol{y}\rangle = \langle \boldsymbol{x}|T^*\boldsymbol{y}\rangle \qquad \text{for all } \boldsymbol{x} \text{ and } \boldsymbol{y} \in \mathcal{H}.$$

There are two special classes of transformations which are of interest to us:

1. A square complex matrix T is called Hermitian, or self-adjoint, if it is equal to its conjugate transpose: $T = T^*$.

2. A square complex matrix T is said to be ***unitary***, if its inverse is equal to its conjugate transpose; $T^{-1} = T^*$. That is if $TT^* = T^*T = \mathbb{I}$.

Several important facts about ***unitary*** and ***Hermitian*** matrices can be proved.

Theorem 2.1 If T is a complex $n \times n$ ***unitary*** matrix then $\langle T\boldsymbol{x}|T\boldsymbol{y}\rangle = \langle \boldsymbol{x}|\boldsymbol{y}\rangle$ for all $\boldsymbol{x}$ and $\boldsymbol{y}$ in $\mathcal{H}$.

Proof. Let $\boldsymbol{x} = (x_1\ x_2 \ldots x_n)^T$ and $\boldsymbol{y} = (y_1\ y_2 \ldots y_n)^T \in \mathcal{H}$, then by properties of a unitary matrix operator it follows $\langle T\boldsymbol{x}|T\boldsymbol{y}\rangle = (T\boldsymbol{x})^* T\boldsymbol{y} = \boldsymbol{x}^* T^* T\boldsymbol{y} = \boldsymbol{x}^* T^{-1} T\boldsymbol{y} = \boldsymbol{x}^*\boldsymbol{y} = \langle \boldsymbol{x}|\boldsymbol{y}\rangle$ ■

[4] An operator is a mathematical instructor which is acting on the function that follows it.

It follows from Theorem 2.1 that a unitary matrix is also an isometry i.e. the distance is preserved between two vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ after a map by a *unitary* matrix *T*, which can be shown by following:

$$|T\boldsymbol{x} - T\boldsymbol{y}|^2 = \langle T(\boldsymbol{x}-\boldsymbol{y})|T(\boldsymbol{x}-\boldsymbol{y})\rangle = (\boldsymbol{x}-\boldsymbol{y})^* T^{-1} T(\boldsymbol{x}-\boldsymbol{y}) = \langle(\boldsymbol{x}-\boldsymbol{y})|(\boldsymbol{x}-\boldsymbol{y})\rangle = |\boldsymbol{x}-\boldsymbol{y}|^2.$$

Theorem 2.2 For a ***unitary*** matrix *T*, eigenvalues λ have unit magnitude i.e. eigenvalues $\lambda \in \mathbb{C}$: $|\lambda| = 1$.

Proof. For an eigenvector $\boldsymbol{x} = (x_1\ x_2 \dots x_n)^T$, such that $T\boldsymbol{x} = \lambda\boldsymbol{x}$ we have by unitary property and Theorem 2.1:

$$\langle \boldsymbol{x}|\boldsymbol{x}\rangle = \langle T\boldsymbol{x}|T\boldsymbol{x}\rangle = (\lambda\boldsymbol{x})^*\lambda\boldsymbol{x} = (\lambda^*\lambda)\boldsymbol{x}^*\boldsymbol{x} = \lambda^*\lambda\langle \boldsymbol{x}|\boldsymbol{x}\rangle.$$

Since $\langle \boldsymbol{x}|\boldsymbol{x}\rangle \neq 0$ and $(\lambda^*\lambda - 1)\langle \boldsymbol{x}|\boldsymbol{x}\rangle = 0 \Rightarrow \lambda^*\lambda = |\lambda|^2 = 1$ ■

Theorem 2.3 The *eigenvalues* of a Hermitian matrix are real.

Proof. Let λ be an eigenvalue with the corresponding eigenvector $\boldsymbol{x} \neq 0$ of a Hermitian matrix *T*, then by Definition 2.6 and property of Hermitian operator:

$$\lambda\langle \boldsymbol{x}|\boldsymbol{x}\rangle = \langle \lambda\boldsymbol{x}|\boldsymbol{x}\rangle = \langle T\boldsymbol{x}|\boldsymbol{x}\rangle = \langle \boldsymbol{x}|T^*\boldsymbol{x}\rangle = \langle \boldsymbol{x}|T\boldsymbol{x}\rangle = \langle \boldsymbol{x}|\lambda\boldsymbol{x}\rangle = \lambda^*\langle \boldsymbol{x}|\boldsymbol{x}\rangle.$$

Because $\boldsymbol{x} \neq 0$ it must be true $\lambda = \lambda^* \Rightarrow \lambda \in \mathbb{R}$. ■

Without any proof we will state an important theorem which combines *unitary* and *Hermitian* matrices.

Definition 2.7 A square complex matrix *T* is said to be ***unitary diagonalizable*** if there exists a *unitary* matrix *B* which diagonalizes *T*, *i.e.* $B^*TB = D$ where *D* is a diagonal matrix.

Theorem 2.4 Every *Hermitian* $n \times n$ matrix has an orthonormal set of *n* eigenvectors and is unitarily diagonalizable by a $n \times n$ matrix whose column vectors form an orthonormal set of eigenvectors of *the Hermitian* matrix ■

Let us now introduce the notation for a linear operator which acts on complex functions in $L_2(a,b)$ space.

Definition 2.8 Let f and g be two functions in $L_2(a,b)$. The quadratic form of a linear operator *T* denoted by $\hat{T}$ is a linear transformation on $L_2(a,b)$ with inner product defined by:

$$\langle f|\hat{T}g\rangle = \int_a^b f^*(x)\hat{T}g(x)dx.$$

We will see further on that in physics we are interested in operators which has following property, equivalent to a *Hermitian* matrix. An operator $\hat{T}$ in $L_2(a,b)$ is called symmetric or just *Hermitian* if following equality holds:

$$\langle f|\hat{T}g\rangle = \langle \hat{T}f|g\rangle.$$

3. On quantum mechanical representation and its principles

In this part we shall present some general principles of quantum mechanics. [**8** pp. 194-231] [**11** pp. 3-2 – 3-4] But before doing so let us mention some facts about notation called *Dirac bracket notation* after Paul Dirac. It is widely used in theoretical physics and

mathematics and we have already introduced it in Definition 2.1 as inner product notation $\langle . . | . . \rangle$. The symbol $\langle . . |$ is called *bra* while $| . . \rangle$ is called *ket* and together they will form bracket $\langle . . | . . \rangle$. Continuing using the bracket notation we can now introduce the general principles of quantum mechanics.

3.1 The principles of quantum mechanics

In quantum mechanics a state of an event, object or a system of objects can be described by complex functions in a Hilbert space[5]. The transition between some possible states is connected to the transition probability. Because the probability is always real and is between [0,1] we have the following principle to guarantee a real outcome despite quantum mechanical states are complex valued.

Principle 1.

Let ψ_1 and ψ_2 belong to the Hilbert space. The probability that an object will be at a state ψ_2, when first being in the state ψ_1, is the ***absolute square*** *of a complex number called the probability amplitude*[6].

$$P_{r\to s} = |\langle \psi_2 | \psi_1 \rangle|^2.$$

We see that $P_{r\to s} \in [0,1]$ which is deduced from that absolute square of a complex scalar is real. The first principle states that two functions, which represent two quantum mechanical states, are square integrable and limited. The introduction of probability is important here because it gives us a way to interpret the probability amplitude.[7]

If we have an event in state ψ_1 which has several routes to end up in a state ψ_2 we might ask us what is the *probability amplitude* for an event to go by some particular route? Let us define the route as an event with the quantum mechanical state α. Then we have by Principle 1 three events with the following probability amplitudes:

$$Events \begin{cases} A & P_A \to & \langle \alpha | \psi_1 \rangle & from\ state\ \psi_1\ to\ \alpha \\ B & P_B \to & \langle \psi_2 | \alpha \rangle & from\ state\ \alpha\ to\ \psi_2 \\ C & P_C \to & \langle \psi_2 | \psi_1 \rangle_\alpha & from\ state\ \psi_1\ to\ \psi_2\ by\ state\ \alpha \end{cases}$$

Probability amplitude for event *C* is then given by $P_C = P_A P_B$. The events *A* and *B* are said to be *independent* which is equivalent to say: $P_{(A\cap B)} = P_A P_B$. Let us put this as a principle

Principle 2.

Probability amplitude for an event that is in state ψ_1 and goes by some particular route, defined by state α, to end up in state ψ_2 is the product of the amplitude to go part way $\langle \alpha | \psi_1 \rangle$ with the amplitude to go the rest way $\langle \psi_2 | \alpha \rangle$.

$$\langle \psi_2 | \psi_1 \rangle_\alpha = \langle \psi_2 | \alpha \rangle \langle \alpha | \psi_1 \rangle.$$

It is not hard to see that if we add all the routes, say $\alpha_1, \alpha_2, \ldots \alpha_i$, from ψ_1 to ψ_2 we should end up with a total probability amplitude go from state ψ_1 to ψ_2 by all routes possible.

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[5] Technically a Hilbert space, is as stated by Definition 2.2, a complete inner product space. The collection of square integrable functions $L_2(a,b)$ is therefore only one possible Hilbert space. But since physicist and many mathematicians often refer to $L_2(a,b)$ space when saying Hilbert space we will adopt same standard when dealing with quantum mechanics.

[6] Observe that "probability amplitude" is ***not*** *the same as "probability". The probability amplitude is in general a complex number whereas probability is defined on a real interval.*

[7] Some basic definitions and theorems from the theory of probability are stated in appendix A4.

Principle 3.

Probability amplitude for an event which has several routes, $\alpha_1, \alpha_2, \ldots \alpha_i$, from state ψ_1 to state ψ_2 is the sum of the amplitudes for the routes considered separately.

$$\langle \psi_2 | \psi_1 \rangle = \sum_i \langle \psi_2 | a_i \rangle \langle a_i | \psi_1 \rangle.$$

By combining the three main principles we get the probability for an event from state ψ_1 to state $\psi_2$undertaking all possible routes and partial routs as:

$$|\langle \psi_2 | \psi_1 \rangle|^2 = \left| \sum_{all\ index} \langle \psi_2 | k_l \rangle \langle k_l | e_q \rangle \ldots \langle d_n | c_m \rangle \ldots \langle b_j | a_i \rangle \langle a_i | \psi_1 \rangle \right|^2.$$

We will now put the idea by **L. de Broglie**, which is all moving objects have wave characteristics, in a mathematical form. Developed by E. Schrödinger we got the Schrödinger equation which explicitly tells that a quantum mechanical state is a function of position and time.

Principle 4. **(The Schrödinger equation)**

To an ensemble of physical system one can associate a wave function which is in general complex. The wave function contains all the information that can be known about the ensemble.

The time evolution of the wave function of a physical system is determined by the time dependent Schrödinger equation, which is a partial differential equation. In one dimension we can express the time dependent Schrödinger equation on a wave function $\Psi(x,t)$ by its partial derivatives:

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

In this equation *i* is the square root of -1, $\hbar$ is Planck's constant divided by 2π, *m* is the mass of the system and *V* is the potential, which is real, describing the interaction between the system by the rest of the surrounding world.[8]

Principle 5. **(The Heisenberg's uncertainty principle in one dimension)**

It is not possible to know both the exact momentum (p) and the exact position (x) of an object at the same time. The minimum uncertainty is quantitatively described by:

$$\Delta_p \Delta_x \geq \frac{\hbar}{2},$$

Were Δ_p is the deviation in momentum and Δ_x is the deviation in position. As before $\hbar$ is Planck's constant divided by 2π. The fifth principle tell us that no matter how well one measures speed (momentum) and position of an object one will end up at least to be uncertain in $(\hbar/2)$ magnitude when measure speed and position at the *same time*.

[8] A more elaborate description of the Schrödinger equation and its connection to the classical wave equation is presented in appendix A1.

3.2 Arbitrary quantum mechanical system

In general, for an arbitrary quantum mechanical system, let the system be represented by a function $\Psi(\boldsymbol{x}, t)$ living in Hilbert space. Define $\boldsymbol{x}$ as position vector in $\mathbb{R}^n$ and t as time parameter belonging to $\mathbb{R}$. It now follows from *Principle 1* that integrating a quantum mechanical state $\Psi(\boldsymbol{x}, t)$ over the whole volume $\mathbb{R}^n$ equals unity:

$$|\langle\Psi|\Psi\rangle|^2 = \int |\Psi(\boldsymbol{x}, t)|^2 d\boldsymbol{x} \;=\; 1. \tag{3.2}$$

Physically (3.2) means that probability of finding, somewhere in real space $\mathbb{R}^n$ and at all times, an object described by a quantum mechanical state $\Psi(\boldsymbol{x}, t)$ must be 1.

Besides being square integrable, Ψ must be continuous to give a physically meaningful result. One might observe that there is no integration in (3.2) with respect to time parameter *t*. It can be explicitly proven that the probability for a quantum mechanical state, described by the Schrödinger equation, evolving in time is preserved i.e.

$$\frac{d}{dt}\int |\Psi(\boldsymbol{x}, t)|^2 d\boldsymbol{x} = 0.$$

We might be interested in some physical observable quantities like speed or position of an object represented by the Schrödinger equation. Such observables are represented in quantum physics by symmetric or hermitian operators (see Definition 2.8).[9] The expectation value for a hermitian operator follows same notation as expectation value of a function of a random variable defined in appendix A4. We have also showed by Theorem 2.3 that the eigenvalues of a hermitian matrix have to be real. Same follows for a hermitian operator where the eigenvalues representing determinate states are real. The expectation value of a hermitian operator, which is an average of eigenvalues, is therefore also real. Why is this conclusion so important? We will see in the next section that the total energy of an object (in motion much less than speed of light) can be represented by Hamiltonian operator ($\hat{H}$) which is hermitian with eigenvalues representing the energy *E*. The time independent Schrödinger equation (see appendix A2.1) can be written as:

$$\hat{H}\psi_n = E_n\psi_n,$$

Where E_n is an eigenvalue corresponding to eigenfunction ψ_n. When we measure the energy of a quantum mechanical system we are guaranteed by Theorem 2.3 to get a real energy value E_n. In probabilistic terms we say that the wave equation Ψ collapses to give one of the possible eigenvalues E_n.

4. Introduction to quantum mechanical scattering theory.

In classical physics scattering is associated with moving objects which interact and then move apart. In quantum mechanics, moving objects are associated with the wave function which is described by the Schrödinger equation "*Principle 4*". When studying scattering problems we are therefore interested in finding solutions to partial differential equations which describe different quantum mechanical states. The standard case is that several particles come together from an infinite large distance away. They collide or maybe react and then scatter away to infinity again. The solutions to the differential equations tell which directions the particles are most likely to go. An equivalent way of describing the same problem is by applying the general principles of quantum mechanics. Suppose we

[9] For example the momentum operator *(p)* tells to differentiate the wave function $\psi(x)$ with respect to position variable *x* and then multiply the result by $-i\hbar$.

have an arbitrary potential structure which causes scattering of a particle when interacting with it. We can label the various position on the potential structure by an index *i*, where *i* runs over the integer *N*. For any particular *i*, the amplitude that the particle arrives at a particle counter C placed in a fixed position *j* denoted as $\langle\psi_C|\psi_j\rangle_i$, is the amplitude that the particle gets from the source in initial state ψ_0 to position in state ψ_i, multiplied by the scattering amplitude A_{ij}:

Probability amplitude to go from ψ_0 *to* ψ_C *by position i* : $\quad \langle\psi_C|\psi_j\rangle_i = A_{ij}\langle\psi_i|\psi_0\rangle.$

The total probability amplitude to go from ψ_0 *to* ψ_C is the sum over all the positions *i*:

$$\sum_{i=1}^{N}\langle\psi_C|\psi_j\rangle_i = \sum_{i=1}^{N} A_{ij}\langle\psi_i|\psi_0\rangle. \tag{4.0}$$

Because we are in (4.0) adding amplitudes of scattering from index *i* with different space positions, the amplitudes will have different phases giving rise to interference. Now, the probability of finding the particle before scattering, somewhere in space, must be 1. This is equal to the probability of finding same particle after the scattering. We have therefore equality of probabilities before and after scattering. If $P_{in}(\boldsymbol{s})\boldsymbol{ds}$ is the probability to find particles in a small space interval $\boldsymbol{ds}$ before and $P_{out}(\boldsymbol{s})\boldsymbol{ds}$ is after, we have:

$$\int P_{in}(\boldsymbol{s})\boldsymbol{ds} = \left|\sum_{\boldsymbol{j}}\sum_{i=1}^{N} A_{ij}\langle\psi_i|\psi_0\rangle\right|^2 = \sum_{\boldsymbol{j}}\sum_{i=1}^{N}\langle\psi_C|\psi_j\rangle_i = \int P_{out}(\boldsymbol{s})\,\boldsymbol{ds} = 1.$$

The different quantum mechanical states in expression (4.0) can be described by the Schrödinger equation for which we are interested in finding a solution. In particular, we are studying what is called the *spectrum* of a linear operator corresponding to the Schrödinger equation. Discrete spectrum is corresponding to bound states while continuous spectrum is corresponding to scattering states of the Schrödinger equation. The long time asymptotic of the scattering states is then described by a map, called ***S***-matrix, $\boldsymbol{S} : \mathcal{H} \to \mathcal{H}$. For example, the time independent Schrödinger equation (see appendix A2.2) can be written as: [10]

$$\hat{H}\psi_1(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi_1(x)}{\partial x^2} + V(x)\psi_1(x) = E\psi_1(x). \tag{4.1}$$

Here we use the correspondence between classical mechanics and quantum mechanics In (4.1) E stands for the eigenvalue and $\psi_1$for the eigenfunction. The solution to the Schrödinger equation, (4.1), which is a second-order linear ordinary differential equation, is generally complex-valued. Consider first $V(x) = 0$, with general solution to the equation (4.1) is:

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}, \qquad A, B \in \mathbb{C},\ k = \frac{\sqrt{2mE}}{\hbar}. \tag{4.2}$$

Tacking on the time dependence on (4.2), as stated in appendix A2.2, which is $e^{-iEt/\hbar}$, we get the time dependent wave function:[11]

[10] The Hamiltonian operator $\hat{H}$ in *x-variable* is obtained by the substitution of momentum operator $\hat{p} \to \frac{\hbar}{i}\frac{\partial}{\partial x}$ into Hamiltonian: $\frac{p^2}{2m} + V(x)$, which gives: $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

[11] Actually we have a small problem here because the wave equation describing a scattering state in (4.2) is not part of the $L_2(a,b)$ space i.e. not normalizable. A wave packet, constituted by a set of individuals waves, is on the other hand normalizable and by **Theorem A4.4** (see **appendix A4**) fully

$$\Psi_1(x,t) = (Ae^{ikx} + Be^{-ikx})e^{-iEt/\hbar}. \quad (4.3)$$

Now, let us introduce potential $V(x) \neq 0$ which gives rise to transformation of the scattering state in (4.3). Because there is a time parameter *t* we may introduce an evolution operator $U(t_2, t_1)$ **[8** p. 232 **]** which is a time dependent transforms a state by the following rule:

$$\Psi_2(x,t_2) = U(t_2,t_1)\Psi_1(x,t_1),$$

with the definition of $U(t_1,t_1) = I$. The $\boldsymbol{S}$-matrix is the time limit of the evolution operator $U(t_2,t_1)$ i.e.

$$\lim_{\substack{t_1\to-\infty \\ t_2\to\infty}} U(t_2,t_1) = \boldsymbol{S}.$$

The scattering transformation of a quantum mechanical state can then be written as:

$$\Psi_1\boldsymbol{S} = \Psi_2. \quad (4.4)$$

The conservation of probability demands that $\langle\Psi_1|\Psi_1\rangle = \langle\Psi_2|\Psi_2\rangle$. If we take the absolute square of both sides of expression (4.4) we see that $\Psi_2^*\Psi_2 = \Psi_1^*\boldsymbol{S}^*\boldsymbol{S}\Psi_1$. It follows that $\boldsymbol{S}^*\boldsymbol{S} = \mathbb{I}$ which means that the $\boldsymbol{S}$-matrix is unitary.

We will from now on concentrate on to show how to construct $\boldsymbol{S}$-matrix from some idealized scattering problems and its connection to probability conservation. Before we first deal with the one-dimensional scattering problem let us mention some facts about idealized scattering in experimental physics.

In an idealized scattering experiment we have a particle (P) with a defined momentum and which is scattered from a target (T) with a well defined shape. As a result of the collision there are several possible outcomes:

1. An elastic collision where momentum of $P + T$ is conserved.
2. An inelastic collision where some kinetic energy of $P + T$ is transformed.
3. An absorption where $P + T$ is transformed into a new particle.

In this paper we will limit our analysis to only elastic collisions; both energy, momentum and the number of particles are conserved. In particular our point of view will be from a theoretical perspective, where we first treat one dimensional scattering problem and expand the analysis to the three dimensional scattering problem.

4.1 One dimensional quantum mechanical scattering

Consider a schematic situation where an object described by state Ψ_1, is scattered by a potential *V(x)* at time *t* which transforms the state Ψ_1 into another scattered state Ψ_2. We can divide the situation into three regions as seen in *Fig. 4.1*.

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defined by its continuous distribution. But it would be too much for us to describe a configuration of waves, why we only deal with a wavelength at a time.

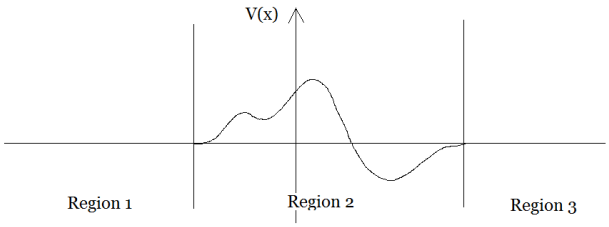

Figure 4.1. Scattering from an arbitrary localized potential.

Outside the potential, in the region 1 and 3, the Schrödinger equation has following time independent form where $V(x) = 0$:

$$\text{Region 1:} \quad \frac{\partial^2 \psi_1}{\partial x^2} = -\frac{2m}{\hbar^2} E\psi_1 \tag{4.5}$$

$$\text{Region 3:} \quad \frac{\partial^2 \psi_3}{\partial x^2} = -\frac{2m}{\hbar^2} E\psi_3 \tag{4.6}$$

The solutions to the equation (4.5) and (4.6) are:

$$\psi_1 = Ae^{ik_1 x} + Be^{-ik_1 x} \quad A, B \in \mathbb{C} \tag{4.7}$$

$$\psi_3 = Fe^{ik_1 x} + Ge^{-ik_1 x} \quad F, G \in \mathbb{C}. \tag{4.8}$$

Where k_1 is the wave number of de Broglie wave representing the object:[12]

$$k_1 = \frac{\sqrt{2mE}}{\hbar}.$$

Recall from appendix A2.2 that adding the time dependence $e^{-iEt/\hbar}$ gives rise to a wave function propagating to either left or right depending on the time independent function:

$$\Psi_1(x,t) = Ae^{ik_1\left(x - \frac{\hbar k_1}{2m}t\right)} + Be^{-ik_1\left(x + \frac{\hbar k_1}{2m}\right)t}. \tag{4.9}$$

We can therefore interpret *A* and G as incident wave amplitudes from left respective right side as in *Fig. 4.1*. By the potential *V(x)* the incident waves are partially reflected and transmitted with the wave amplitudes *B* and *F*.

Inside the barrier the Schrödinger equation reads:

$$Region\ 2: \quad \frac{\partial^2 \psi_2}{\partial x^2} = \frac{2m}{\hbar^2}(V(x) - E)\psi_2 \tag{4.10}$$

The solution to the equation (4.10) depends on whether $(V(x) - E)$ has positive or negative sign (or zero). It is not in our purpose to go through all possibilities and therefore we limit our analysis to the case where $(V(x) - E)$ is constant and positive. In that case the solution to equation (4.10) is:[13]

[12] Actually an object cannot be just represented by a single probability wave. In that case it would be everywhere. Instead we are talking about a wave packet, a packet with individual waves in superposition. For our purpose it is fully enough to study one wave individually. However, example of numerical studies of wave packets scattering off different wells and barriers can be found in [19].

[13] Observe that since the exponents are real of function (4.11) it does not oscillate and therefore cannot represent a moving object defined by de Broglie wave. The probability density, which is

$$\psi_2 = Ce^{k_2 x} + De^{-k_2 x} \qquad C, D \in \mathbb{C},\ k_2 = \frac{\sqrt{2m(V-E)}}{\hbar}. \tag{4.11}$$

Now, we must have both ψ and its derivative to be continuous. This implies *four boundary conditions* because there are three regions with two splits dividing the regions (see *Fig. 4.1*).

$$Between\ region\ 1\ and\ 2,\ x = a_1: \begin{cases} \psi_1 = \psi_2 \\ \frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \end{cases} \tag{4.12}$$

$$Between\ region\ 2\ and\ 3,\ x = a_2: \begin{cases} \psi_2 = \psi_3 \\ \frac{d\psi_2}{dx} = \frac{d\psi_3}{dx} \end{cases} \tag{4.13}$$

By substituting ψ_1, ψ_2 and ψ_3 from equation (4.7), (4.11) and (4.8) into boundary conditions (4.12) and (4.13) we will end up in a system of equations:

$$Ae^{ik_1 a_1} + Be^{-ik_i a_1} = Ce^{k_2 a_1} + De^{-k_2 a_1} \tag{4.14}$$

$$ik_1 Ae^{ik_1 a_1} - ik_1 Be^{-ik_i a_1} = k_2 Ce^{k_2 a_1} - k_2 De^{-k_2 a_1} \tag{4.15}$$

$$Ce^{k_2 a_2} + De^{-k_2 a_2} = Fe^{ik_1 a_2} + Ge^{-ik_1 a_2} \tag{4.16}$$

$$k_2 Ce^{k_2 a_2} - k_2 De^{-k_2 a_2} = ik_1 Fe^{ik_1 a_2} - ik_1 Ge^{-ik_1 a_2}\ . \tag{4.17}$$

We can write the above equation system in a more compact way as:

$$\begin{pmatrix} e^{ik_1 a_1} & e^{-ik_1 a_1} & -e^{k_2 a_1} & -e^{-k_2 a_1} & 0 & 0 \\ ik_1 e^{ik_1 a_1} & -ik_1 e^{-ik_i a_1} & -k_2 e^{k_2 a_1} & k_2 e^{-k_2 a_1} & 0 & 0 \\ 0 & 0 & e^{k_2 a_2} & e^{-k_2 a_2} & -e^{ik_1 a_2} & -e^{-ik_1 a_2} \\ 0 & 0 & k_2 e^{-k_2 a_2} & -k_2 e^{k_2 a_2} & -ike^{ik_1 a_2} & ik_1 e^{-ik_1 a_2} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \\ F \\ G \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Let us for simplicity deal with a location of the potential which has its position between $a_1 = 0,\ a_2 = L$. This implies somewhat easier matrix than above stated:

$$\begin{pmatrix} 1 & 1 & -1 & -1 & 0 & 0 \\ ik_1 & -ik_1 & -k_2 & k_2 & 0 & 0 \\ 0 & 0 & e^{-k_2 L} & e^{k_2 L} & -e^{ik_1 L} & -e^{-ik_1 L} \\ 0 & 0 & k_2 e^{-k_2 L} & -k_2 e^{k_2 L} & -ike^{ik_1 L} & ik_1 e^{-ik_1 L} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \\ F \\ G \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{4.18}$$

Usually, in experimental physics, there is only incoming wave from one side. Let us therefore put $G = 0$ which makes it only possible for a transmitted wave with amplitude *F*. Now, to show the probability conservation principle we need to calculate the transmission probability (*T*) and reflection probability (*R*) which are defined as:

$$T = \frac{|F|^2}{|A|^2}\ , \qquad R = \frac{|B|^2}{|A|^2}.$$

The first step is to calculate *F/A* and *B/A* which can be done by observing that *A* and *B* are functions of *C* and *D* which are in turn functions of just *F*:

---

square of the function (4.11), is certainly real and therefore there is a real probability of finding the object within the barrier!

$$\begin{cases} A + B = C + D \\ ik_1(A - B) = k_2(C - D) \end{cases} \rightarrow \begin{cases} A = C\left(\frac{k_2 + ik_1}{2ik_1}\right) + D\left(\frac{ik_1 - k_2}{2ik_1}\right) \\ B = C\left(\frac{ik_1 - k_2}{2ik_1}\right) + D\left(\frac{k_2 + ik_1}{2ik_1}\right) \end{cases}, \quad (4.19a)$$

$$\begin{cases} Fe^{ik_1L} = Ce^{k_2L} + De^{-k_2L} \\ ik_1Fe^{ik_1L} = k_2(Ce^{k_2L} - De^{-k_2L}) \end{cases} \rightarrow \begin{cases} C = F(e^{ik_1L}e^{-k_2L}\left(\frac{k_2 + ik_1}{2k_2}\right) \\ D = F(e^{ik_1L}e^{k_2L}\left(\frac{k_2 - ik_1}{2k_2}\right) \end{cases}. \quad (4.19b)$$

By replacing *C* and *D* in equation (4.19a) by formula for *C* and *D* in (4.19b) we will obtain the following ratios for *F/A* and *B/A*:

$$\frac{F}{A} = \frac{4ik_1k_2e^{-ik_1L}e^{k_2L}}{e^{2k_2L}(k_1 + ik_2)^2 - (k_1 - ik_2)^2}, \quad (4.20a)$$

$$\frac{B}{A} = \frac{(e^{2k_2L} - 1)(k_1^2 + k_2^2)}{e^{2k_2L}(k_1 + ik_2)^2 - (k_1 - ik_2)^2}. \quad (4.20b)$$

Expression (4.20a) can be rewritten as:

$$\left(\frac{F}{A}\right)^{-1} = \frac{e^{2k_2L}(k_1 + ik_2)^2 - (k_1 - ik_2)^2}{4ik_1k_2e^{-ik_1L}e^{k_2L}} = e^{ik_1L}\left[\frac{e^{k_2L}(k_1 + ik_2) - e^{-k_2L}(k_1 - ik_2)}{4ik_1k_2}\right]$$

$$= e^{ik_1L}\left[\frac{k_2^2 + 2ik_1k_2 - k_1^2}{4ik_1k_2}e^{-k_2L} - \frac{k_2^2 - 2ik_1k_2 - k_1^2}{4ik_1k_2}e^{k_2L}\right]$$

$$= e^{ik_1L}\left[\frac{k_2^2 - k_1^2}{4ik_1k_2}e^{-k_2L} - \frac{k_2^2 - k_1^2}{4ik_1k_2}e^{k_2L} + \frac{2ik_1k_2}{4ik_1k_2}e^{-k_2L} + \frac{2ik_1k_2}{4ik_1k_2}e^{k_2L}\right]$$

$$= e^{ik_1L}\left[\left(\frac{k_2^2 - k_1^2}{4ik_1k_2}\right)(e^{-k_2L} - e^{k_2L}) + \frac{e^{k_2L} + e^{-k_2L}}{2}\right]$$

$$= e^{ik_1L}\left[2i\left(\frac{k_2^2 - k_1^2}{4k_1k_2}\right)\left(\frac{e^{k_2L} - e^{-k_2L}}{2}\right) + \left(\frac{e^{k_2L} + e^{-k_2L}}{2}\right)\right]$$

$$= e^{ik_1L}\left[i\left(\frac{k_2^2 - k_1^2}{2k_1k_2}\right)\sinh(k_2L) + \cosh(k_2L)\right].$$

We are now able to express the transmission probability as ratios between square of probability amplitudes F/A. The complex conjugate of F/A which we denote by $(F/A)^*$ multiplied by (F/A) gives:

$$T^{-1} = \left(\frac{F}{A}\right)^{-1}\left(\frac{F^*}{A^*}\right)^{-1} = \frac{\cosh^2(k_2L) + (k_2^2 - k_1^2)^2\sinh^2(k_2L)}{4k_1^2k_2^2}$$

Utilizing the hyperbolic identity, $\cosh^2 x + \sinh^2 x = -1$, the expression above for transmission coefficient can be simplified further to give:

$$T = \left[1 + \frac{(k_1^2 + k_2^2)^2\sinh^2(k_2L)}{4k_1^2k_2^2}\right]^{-1}.$$

Using same method as when obtaining the transmission coefficient it can be shown that (4.20b) leads to the reflection coefficient

$$R = \left[1 + \frac{4k_1^2k_2^2}{(k_1^2 + k_2^2)^2 \sinh^2(k_2L)}\right]^{-1}.$$

Remember expression for the k_1 and k_2 where

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \quad k_2 = \frac{\sqrt{2m(V-E)}}{\hbar},$$

the transmission and reflection coefficients can be written as

$$T = \left[1 + \frac{V^2 \sinh^2(k_2L)}{4E(V-E)}\right]^{-1} \quad and \quad R = \left[1 + \frac{4E(V-E)}{V^2 \sinh^2(k_2L)}\right]^{-1}.$$

Let us verify the principle of probability conservation which should in this case give $T + R = 1$:

$$T + R = \left[1 + \frac{V^2 \sinh^2(k_2L)}{4E(V-E)}\right]^{-1} + \left[1 + \frac{4E(V-E)}{V^2 \sinh^2(k_2L)}\right]^{-1}$$

$$= \frac{4E(V-E)}{4E(V-E) + V^2 \sinh^2(k_2L)} + \frac{V^2 \sinh^2(k_2L)}{4E(V-E) + V^2 \sinh^2(k_2L)} = 1.$$

4.2 Generalization of quantum mechanical scattering in one dimension

The case study of one dimensional scattering under restrictions of $V(x) > 0$ in section 4.1 can be generalized to arbitrary localized potential.[14] In region 1 and 3 (see Fig. 4.1) the potential energy is $V(x) = 0$. This means the solutions to the time independent Schrödinger equations are:

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \tag{4.21}$$

$$\psi_3 = Fe^{ik_1x} + Ge^{-ik_1x} \tag{4.22}$$

In region 2 the potential energy is $V(x)$ and the Schrödinger equation reeds:

$$\frac{\partial^2\psi_2}{\partial x^2} + \frac{2m}{\hbar^2}(V(x) - E)\psi_2 = 0. \tag{4.23}$$

A general solution to the linear second order differential equation (4.23) is of the form:

$$\psi_2 = Cf(x) + Dg(x) \qquad C, D \in \mathbb{C}, \tag{4.24}$$

where both $f(x)$ and $g(x)$ are two linear and independent solutions. The rest of the problem is about to combine region 1 and 2 by two boundary conditions and region 2 and 3 by another two boundary conditions:

$$x = x_1 \quad \begin{cases} \psi_1 = \psi_2 \\ \dfrac{\partial\psi_1}{\partial x} = \dfrac{\partial\psi_2}{\partial x} \end{cases}$$

[14] In our analysis we are treating only one wave function.

$$x = x_2 \quad \begin{cases} \psi_2 = \psi_3 \\ \dfrac{\partial \psi_2}{\partial x} = \dfrac{\partial \psi_3}{\partial x} \end{cases}$$

Two of the conditions can be used to eliminate *C* and *D* which will lead to *B* and *F* can be solved in terms of *A* and *G*. We can therefore construct a 2 x 2 scattering matrix (***S***-matrix) which tells us the relation between the incoming components of wave (*A* and *G*) and outgoing components of wave (*B* and *F)*:

$$\binom{B}{F} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \binom{A}{G} \quad \rightarrow \quad \psi_{out} = \boldsymbol{S}\psi_{in}, \tag{4.25}$$

$$Where: \quad \psi_{in} = \binom{A}{G}, \quad \psi_{out} = \binom{B}{F}.$$

The law of energy conservation demands conservation of probability, as stated in (3.2). This means in quantum mechanical notation $\psi_{in}^* \psi_{in} = \psi_{out}^* \psi_{out}$. But since the relation (4.25) holds the following must be true for one dimensional scattering problem:

$$\psi_{in}^* \psi_{in} = \psi_{out}^* \psi_{out} = \psi_{in}^* \boldsymbol{S}^* \boldsymbol{S} \psi_{in} \quad \Rightarrow \quad \boldsymbol{S}^* \boldsymbol{S} = \mathbb{I}, \tag{4.26}$$

Which leads to the following equation $(|A|^2 + |G|^2) = (|B|^2 + |F|^2)$.

In a typical formulation of scattering described in section 4.1 we only have incident wave coming from one side of the potential. But we can as well think of two incident waves with the same wave number coming from both sides of the potential. In the first case we are able to talk about the reflection (*R*) and transmission (*T*) coefficients. For example if we let $G = 0$ we have the following expression for (*R*) and (*T*):

$$R = \frac{|B|^2}{|A|^2} = S_{11}^2, \quad T = \frac{|F|^2}{|A|^2} = S_{21}^2.$$

4.3 Quantum mechanical scattering in three dimensions

In classical three dimensional scattering the main problem is to calculate scattering angle when we have a given impact parameter. Consider the case where the collision object is a circle with radius *R* at which we fire a projectile with an impact parameter *b*, see *Fig. 4.2*. Using the angle notation from *Fig. 4.2* we can see that the impact parameter is equal to $b = Rsin(\alpha)$ where $\theta = \pi - 2\alpha$ and therefore:

$$\theta = \begin{cases} 2\cos^{-1}(b/R) & b \leq R \\ 0 & b > R \end{cases}$$

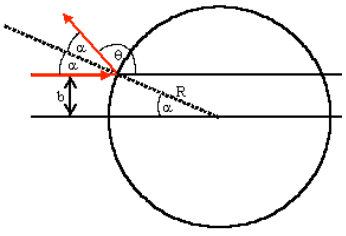

Figure 4.2. Scattering circle.

Expanding to three dimensional view we can introduce so called **differential cross section**, defined as the ratio of an infinitesimal area $d\sigma$, from which there is a projection into a corresponding infinitesimal solid angle $d\Omega$ (see *Fig. 4.*3) or $D(\theta, \varphi) = d\sigma/d\Omega$. In practice we measure the number of particles received ($N_r(\theta, \varphi)$) by a counter in a certain time interval and in some solid angle (θ, φ). If we know how many particles per time unit

are crossing a unit area, normal to the direction of incident say J_i, we are able to calculate the differential cross section by:

$$D(\theta,\varphi) = \frac{d\sigma}{d\Omega} = \frac{N_r(\theta,\varphi)}{J_i}.$$

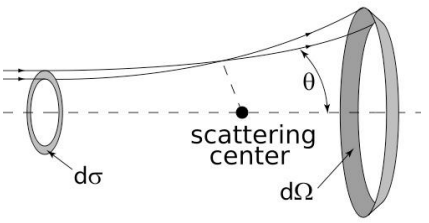

Figure 4.3 Schematic scattering.

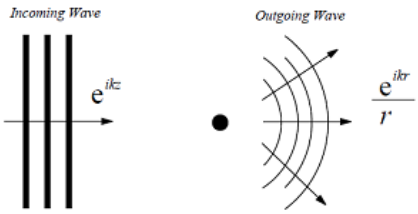

Figure 4.4 QM scattering 2-dimension.

From the differential cross section we can obtain the total cross section of a collision object, which typically depends on the energy of the incoming particle and the collision object's form [**18** pp. 24-25**]**, as:

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int D(\theta,\varphi) d\Omega\,. \tag{4.27}$$

Let us now go over to quantum theory of scattering and imagine a simple configuration where a plane wave, defined by e^{ikz} and traveling in *z*-direction, representing an electron, atom or another particle, travelling towards an object represented by a potential $V(\boldsymbol{r})$, see *Fig. 4.4* for a 2-dimensional example. After interaction with the potential there is an outgoing (in this example) spherical wave with the energy concentration proportional to $e^{ik\boldsymbol{r}}/r$. The wave carries a factor of $1/r$ because of the energy conservation law. The task for us now is to solve the Schrödinger equation for different configurations and find the probability amplitude for respective outgoing waves. We know that the solution must be similar to:

$$\psi(\boldsymbol{r},\theta,\varphi) \approx A\left(e^{ikz} + \frac{f(\theta,\varphi)e^{ik|\boldsymbol{r}|}}{|\boldsymbol{r}|}\right). \tag{4.28}$$

As before k is related to energy of the incident particle as $k = \sqrt{2mE}/\hbar$. The so called scattering amplitude $f(\theta,\varphi)$, which is related to the S-matrix, has a close connection to the differential cross section. By analyzing the problem in probability measurement we have in case for large $\boldsymbol{r}$:

$$dP_{in} = \left|Ae^{ikz}\right|^2 dV_\sigma = \left|\frac{Af(\theta,\varphi)e^{ikr}}{r}\right|^2 dV_\Omega = dP_{sc}\,,$$

where dP_{in} is the probability of a particle being in a small volume around part of cross section dV_σ and dP_{sc} is the probability of finding the scattered particle in a small volume dV_Ω. We have in fact following notation:

$$\int dP_{in} = \int \left|Ae^{ikz}\right|^2 dV_\sigma = \int \left|\frac{Af(\theta,\varphi)e^{ikr}}{r}\right|^2 dV_\Omega = \int dP_{sc} = 1.$$

But $dP_{in} = dP_{sc}$ which in our notation reads:

$$dP_{in} = |A|^2 dz d\sigma = \frac{|A|^2|f(\theta,\varphi)|^2}{r^2} dz r^2 d\Omega = dP_{sc}\,. \tag{4.29}$$

By using formulation (4.27) and equation (4.29) it follows that $d\sigma = |f(\theta,\varphi)|^2 d\Omega$ and therefore:

$$D(\theta,\varphi) = |f(\theta,\varphi)|^2\,. \tag{4.30}$$

In other words the differential cross section is equal to the absolute square of scattering amplitude.

There are two main techniques of finding solutions to scattering problems: partial wave analysis [**8** pp. 595-599] and Born approximation [**8** pp. 615-618]. In the following we will use the techniques of partial wave analysis for calculating the scattering amplitude.

Let us begin by observing that solution to the three-dimensional Schrödinger equation for different potential functions has vast set of solutions. We will therefore limit ourselves to the potentials which are typically functions of the distance from the origin. It is then more convenient to go from cartesian (*x, y, z*) to spherical coordinates (*r, θ, φ*). By limitation to a spherically symmetrical potential $V(\boldsymbol{r})$ we can now allow us to use the method of separable solution to the three-dimensional Schrödinger equation. Referring to appendix A2.3 the wave equation described by the Schrödinger equation with symmetrical potential $V(\boldsymbol{r})$ has separable solutions of following form in spherical coordinates:

$$\Psi(r,\theta,\varphi) = R_l(r)Y_l^m(\theta,\varphi),$$

where $R_l(r)$ is a function of distance from the origin and $Y_l^m(\theta,\varphi)$ is the function of polar angle θ, and azimuthal angle φ. The values m and l in Y_l^m are standing for magnetic quantum number (m) respectively azimuthal quantum number (l).[15] The radial solution $R_l(r)$ satisfies the radial equation (see appendix A2.3 eq. A2.3e):

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r)-E) = l(l+1). \tag{4.31}$$

By introducing $u(r) = rR(r)$, so that $dR/dr = [r(du/dr) - u]/r^2$ and $(d/dr)[r^2(dR/dr)] = r(d^2u/dr^2)$, we can write (4.31) in the following form:[16]

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu. \tag{4.32}$$

The solution to equation (4.32) depends on $V(r)$. If we consider the case when potential is localized, which means $V(r) = 0$ if $r > a$ where $a \in \mathbb{R}$, we are dealing with two regions. In the region where $V(r) = 0$ the radial equation becomes:

$$\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}u = -k^2u \qquad k = \sqrt{2mE}/\hbar. \tag{4.33}$$

The general solution, for arbitrary integer l, to the equation (4.33) is a combination of spherical **Bessel** ($j_l(x)$) and **Neumann** ($n_l(x)$) functions of order l [**9** p.142, **16** pp.540-543]:

$$u(r) = r\big(Aj_l(kr) + Bn_l(kr)\big), \quad A, B \in \mathbb{C}, \tag{4.34}$$

where spherical Bessel and Neumann functions are defined as follows:

$$j_l(x) = (-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\frac{\sin(x)}{x}, \qquad n_l(x) = -(-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\frac{\cos(x)}{x}.$$

[15] Observe *m* does not stand for the physical unit mass in this case.

[16] The equation (4.31) is called radial equation and is identical in form to the one dimensional Schrödinger equation (see *Principle 4*, part 3) except $\left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]$, which is called effective potential, and containing an extra term.

The problem is that neither spherical Bessel nor Neumann function represents a complex wave function as stated in (4.28). The solution to the problem is to apply spherical **Hankel functions** of first and second kind:[17]

$$h_l^{(1)}(x) = j_l(x) + in_l(x), \quad h_l^{(2)}(x) = j_l(x) - in_l(x), \tag{4.35}$$

We are interested in asymptotic behavior (large r) of spherical Hankel functions. For the first kind Hankel function $h_l^{(1)} \to (-i)^{l+1}e^{ikr}/r$ and the second kind Hankel function $h_l^{(2)} \to i^{l+1}e^{-ikr}/r$, when r goes to infinity. Because we are interested in an outgoing probability wave we use the spherical Hankel function of first kind. The solution to the radial equation (4.33) is proportional to $h_l^{(1)}(kr)$ or $R_l(r) \sim h_l^{(1)}(kr)$.

The exact probability wave function in region where $V(r) = 0$ can now be written as:

$$\Psi(r,\theta,\varphi) = A\left(e^{ikz} + \sum_{l,m} C_{l,m} h_l^{(1)}(kr) Y_l^m(\theta,\varphi)\right), \tag{4.36}$$

where the first complex term is the *incident plane wave* and the second series term is the *scattered wave* where $C_{l,m}$is the product coefficients for $h_l^{(1)}(kr)Y_l^m(\theta,\varphi)$. Now we have to deal with angular wave function $Y_l^m(\theta,\varphi)$ which is proportional to (see appendix A2.3):

$$Y_l^m(\theta,\varphi) \sim Ae^{im\varphi} + Be^{-im\varphi} P_l^m(\cos(x)),$$

where P_l^m is the **Legendre function** defined in appendix A2.3. The normalized angular wave function $Y_l^m(\theta,\varphi)$ is called spherical harmonic:

$$Y_l^m(\theta,\varphi) = c\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}e^{im\varphi}P_l^m(\cos(x)), \tag{4.37}$$

where $c = (-1)^m$ for $m \geq 0$ and $c = 1$ for $m < 0$. Because we have limited ourselves to spherically symmetric potential there is no dependence of variable φ in the outgoing wave function (4.37). This means m is equal to zero which gives us following spherical harmonic function:

$$Y_l^0(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos(\theta)).$$

The product coefficient $C_{l,m}$ in function (4.36) is then reduced to $C_{l,0} = i^{l+1}k2\sqrt{\pi(2l+1)}a_l(k)$ [**9** p. 402], where $a_l(k)$ is called the partial wave amplitude. We can now write the wave function in (4.36) as follows:

$$\Psi(r,\theta) = A\left(e^{ikz} + k\sum_{l=0}^{\infty} i^{l+1}(2l+1)a_l(k)h_l^{(1)}(kr)P_l(\cos(\theta))\right). \tag{4.38}$$

In the limit of large distance from the origin of the potential we know that the Hankel function $h_l^{(1)} \to (-i)^{l+1}e^{ikr}/r$. This means:

$$\Psi(r,\theta) \approx A\left(e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right),$$

[17] This is analogous to linear combination of e^{ix} and e^{-ix} in case when we want to express the harmonic functions $sin(x)$ and $cos(x)$.

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) a_l(k) P_l(\cos(\theta)).$$

Remember that $\sigma = \int D(\theta,\varphi) d\Omega$ and $D(\theta,\varphi) = |f(\theta,\varphi)|^2$, we have now a way to calculate the total scattering cross section as function of $f(\theta)$. With the orthogonality relation:

$$\int P_l(\cos(\theta))\, P_{l'}(\cos(\theta)) d\Omega = \frac{4\pi}{2l+1} \delta_{ll'},$$

where $\delta_{ll'} = 1$ if $l = l'$and $\delta_{ll'} = 0$ if $l \neq l'$, we can express σ by:

$$\sigma = \sum_{ll'} (2l+1)(2l'+1) a_l^*(k) a_{l'}(k) \int P_l(\cos(\theta))\, P_{l'}(\cos(\theta)) d\Omega =$$

$$= 4\pi \sum_{l=0}^{\infty} (2l+1) |a_l(k)|^2.$$

To calculate $a_l(k)$ one need to solve the Schrödinger equation in the region where $V \neq 0$ and match the solution to the solution of (4.38) using right boundary conditions as in one dimensional scattering analysis. It is not in our scope to make all the necessary and in many times advance calculations to get an explicit formula for $a_l(k)$. The interested reader is advised to consult [8] or [9].

5 Discussion

We have now looked on the quantum mechanical scattering theory by a brief analysis of one and three dimensional problems. In section 2 we presented the mathematical frame of reference upon which the quantum mechanical scattering theory is based. In section 3 we presented the principles on which quantum mechanics is based. In particular the main principles of quantum mechanics gave us the ability to understand how to deal with *probability amplitude*. The main result which followed from previous section 4, on quantum mechanical scattering theory, was that a scattering matrix must be unitary to ensure that energy and probability amplitude were conserved. The construction of scattering matrix for simple case as one dimensional problem involve solving the Schrödinger equation and application of correct boundary conditions. Whereas the three dimensional scattering problem, even in simple cases with spherical symmetrical potential, give rise to complicated solution to the Schrödinger equation.

An important distinction we would like to stress is the difference between analyzing a problem by a deterministic model, as we have done in solving the Schrödinger equation, and a probabilistic model. A differential equation may well describe a random phenomenon, although the equation does not capture any of the randomness involved in the real problem. A differential equation can not tell us why a particle has chosen to scatter into one direction or another. It only tells us the average behavior of the scattering phenomenon. We can only point out a random phenomenon by its distribution which we observe. In the case of one dimensional scattering the distribution is binomial; reflection or transmission. In the case of three dimensional scattering we may have a continuous distribution over spherical angles θ, φ (scattering problem described in section 4.3 by function (4.30)) or a discrete distribution in case of limited number of scattering channels.

Further questions which might be interested to examine are connected to the set of all unitary scattering matrices characterized by some given conditions. For example we might be interested in construction of a physical devise which gives a certain distribution of scattered amplitudes. Relevant applications are different efficient photon radiation and collection techniques. One example which is widely used in our everyday lives is *light emmitin-diod*. More advanced applications are; micropillar cavity [22], light guiding nanowires [23] and apertured microcavity [24]. All these applications are based on proper understanding of scattering theory.

Appendices

A1 Mathematical description of wave motion

In this section we formulate mathematical description for wave motion in general. Further on we concentrate on a special case of wave motion, the harmonic wave. The importance of harmonic wave comes from its physical representation.

A1.1 Wave equation [14 pp.94-96]

To begin with let us define a one dimensional pulse of arbitrary shape. One can set the pulse moving along *x*-axis to the right of the origin with speed v. The shape of the pulse stays the same but changes the location on the *x*-axis as time goes by. In mathematical form the moving pulse is described by a time-dependent function which has the form of $f(x-vt)$.

By definition any function represented by $\psi = f(x-vt)$ is a pulse traveling in positive x-direction. If the pulse moves to the left the sign of v must be reversed so we might write in general

$$f(x+vt) + g(x-vt). \tag{A1.1a}$$

Theorem A1.1. In general a *one dimensional wave function satisfies following differential equation:*

$$\frac{\partial^2\psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \tag{A1.1b}$$

Proof. For $\psi = f(h)$ where $h = (x-vt)$ we can calculate the partial derivatives as follow:

Derivative with respect to *x*:

$$\frac{\partial\psi}{\partial x} = \frac{\partial f}{\partial h}\frac{dh}{dx} = \frac{\partial f}{\partial h}.$$

Second derivate with respect to *x*:

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\right) = \frac{\partial}{\partial h}\left(\frac{\partial\psi}{\partial x}\right)\frac{dh}{dx} = \frac{\partial}{\partial h}\left(\frac{\partial f}{\partial h}\right) = \frac{\partial^2 f}{\partial h^2}.$$

First time derivative:

$$\frac{\partial\psi}{\partial t} = \frac{\partial f}{\partial h}\frac{dh}{dt} = -v\frac{\partial f}{\partial h}.$$

Second time derivative:

$$\frac{\partial^2\psi}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial\psi}{\partial t}\right) = \frac{\partial}{\partial h}\left(\frac{\partial\psi}{\partial t}\right)\frac{dh}{dt} = \frac{\partial}{\partial h}\left(-v\frac{\partial f}{\partial h}\right)(-v) = v^2\frac{\partial^2 f}{\partial h^2}.$$

Comparing the second partial derivatives we get the statement (A1.1b). ■

A1.2 Harmonic waves [14 pp. 96-97]

An important representation of wave in physics is the harmonic one which is characterized by a periodicity. The most familiar are the sine and cosine functions,

$$\psi = Asin[k(x \pm vt)], \quad or \quad \psi = Acos[k(x \pm vt)] \tag{A1.2a}$$

Where *A* and *k* are constants. Because the only difference between sine and cosine is the phase of $\pi/2$ it is sufficient for us to treat only one of the functions.

Definition A1.1. *Relationships of wave parameters:*

- *The constant k is related to the wavelength λ as* $k = 2\pi/\lambda$.
- *The time period T is related to the wavelength λ as* $vT = \lambda$., *where* v *is the wave velocity.*
- *The angular frequency ω is related to the wavelength λ as* $\omega = 2\pi\, v/\lambda$

By Definition A1.1 we can express the harmonic functions in (A1.2a) in different ways:

$$Asin[k(x \pm vt)] = Asin\left[2\pi\left(\frac{x}{\lambda} \pm \frac{t}{T}\right)\right] = Asin[(kx \pm \omega t)].$$

A1.3 Harmonic waves in three-dimensional space [14 pp. 100-102]

Definition A1.2. *Let* $\vec{\boldsymbol{r}}$ *be the vector representing an arbitrary point in space and* $\vec{\boldsymbol{k}}$ *represent a vector with magnitude* $2\pi/\lambda$ *which is pointing in the direction of propagation of the wave. Similar to one dimension we write :*

$$\psi = Asin\left(\vec{\boldsymbol{k}} \cdot \vec{\boldsymbol{r}} \pm \omega t\right) \tag{A1.3a}$$

The partial differential equation which is satisfied by the harmonic wave in **(A1.3a)** is a generalization of equation (A1.1b) and has following form:

$$\Delta\psi = \frac{1}{v}\frac{\partial^2\psi}{\partial t^2},$$

where Δ is the Laplacian in cartesian coordinates defined as: $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$.

Using Eulers's formula the function in (A1.3a) can be expressed as imaginary part of the complex function

$$\psi = Im\ \left(Ae^{i(\vec{r}\cdot\vec{k}-\omega t)}\right) \tag{A1.3b}$$

This will simplify many calculations because it is easier to work with exponential functions than with trigonometric.

A2 The Schrödinger equation

A2.1 The Schrödinger equation in one dimension

The Schrödinger equation can be arrived in many different ways but it cannot be derived from already known physical principles [8,9,12]. We will here show one way to get the equation by starting from a freely moving particle interpreted by **L. de Broglie's** point of view as a wave described in appendix A1. Assume a wave function (A1.3a), mentioned in section A1.3, but for simplicity only in one dimension (*x-axis*) as moving in + *x direction*, which can be written as:

$$\Phi = Ae^{i\left(\frac{2\pi}{\lambda}t-\omega t\right)}.$$

We can now rewrite the above written function by implementing what we have already stated in *section 1* about the energy of a particle and its wavelength:

$$E = hf = 2\pi\hbar f \quad \text{and} \quad \lambda = \frac{2\pi\hbar}{p}.$$

This gives us the wave function for a freely moving particle:

$$\Phi = Ae^{i/\hbar(\,px-Et)}. \tag{A2.1a}$$

The expression for the wave function (A2.1a) is correct only for freely moving particles which means potential $V = 0$. By restricting the motion of the freely moving particle by some local potential $V(x,t) \neq 0$, in general a function of position *x* and time *t*, we get by the classical physics the total energy of the particle as sum of its potential and kinetic energy. For non relativistic energies (particle speed much lower than speed of light) the total energy is given by:

$$E = \frac{p^2}{2m} + V(x,t). \tag{A2.1b}$$

What we now will do is to obtain the fundamental difference equation for a wave function Ψ, which we can solve for a specific situation involving potential restriction. Let us begin by differentiating equation (A2.1a) twice with respect to *x*, which gives:

$$\frac{\partial^2\Phi}{\partial x^2} = -\frac{p^2}{\hbar^2}\Phi \quad \rightarrow \quad p^2\Phi = -\hbar^2\frac{\partial^2\Phi}{\partial x^2}. \tag{A2.1c}$$

Differentiating equation (A2.1a) once with respect to *t* gives:

$$\frac{\partial\Phi}{\partial t} = -\frac{iE}{\hbar}\Phi \quad \rightarrow \quad E\Phi = -\frac{\hbar}{i}\frac{\partial\Phi}{\partial t}. \tag{A2.1d}$$

Multiplying both sides of equation **(**A2.1b) by Φ and substituting for $E\Phi$ and $p^2\Phi$ from equation (A2.1c) and (A5.1d) respectively we obtain following equation:

$$i\hbar\frac{\partial\Phi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Phi}{\partial x^2}.$$

Remember the classical expression for the total energy in (A2.1b), we can now use the quantum mechanical equivalence which is the operator in (A2.1d) for energy E. The operator for momentum p is given in (A2.1c). We will get the time dependent Schrödinger equation for the wave function Ψ as:

$$E\Psi = \frac{p^2\Psi}{2m} + V(x,t)\Psi \;\rightarrow\; i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi.$$

A2.2 Separation of variables to solve the Schrödinger equation

In many physical problem formulations the potential energy *V* is independent of time. In that case the Schrödinger equation can be solved by the method of *separation of variables*. We are looking for solutions to the Schrödinger equation which are products

$$\Psi(x,t) = \psi(x)\varphi(t), \tag{A2.2a}$$

where ψ is a function of only *x* and φ is a function of only *t*. Substituting the expression in (A2.2a) into the Schrödinger equation and dividing by $\Psi = \psi\varphi$ we will obtain:

$$i\hbar\frac{1}{\varphi}\frac{d\varphi}{dt} = -\frac{\hbar}{2m}\frac{d^2\psi}{dx^2}\frac{1}{\psi} + V(x). \qquad \text{(A2.2b)}$$

Because the left side of the equation **(A2.2b)** is a function of just *t* and the right side is a function of *x*, both sides must be constant. In fact it turns out that the constant in equation **(A2.2b)** is related to the energy of the system [**9** pp. 26-27]. Now we have made a partial differential equation into two ordinary differential equations:

1. $E = i\hbar\frac{1}{\varphi}\frac{d\varphi}{dt} \quad or \quad \frac{Edt}{i\hbar} = \frac{d\varphi}{\varphi}$

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

The first equation can be solved by standard methods with an integration of both sides to get $\varphi(t) = e^{-iEt/h}$. The second equation, which is a time independent Schrödinger equation, can be solved when the potential *V(x)* is specified.

A2.3 Separation of variables to solve the Schrödinger equation in spherical coordinates

In three dimensions the Schrödinger equation has following form:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar}{2m}\nabla^2\Psi + V\Psi, \qquad \text{(A2.3a)}$$

Changing from cartesian coordinates to spherical coordinates (r, θ, φ) the Laplacian takes the following form:

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\left(\frac{\partial^2}{\partial\varphi^2}\right). \qquad \text{(A2.3b)}$$

Putting the Laplacian in (A2.3b) into the three dimensional Schrödinger equation (A2.3a) and we may look for solutions to the separable equation of following form:

$$\Psi(r, \theta, \varphi) = R(r)\Theta(\theta)\Phi(\varphi). \qquad \text{(A2.3c)}$$

The partial derivatives are:

$$\frac{\partial\Psi}{\partial r} = \frac{dR}{dr}\Theta\Phi \qquad \frac{\partial\Psi}{\partial\theta} = \frac{d\Theta}{d\theta}R\Phi \qquad \frac{\partial^2\Psi}{\partial\varphi^2} = \frac{d^2\Phi}{d\varphi^2}R\Theta. \qquad \text{(A2.3d)}$$

Substituting the expression (A2.3c) and the three derivatives (A2.3d) in the Schrödinger equation (A2.3a), thereafter dividing entire equation by $\Psi = R\Theta\Phi$ and multiplying by $(-2mr^2/\hbar^2)$ we end up with the following equation:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}(V(r) - E) + \frac{1}{\Theta}\left(\frac{1}{\sin(\theta)}\frac{d}{d\theta}\left(\sin(\theta)\frac{d\Theta}{d\theta}\right)\right) + \frac{1}{\Phi}\left(\frac{1}{\sin^2(\theta)}\frac{d^2\Phi}{d\varphi^2}\right) = 0.$$

As with the one dimensional analysis (see equation (A2.2b)) we can divide the above written equation into two equations equal to a constant:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}(V(r)-E)=k, \tag{A2.3e}$$

$$\frac{1}{\Theta}\left(\frac{1}{\sin(\theta)}\frac{d}{d\theta}\left(\sin(\theta)\frac{d\Theta}{d\theta}\right)\right)+\frac{1}{\Phi}\left(\frac{1}{\sin^2(\theta)}\frac{d^2\Phi}{d\varphi^2}\right)=-k. \tag{A2.3f}$$

It can be proved that the constant k is equal to $l(l+1)$, where l is an nonnegative integer. The equation (A2.3e), which is called the **radial equation**, can only be solved when we know the form of the potential $V(r)$. The equation (A2.3f) can be divided once more into following parts after multiplication by $\sin^2(\theta)$:

$$\frac{1}{\Theta}\left(\sin(\theta)\frac{d}{d\theta}\left(\sin(\theta)\frac{d\Theta}{d\theta}\right)\right)+l(l+1)\sin^2(\theta)=-\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}.$$

Both sides are constant which we may set to q. It can be proved that $q=m^2$, where m is an integer. The separation constant m^2 in above equation gives following equations:

$$\frac{1}{\Theta}\left(\sin(\theta)\frac{d}{d\theta}\left(\sin(\theta)\frac{d\Theta}{d\theta}\right)\right)+l(l+1)\sin^2(\theta)=-m^2 \tag{A2.3g}$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=-m^2 \tag{A2.3h}$$

Equation (A2.3h) can be directly solved to generate following solutions:

$$\Phi(\varphi)=Ae^{im\varphi}+Be^{-im\varphi}\quad where\ A,B\in\mathbb{C}$$

Somewhat difficult is to solve equation (A2.3g) so we will just state the solution which is given in [9 p.136]:

$$\Theta(\theta)=AP_l^m(\cos(\theta)),$$

Where P_l^m is the **Legendre function** defined by:

$$P_l^m(x)=(1-x^2)^{\frac{|m|}{2}}\left(\frac{d}{dx}\right)^{|m|}P_l(x),$$

and P_l is the **Legendre polynomial** of the l^{th} order, defined by the **Rodrigues formula**:

$$P_l(x)=\frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l(x^2-1)^l.$$

A3 A mathematical definition of a complete vector space

Definition A3.1 *A **metric space** is a set X with a real-valued function $d: X\times X\to\mathbb{R}_+$ such that for every $x,y,z\in X$:*

- $d(x,y)\geq 0$ *and*
- $d(x,y)=0$ *if and only if* $x=y$
- $d(x,y)=d(y,x)$
- $d(x,y)\leq d(x,z)+d(y,z)$.

The metric space is an abstraction of the distance between two points in space. This creates a fundamental question of closeness of points and, in a broader view, completeness of a metric space. To deal with this questions let us define convergence.

Definition A3.2 *If for some x and for any positive real number ϵ there exists a natural number N, such that $d(x_n, x) < \epsilon$ when $n > N$, we say that the sequence $\{x_n\}_{n=1}^{\infty}$* ***converges*** *to x. Written as* $\lim_{n\to\infty} x_n = x$.

Often it is not easy to tell about convergence of a sequence from Definition A3.2. However, the next best thing to do is to see whether the points of a sequence get closer with larger *n*. Let's therefore define a Cauchy sequence.

Definition A3.3 *A* ***Cauchy sequence*** *is a sequence for which $x \in X$ shows following property:* $\lim_{m,n\to\infty} d(x_m, x_n) = 0$

A sequence that converges is necessary a Cauchy which can be shown by the following:

$$|x_m - x_n| - |x_m - x + x - x_n| \leq |x_m - x| + |x - x_n| < \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon$$

We have here used the Definition A3.2 of convergence and triangle inequality.

Definition A3.4 *A* ***complete*** *metric space is one in which every Cauchy sequence converges.*

An example of a metric space which is not complete but where we have a Cauchy sequence is the set of rational numbers $\mathbb{Q}$ with respect to the absolute value metric i.e. $d(x, y) = |x - y|$. If we take the sequence of rational numbers $x_n = \sum_{k=1}^{n}(1 + 1/k)^k$ the sum is well known to converge to the base of natural logarithm *e*, which is an irrational number. But *e* is not part of $\mathbb{Q}$ which means that $\mathbb{Q}$ is not complete.

We now define a Euclidian metric space often represented by vectors.

Definition A3.5 *A* ***vector space*** *V is a set of objects called vectors with the following properties:*

1) *For every vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ in V we have corresponding binary operation with the vector-result which is also in V*
   a) $\vec{a} + \vec{b} = \vec{b} + \vec{a}$ (*where* $\vec{a} + \vec{b} \in V$)
   b) $\vec{a} + (\vec{b} + \vec{c}) = (\vec{a} + \vec{b}) + \vec{c}$
   c) $\vec{a} + \vec{0} = \vec{a}$ ($\vec{0}$ is a unique zero-vector)
   d) $\vec{a} + (-\vec{a}) = \vec{0}$

2) *For scalars $k, \alpha \in \mathbb{C}$ we have a corresponding vector in V with following properties:*
   a) $k(\alpha\vec{b}) = k\alpha\vec{b}$
   b) $1\vec{b} = \vec{b}$

3) *Distributive laws:*
   a) $k(\vec{a} + \vec{b}) = k\vec{a} + k\vec{b}$
   b) $(k + \alpha)\vec{b} = k\vec{b} + \alpha\vec{b}$

Definition A3.6 *The vectors $\overrightarrow{a_1}, \overrightarrow{a_2}, \ldots, \overrightarrow{a_n}$ are said to be* ***linearly independent*** *if for scalars $\alpha_i \in \mathbb{C}$, the relation $\sum_{i=1}^{n} \alpha_i \overrightarrow{a_n} = 0$ implies $\alpha_i = 0$ for all i.*

Definition A3.7 *A* ***complete vector space*** *V is a vector space for which every Cauchy sequence of vectors in V has a limit vector in V.*

A.4 Basics in probability theory

The basic idea behind the probability theory is the *probability space* and the *stabilization of the relative frequencies*. If we perform, what is called, *independent* repetitions of an unchanged *random* experiment we will get a countable set, an integer number *B,* for as many times as an event occurred and continue add 1 to the set for every time the event occurs. Let then $T_n(B)$ denote the number of occurrences of *B* in the first *n* trials, and $R_n(B)$ the relative frequency whit the following relation; $R_n(B) = T_n(B)/n$. We will empirically observe the stabilization of the relative frequencies as $R_n(B)$ converges to some *real* number as $n \to \infty$. To be more precise let us build up some definitions and outline some basic properties in probability theory which will be of importance for us when dealing with theory of quantum mechanics. A more rigorous treatment of probability can be found in most books for graduate courses in probability as example **[7]**.

Definition A4.1 *The triple (Ω,F,P) is a* probability space *if*

- *Ω is the sample space.*
- *F is a collection of events - or the subsets of* $\boldsymbol{\Omega}$.[18]
- *P is a probability measure, which means that P satisfies the following three axioms of Kolmogorov:*

  1. *For any A* $\in F$*, there exists a number P(A)* ≥ 0*; the probability of A.*
  2. $P(\Omega) = 1$.
  3. *Let* $\{A_n, n \geq 1\}$ *be disjoint. Then* A_n is countable additive:

$$P\left(\bigcup_1^\infty A_n\right) = \sum_1^\infty P(A_n)\,.$$

Definition A4.2 *The events* $\{A_k, 1 \leq k \leq n\}$ *are independent if and only if*

$$P\left(\bigcap A_{i_k}\right) = \prod P\left(A_{i_k}\right),$$

where intersections and products are to be taken over all subsets of $\{1, 2, \ldots, n\}$.

Definition A4.3 A random variable *X* is a *(measurable) function from the sample space Ω to* $\mathbb{R}$*;* $X : \Omega \to \mathbb{R}$.

The inverse image of any subset A of R *is a subset of F:*

$$X^{-1}(A) = \{\omega : X(\omega) \in A\} \in F \quad for\ all\ A \in \mathrm{R}.$$

Definition A4.4 To each random variable *X* there is an *induced probability* $\mathbb{P}$:

$$\mathbb{P}(A) = P(X^{-1}(A)) = P(\{\omega : X(\omega) \in A\}) \quad for\ all\ A \in \mathrm{R}.$$

By Definition 4.3 and 4.4 we have actually described a map from (*Ω,F,P*) to $(\mathbb{R}, \mathrm{R}, \mathbb{P})$ which can be showed to satisfy Kolmogorov's axioms. The importance of this fact should be stated in a theorem.

Theorem A4.1 *The* induced *space* $(\mathbb{R}, \mathrm{R}, \mathbb{P})$ *with* $\mathbb{P}$ *defined by* Definition A4.4 *is a probability space.*

[18] To be more formal *F* is an *σ-algebra of sets.* But for our purposes it is fully enough to define *F* as a collection of events as subsets of *Ω*.

Actually there is no reason for us to go between the two probability spaces when in fact we are just interested in the random variable *X*. We shall henceforth, for convenient reason, write $P(X \in A)$ instead of $\mathbb{P}(A) = P(\{\omega : X(\omega) \in A\})$.

Definition A4.5 *Let A and B be two events, and suppose that P(A) > 0. The* conditional probability of *B* given *A is defined as*

$$P(B|A) = \frac{P(B \cap A)}{P(A)}.$$

If conditional probability of an event *B* does not depend on a given event *A* we say event *B* and *A* are independent.

Definition A4.6 *A random variable X said to be* degenerate *if:*

$$\textit{for some } a \in \mathbb{R},\ P(X = a) = 1.$$

The degenerality is treated as some kind of axiom in quantum mechanics. When one measures an observable of a quantum mechanical system the probability wave is said to collapse to give only one value; a degenerate state.

Definition A4.7 *Expectation value of a random variable X respectively continuous random variable Y is*

$$E(X) = \sum_{-\infty}^{\infty} x p_X(x) \qquad \textit{respectively} \qquad E(Y) = \int_{-\infty}^{\infty} y f_Y(y) dy$$

Where $p_X(x)$is probability to get an outcome *x* from a random variable *X* and $f_Y(y)dy$ is the limit of probability to get an outcome in the infinitesimal surround of *y* from a random variable *Y*.

Definition A4.8 *Variance, or spread, of a random variable X is defined by:*

$$E(X^2) - E(X).$$

References

[1] L. de Broglie, "Recherches sur la théorie des quanta" [On the Theory of Quanta]. *Annales de Physique* **10** (3): 22–128 (1925), Translated version.

[2] W. Heisenberg, *Physical Principles of Quantum Theory*. *Chicago Univ*. Press, Chicago (1930).

[3] E. Schrödinger, "Quantisierung als Eigenwertproblem; von Erwin Schrödinger". *Annalen der Physik*, 361–377 (1926).

[4] E. Schrödinger, "An Undulatory Theory of the Mechanics of Atoms and Molecules". *Physical Review*, **28** (6): 1049–1070 (1926).

[5] P. A. M. Dirac, *The Principles of Quantum Mechanics*, *Oxford Univ*. Press (1930).

[6] A. N. Kolmogorov, *Grundbegriffe der Wahrscheinlichkeitsrechnung*, *Springer Verlag*, Berlin (1933).

[7] Probability: A graduate course (*second ed.*), A. Gut, Springer, 2013, ISBN 978-1-4614-4708-5 (e-book).

[8] Quantum Mechanics (*second ed.*), B.H. Bransden and C.J. Joachain, Pearson Prentice Hall, 2000, ISBN 0-582-35691-1.

[9] *Introduction to Quantum Mechanics (2nd ed.*), D. J. Griffiths, Prentice Hall, 2005, ISBN 0-13-191175-9.

[11] Feynman Lectures on Physics (Vol. 3,), R. Feynman, R.B. Leighton, M. Sands, Addison-Wesley, 1989, ISBN 0-201-51005-7.

[12] Concepts of MODERN PHYSICS (*sixth ed.*), A. Beiser, McGraw-Hill, 2003, ISBN 007-123460-8.

[13] University Physics (*ninth ed*.), H.D. Young and R.A. Freedman, *Addison-Wesley*, 1996, ISBN 0-201-31132-1.

[14] Introduction to Optics (*third ed.*), F.L Pedrotti, L.M Pedrotti, L.S. Pedrotti, *Pearson Prentice Hall*, 2007, ISBN 0-13-197133-6.

[15] Elementary Linear Algebra (*tenth ed.*), H. Anton and C. Rorres, *John Wiley & Sons*, 2011, ISNB 978-0-470-56157-7.

[16] Mathematical Physics, S. Hassani, *Springer*, 1998, ISBN 978-0-387-98579-4.

[17] Felix Bloch, *Physics Today*, **29** (12) (23 December 1976).

[18] Nuclear Physics, John Lilley, *John Wiley & Sons*, 2006, ISBN 0-471-97936-8.

[19] J. L. Schwartz, *American Journal of Physics*, **35** (177) (1967).

[20] P. W. Hawkes, *Physics Today*, **43** (7): 84–85 “Ernst Ruska” (July 1990).

[21] G. Binnig, H. Rohrer, *IBM Journal of Research and Development*, **30**: 4 (1986).

[22] J. M. Gérard, B. Sermage, B. Gayral, B. Legrand, E. Costard, and V. Thierry-Mieg, *Phys. Rev*. Lett. **81**, 1110 (1998).

[23] J.Claudon, J.Bleuse, N. S. Malik, M. Bazin, P. Jaffrennou, N. Gregersen, C.Sauvan, P. Lalanne and J.M. Gérard. *Nature Photonics* Vol. 4, 174 (2010).

[24] S. Strauf, N. G. Stoltz, M. T. Rakher, L. A. Coldren, P. M. Petroff and D. Bouwmeester. Nature Photonics Vol 1, 704-708 (2007).