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Quantum Mechanics

Lecture Notes

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Chapter 1

Postulates of Quantum Mechanics

1.1 Postulates

1. The state of a quantum system at time t is represented by a normalized vector $|\psi(t)\rangle$ belonging to some Hilbert space.
2. A physical observable is represented by a linear, hermitian operator \hat{O} .
3. The only possible result of a measurement of an observable is one of the eigenstates o_i of the corresponding operator \hat{O} .
4. The probability for measuring the value o_j is $P_{o_j} = |\langle o_j | \psi(t) \rangle|^2$, where $|o_j\rangle$ is the normalized eigenvector of \hat{O} corresponding to the eigenvalue o_j .
5. After a measurement of \hat{O} that yields the result o_j , the quantum system is in a new state that is the normalized projection of the original state vector onto the vector corresponding to the result of the measurement:

$$|\psi'\rangle = \frac{\hat{P}_j |\psi\rangle}{\sqrt{\langle \psi | \hat{P}_j | \psi \rangle}}, \quad (1.1)$$

where $\hat{P}_j = |o_j\rangle \langle o_j|$ is the projection operator onto the eigenket $|o_j\rangle$ corresponding to the eigenvalue o_j .

6. The time evolution of a state is given by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle, \quad (1.2)$$

where the Hamiltonian operator \hat{H} represents the energy observable of the system.

1.2 Stern-Gerlach experiment

The experiment was first carried out by O. Stern and W. Gerlach in 1922. Fig. 1.1 shows a schematic diagram of the apparatus. A collimated beam of silver atoms is produced by evaporating silver in a hot oven and selecting those atoms that pass through a series of narrow slits. The beam is then directed between the poles of a magnet producing an inhomogeneous magnetic field. When a neutral atom with a magnetic moment $\vec{\mu}$ enters the magnetic field \vec{B} , it experiences a force

$$\vec{F} = \nabla(\vec{\mu} \cdot \vec{B}). \quad (1.3)$$

For particles like electron, the magnetic moment is proportional to intrinsic angular momentum (called spin): $\vec{\mu} \propto \vec{S}$. If we call the direction in which the inhomogeneous magnetic field is large the z direction, we see that

$$F_z = \mu_z \frac{\partial B_z}{\partial z} \propto S_z \frac{\partial B_z}{\partial z}. \quad (1.4)$$

Classically, $S_z = |\vec{S}| \cos \theta$, where θ is the angle that the magnetic moment makes with the z axis. Thus S_z should take on a continuum of values ranging from $-|\vec{S}|$ to $+|\vec{S}|$, so we should find a corresponding continuum of deflections. Surprisingly, Stern and Gerlach observed only two deflections. In fact, they measured the component of the intrinsic angular momentum of an electron along the z axis and found it to take only two discrete values, $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$, commonly called "spin up" and "spin down" respectively. Numerically, $\hbar = \frac{h}{2\pi} = 6.582 \times 10^{-16} eV \cdot s$, where h is Planck's constant.

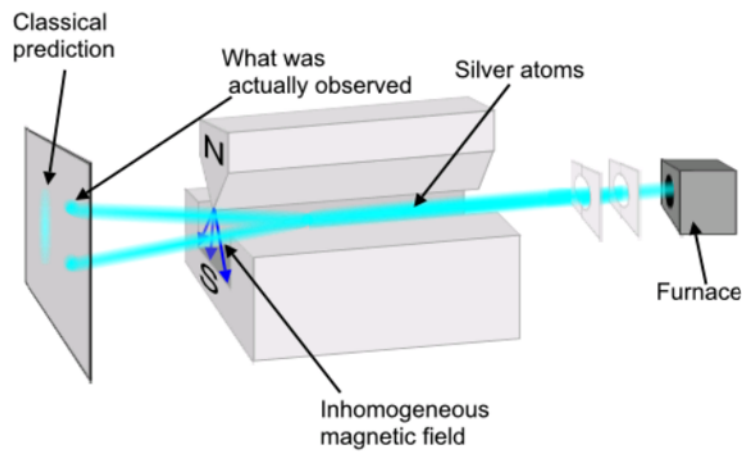


Figure 1.1: Stern-Gerlach experiment [1].

1.3 Five Experiments

Let's turn our attention to five simple experiments that will tell us much about the structure of quantum mechanics. One can think of these experiments as thought experiments in which technical difficulties are hidden.

1.3.1 Experiment 1

Let's say a particle that exits a device in which there is an inhomogeneous magnetic field parallel to the z axis with $S_z = \frac{\hbar}{2}$ is in the state $|+\rangle$ (we discard other particles). The symbol $|+\rangle$, called a ket vector is convenient way of denoting this state. Suppose a beam of particles, each of which is in this state, enters another Stern-Gerlach device with magnetic field in z direction. We find that all particles exit in the state $|+\rangle$ as indicated in fig. 1.2.

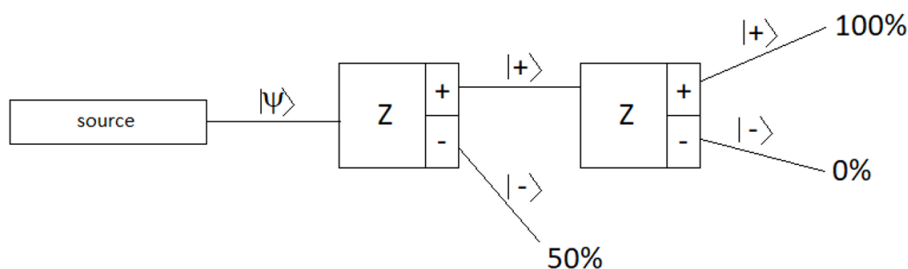


Figure 1.2: Experiment 1

1.3.2 Experiment 2

The first part of this experiment is the same as in experiment 1 i.e. we keep only particles in state $|+\rangle$ coming out of the first SG device. We next send this beam into SG device with inhomogeneous magnetic field oriented along the x axis. We find that 50% of the particles exit the second device with $S_x = \frac{\hbar}{2}$ and are therefore in the state $|+\rangle_x$, while the other 50% exit with $S_x = -\frac{\hbar}{2}$ and are therefore in the state $|-\rangle_x$ (see fig. 1.3). For completeness, we note that if we select the beam of particles exiting the initial SG apparatus in the state $|-\rangle$ instead of $|+\rangle$ and send this beam through the second device, we also find that 50% of the particles yield $\frac{\hbar}{2}$ for a measurement of S_x and 50% yield $-\frac{\hbar}{2}$ for a measurement of S_x .

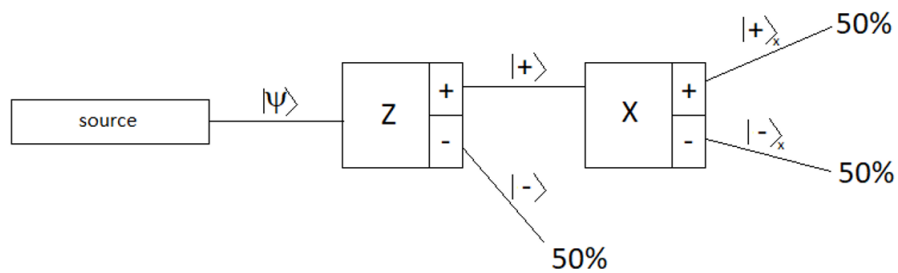


Figure 1.3: Experiment 2

1.3.3 Experiment 3

Let's add a third SG apparatus to experiment 2, but with its inhomogeneous field oriented along the z axis (see 1.4). If we send the beam of particles exiting the second SG device in the state $|+\rangle_x$ through the last device, we find that 50% of the particles exit in the state $|+\rangle$ and 50% exit in the state $|-\rangle$. Initially, none of the particles entering the second device was in the state $|-\rangle$, so the measurement of S_x must have modified the state of the system. Hence, we cannot think of the beam entering the last SG device as comprised of particles with $S_z = \frac{\hbar}{2}$ and $S_x = \frac{\hbar}{2}$ as one might expect.

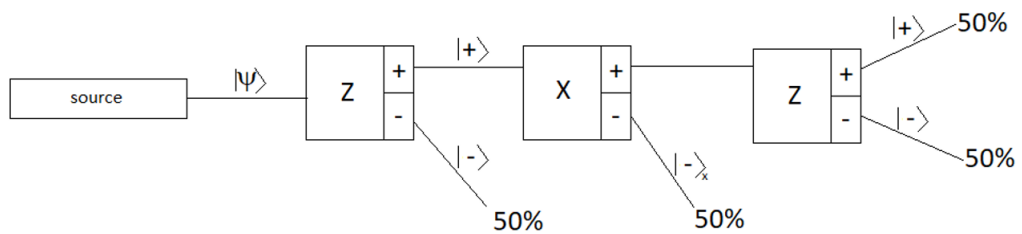


Figure 1.4: Experiment 3

1.3.4 Experiment 4

This experiment is conceptually the same as experiment 3, but this time we keep particles in state $|-\rangle_x$ coming out of the second SG device (see fig. 1.5). Note that we get the same results at the last SG device.

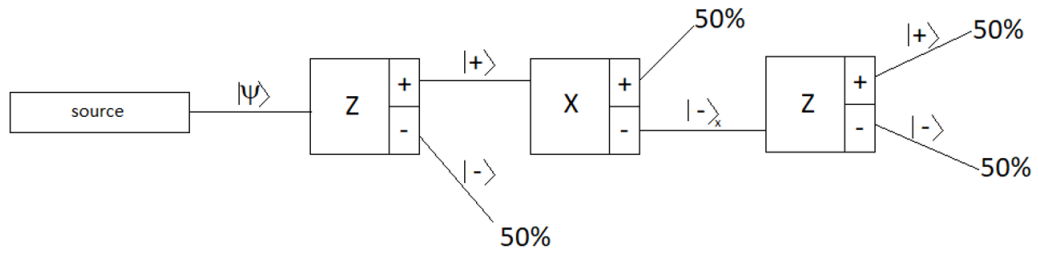


Figure 1.5: Experiment 4

1.3.5 Experiment 5

As in experiment 3, a beam of particles in the state $|+\rangle$ from the first SG apparatus enters the second device with magnetic field along the x axis, but this time we do not block one of the paths. We then send the beam into the third SG device, same as in experiment 3. As indicated in fig. 1.6 we find that 100% of the particles exit the last SG device in the state $|+\rangle$. Before carrying out experiment 5, it may seem obvious (based on results of experiments 3 and 4) that 50% of the particles passing through the last analyzer would be in the state $|+\rangle$ and 50% in the state $|-\rangle$

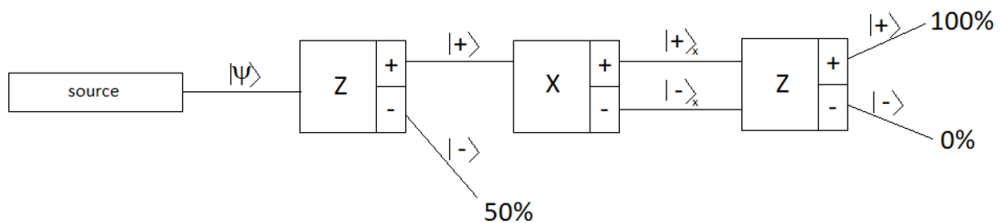


Figure 1.6: Experiment 5

1.4 Quantum State Vectors

The mathematics of quantum mechanics is the mathematics of linear vector spaces. The vector spaces of quantum mechanics are like the ordinary three-dimensional spaces of vectors from elementary physics, except that the scalar

product is complex, the dimension is arbitrary and we use different notation for vectors (Dirac's notation).

The analysis of Stern-Gerlach experiments revealed that there are only two possible values of every experiment of S_z . Let these two results correspond to two vectors $|+\rangle$ and $|-\rangle$. These two vectors form a complete set of basis vectors. Hence, any other ket can be written as a linear combination of the two basis kets:

$$|\psi\rangle = \alpha |+\rangle + \beta |-\rangle. \quad (1.5)$$

From elementary linear algebra we know that for every vector space there is a corresponding dual space of linear functionals. We call elements of this dual space "bra" and denote them as $\langle\psi|$. If $|\psi\rangle$ is a vector as defined in 1.5, then the corresponding bra is defined as

$$\langle\psi| = \alpha^* \langle+| + \beta^* \langle-|. \quad (1.6)$$

The scalar (dot) product in quantum mechanics is most commonly written as the product of a bra and a ket i.e. if we have $|\psi\rangle$ and $\langle\phi|$, then their scalar product is

$$\langle\phi|\psi\rangle. \quad (1.7)$$

Using this notation, we can express orthonormality of $\{|+\rangle, |-\rangle\}$ basis:

$$\begin{aligned} \langle+|+\rangle &= 1, \\ \langle-|-\rangle &= 1, \end{aligned} \quad (1.8)$$

$$\begin{aligned} \langle+|-\rangle &= 0, \\ \langle-|+\rangle &= 0. \end{aligned} \quad (1.9)$$

Notice that when we multiply 1.5 from the left by $\langle+|$, we obtain the first coefficient of $|\psi\rangle$:

$$\langle+|\psi\rangle = \alpha. \quad (1.10)$$

Likewise, it is easy to see that $\langle-|\psi\rangle = \beta$. Hence, we can express $|\psi\rangle$ as

$$\begin{aligned} |\psi\rangle &= \alpha |+\rangle + \beta |-\rangle \\ &= |+\rangle \langle+|\psi\rangle + |-\rangle \langle-|\psi\rangle. \end{aligned} \quad (1.11)$$

Now, let's multiply 1.6 from the right by $|+\rangle$. We obtain

$$\langle\psi|+\rangle = \alpha^*. \quad (1.12)$$

Comparing 1.10 and 1.12 we see that reversing vectors in inner product results in a complex conjugation of the inner product:

$$\langle + | \psi \rangle = \langle \psi | + \rangle^* . \quad (1.13)$$

This is true in general:

$$\langle \phi | \psi \rangle = \langle \psi | \phi \rangle^* . \quad (1.14)$$

Postulate 1 says about a normalized vector. If we apply this normalization requirement to a general state $|\psi\rangle$, then we obtain

$$\langle \psi | \psi \rangle = |\alpha|^2 + |\beta|^2 = 1. \quad (1.15)$$

Now comes the crucial element of quantum mechanics. We postulate that the probability that the quantum state described by the vector $|\psi\rangle$ is measured to be in the corresponding basis state is given by $|\langle + | \psi \rangle|^2$ and $|\langle - | \psi \rangle|^2$ (postulate 4). Thus

$$P_{S_z = \frac{\hbar}{2}} = |\langle + | \psi \rangle|^2, \quad (1.16)$$

and

$$P_{S_z = -\frac{\hbar}{2}} = |\langle - | \psi \rangle|^2. \quad (1.17)$$

1.5 Analysis of Experiments 1 and 2

Let's try to predict the results of experiment 1. All particles that went to the second analyzer were in the state $|+\rangle$. Because we know that the basis states are normalized and orthogonal, the probabilities are

$$\begin{aligned} P_+ &= |\langle + | + \rangle|^2 = 1, \\ P_- &= |\langle - | + \rangle|^2 = 0. \end{aligned} \quad (1.18)$$

We will use the results of the second experiment to figure out how the states $|+\rangle_x$ and $|-\rangle_x$ behave mathematically. Since the vectors $\{|+\rangle, |-\rangle\}$ form a basis, we can express $|+\rangle_x$ and $|-\rangle_x$ as

$$\begin{aligned} |+\rangle_x &= \alpha |+\rangle + \beta |-\rangle, \\ |-\rangle_x &= \delta |+\rangle + \gamma |-\rangle, \end{aligned} \quad (1.19)$$

for some unknown (possibly complex) coefficients: α , β , δ and γ . Notice, that the second SG apparatus found 50% probability of each of the two possible states

$|+\rangle_x$ and $|-\rangle_x$, when the input state was $|+\rangle$. Hence

$$P_{1,+x} = |{}_x\langle + | + \rangle|^2 = |\alpha^*|^2 = |\alpha|^2 = \frac{1}{2}. \quad (1.20)$$

Similarly, we find

$$|\beta|^2 = |\gamma|^2 = |\delta|^2 = \frac{1}{2}. \quad (1.21)$$

Because each coefficient is complex, each has an amplitude and phase. However, the overall phase of a quantum system is not physically meaningful and this fact lets us write the desired states as

$$\begin{aligned} |+\rangle_x &= \frac{1}{\sqrt{2}}(|+\rangle + e^{i\alpha} |-\rangle), \\ |-\rangle_x &= \frac{1}{\sqrt{2}}(|+\rangle + e^{i\beta} |-\rangle). \end{aligned} \quad (1.22)$$

Orthogonality condition leads to

$${}_x\langle - | + \rangle_x = 0 \rightarrow e^{i(\alpha-\beta)} = -1 \rightarrow \alpha - \beta = \pm\pi. \quad (1.23)$$

Since we are free to choose any α and β satisfying 1.23, so let us choose $\alpha = 0$ and $\beta = \pi$. Finally, we obtain

$$\begin{aligned} |+\rangle_x &= \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle), \\ |-\rangle_x &= \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle). \end{aligned} \quad (1.24)$$

We generally use the $\{|+\rangle, |-\rangle\}$ as the preferred basis for writing general states, but we could use any basis we choose. If we were to use $\{|+\rangle_x, |-\rangle_x\}$ basis, then we could express $|\pm\rangle$ kets as

$$\begin{aligned} |+\rangle &= \frac{1}{\sqrt{2}}(|+\rangle_x + |-\rangle_x), \\ |-\rangle &= \frac{1}{\sqrt{2}}(|+\rangle_x - |-\rangle_x). \end{aligned} \quad (1.25)$$

1.6 Matrix Notation

Up to this point we were working in the abstract setting. Now, it's time to simplify things a little bit by providing a concrete representation for vectors and operators. Since $\{|+\rangle, |-\rangle\}$ form a basis in a two-dimensional space, let's express both of them as column vectors:

$$|+\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (1.26)$$

and

$$|- \rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (1.27)$$

Then we can represent kets $|+\rangle_x$ and $|-\rangle_x$ as

$$|+\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad (1.28)$$

and

$$|-\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (1.29)$$

And the general ket

$$|\psi\rangle = \alpha |+\rangle + \beta |-\rangle \quad (1.30)$$

is represented as

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \quad (1.31)$$

We saw earlier that an inner product of a bra and a ket yields a single complex number. In order for the matrix rules of multiplication to be used, a bra must be represented by a row vector. Hence, a bra

$$\langle\psi| = \alpha^* \langle+| + \beta^* \langle-|, \quad (1.32)$$

must be represented as

$$\langle\psi| = (\alpha^* \quad \beta^*). \quad (1.33)$$

Now, the scalar product of $|\psi\rangle$ with its corresponding bra can be expressed as

$$\langle\psi|\psi\rangle = (\alpha^* \quad \beta^*) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = |\alpha|^2 + |\beta|^2. \quad (1.34)$$

1.7 Operators, Eigenvalues, Eigenvectors

An operator is a mathematical object that acts on a ket and transforms it into a new ket:

$$\hat{O}|\psi\rangle = |\phi\rangle \quad (1.35)$$

If $\hat{O}|\psi\rangle = \lambda|\psi\rangle$, where λ is a number, then we say $|\psi\rangle$ is an eigenvector of \hat{O} and λ is its eigenvalue. When we combine the results from previous sections with postulates 2 and 3, we come to the conclusion that eigenvalue equations for the

S_z operator are:

$$\begin{aligned} S_z |+\rangle &= \frac{\hbar}{2} |+\rangle \\ S_z |-\rangle &= -\frac{\hbar}{2} |-\rangle. \end{aligned} \quad (1.36)$$

Using 1.36 we are going to deduce the matrix elements of S_z , which must be 2×2 matrix:

$$S_z = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (1.37)$$

When we substitute 1.26, 1.27 and 1.37 into 1.36 we easily obtain

$$a = \frac{\hbar}{2}, \quad b = 0, \quad c = 0, \quad d = -\frac{\hbar}{2}. \quad (1.38)$$

So the matrix representation of the operator S_z is

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (1.39)$$

Now, consider the general operator \hat{O} , whose matrix representation we would like to determine:

$$\hat{O} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (1.40)$$

To obtain a particular coefficient, we "sandwich" an operator between a bra and a ket:

$$\langle + | \hat{O} | + \rangle = a, \quad \langle + | \hat{O} | - \rangle = b, \dots \quad (1.41)$$

The final result is

$$\hat{O} = \begin{pmatrix} \langle + | \hat{O} | + \rangle & \langle + | \hat{O} | - \rangle \\ \langle - | \hat{O} | + \rangle & \langle - | \hat{O} | - \rangle \end{pmatrix}. \quad (1.42)$$

We call the expression of the form

$$O_{ij} = \langle i | \hat{O} | j \rangle \quad (1.43)$$

a matrix element.

1.8 Hermitian and Projection Operators

So far we have only discussed the action of operators on kets:

$$\hat{A} |\psi\rangle = |\phi\rangle. \quad (1.44)$$

Notice, that in expression 1.44, the operator \hat{A} acts on $|\psi\rangle$ from the left. If we want to define the action of an operator \hat{A} on a bra, we must place it on the right hand side of it:

$$\langle\eta| = \langle\psi|\hat{A}. \quad (1.45)$$

Comparing eq. 1.44 and 1.45 we might suspect, that $\langle\eta|$ should be equal to $\langle\phi|$, but this not the case. Rather the bra $\langle\phi|$ is found by defining a new operator \hat{A}^\dagger that obeys

$$\langle\phi| = \langle\psi|\hat{A}^\dagger. \quad (1.46)$$

We call this new operator \hat{A}^\dagger the Hermitian adjoint of the operator \hat{A} . Even though \hat{A}^\dagger is a completely new operator, it has quite strong connection with operator \hat{A} . to discover it, we multiply both side of equation 1.46 by an arbitrary ket $|\alpha\rangle$:

$$\begin{aligned} \langle\phi|\alpha\rangle &= \langle\alpha|\phi\rangle^* \\ (\langle\psi|\hat{A}^\dagger)|\alpha\rangle &= \left[\langle\alpha|(\hat{A}|\psi\rangle) \right]^* \\ \langle\psi|\hat{A}^\dagger|\alpha\rangle &= \langle\alpha|\hat{A}|\psi\rangle^* \end{aligned} \quad (1.47)$$

The last equation in 1.47 says, that the matrix representing \hat{A}^\dagger is found by transposing and complex conjugating the matrix representing \hat{A} . It may happen that an operator \hat{A} is equal to its Hermitian conjugate:

$$\hat{A} = \hat{A}^\dagger, \quad (1.48)$$

and if this is the case, we call \hat{A} a Hermitian operator. In quantum mechanics, all operators that correspond to physical observables are Hermitian. It is because Hermitian operators have real eigenvalues and their eigenvectors comprise a complete set of basis states.

Another very important class of operators are projection operators. To introduce them, let's look at 1.11

$$\begin{aligned} |\psi\rangle &= \langle+|\psi\rangle|+\rangle + \langle-|\psi\rangle|-\rangle \\ &= |+\rangle\langle+|\psi\rangle + |-\rangle\langle-|\psi\rangle \\ &= (|+\rangle\langle+| + |-\rangle\langle-|)|\psi\rangle \end{aligned} \quad (1.49)$$

Comparing both sides of eq. 1.49 we conclude, that the term in parentheses must be the identity operator:

$$|+\rangle\langle+| + |-\rangle\langle-| = \hat{1}. \quad (1.50)$$

The individual operators $|+\rangle\langle+|$ and $|-\rangle\langle-|$ are called projection operators. Their matrix representation is:

$$\hat{P}_+ = |+\rangle\langle+| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad (1.51)$$

and

$$\hat{P}_- = |-\rangle\langle-| = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (1.52)$$

In general, any operator \hat{P} which is Hermitian and satisfies the relation $\hat{P}^2 = \hat{P}$ is said to be a projection operator.

We found previously that the probability of a measurement is given by the square of the inner product of initial and final states (postulate 4). Using the new projection operators, we can rewrite this probability as

$$\begin{aligned} p_+ &= |\langle+|\psi\rangle|^2 \\ &= \langle+|\psi\rangle^* \langle+|\psi\rangle \\ &= \langle\psi|+\rangle \langle+|\psi\rangle \\ &= \langle\psi|\hat{P}_+|\psi\rangle \end{aligned} \quad (1.53)$$

Using projection operators, we can also describe the change of the quantum state after the measurement (postulate 5):

$$|\psi'\rangle = \frac{\hat{P}_+|\psi\rangle}{\sqrt{\langle\psi|\hat{P}_+|\psi\rangle}} = |+\rangle. \quad (1.54)$$

1.9 Analysis of Experiments 3-5

Let's try to analyze the results of experiments 3-5 using developed tools. We need to discuss the probability that an atom leaving the first analyzer in the $|+\rangle$ state is detected in one of the counters connected to the output ports of the third analyzer. Such a probability involves two measurements at the second and third analyzers. The total probability is the product of the individual probabilities of each measurements. In particular, the probability of measuring an atom at the top most counter is the probability of measuring $S_x = \frac{\hbar}{2}$ at the second analyzer times the probability of measuring $S_z = \frac{\hbar}{2}$ at the third analyzer:

$$P_{upper,+} = |\langle+|+\rangle_x|^2 |\langle+|+\rangle|^2. \quad (1.55)$$

Similarly, we calculate other probabilities:

$$P_{upper,-} = |\langle -|+\rangle_x|^2 |\langle +|+\rangle|^2 \quad (1.56)$$

$$P_{lower,+} = |\langle +|-\rangle_x|^2 |\langle -|+\rangle|^2 \quad (1.57)$$

$$P_{lower,-} = |\langle -|-\rangle_x|^2 |\langle -|+\rangle|^2 \quad (1.58)$$

For experiment 5, both output ports of the second analyzer are connected to the third SG apparatus. Because both states are used, the relevant projection operator is the sum of the two projection operators for each port i. e. \hat{P}_{+x} and \hat{P}_{-x} .

$$|\psi_2\rangle = \frac{(\hat{P}_{+x} + \hat{P}_{-x})|+\rangle}{\sqrt{\langle +|(\hat{P}_{+x} + \hat{P}_{-x})|+\rangle}} = |+\rangle \quad (1.59)$$

The sum of projection operators in 1.59 is equal to the identity operator, hence $|\psi_2\rangle = |+\rangle$. That's why all particles coming out of the third analyzer are in the state $|+\rangle$.

1.10 Mean Value and Standard Deviation

Consider a random variable X with a finite list x_1, x_2, \dots, x_n of possible outcomes, each of which has probability p_1, p_2, \dots, p_n of occurring. The mean value of X is defined as

$$\langle X \rangle = \sum_i x_i p_i. \quad (1.60)$$

Let's calculate the mean value of S_z measurement for spin $\frac{1}{2}$ system:

$$\begin{aligned} \langle S_z \rangle &= \left(\frac{\hbar}{2}\right)p_+ + \left(-\frac{\hbar}{2}\right)p_- \\ &= \frac{\hbar}{2}|\langle +|\psi\rangle|^2 + -\frac{\hbar}{2}|\langle -|\psi\rangle|^2 \\ &= \frac{\hbar}{2}\langle \psi|+\rangle\langle +|\psi\rangle - \frac{\hbar}{2}\langle \psi|-\rangle\langle -|\psi\rangle \\ &= \langle \psi|S_z(|+\rangle\langle +| + |-\rangle\langle -|)|\psi\rangle \end{aligned} \quad (1.61)$$

Since $|+\rangle\langle +| + |-\rangle\langle -|$ is the identity matrix, we obtain

$$\langle S_z \rangle = \langle \psi|S_z|\psi\rangle. \quad (1.62)$$

The above result holds for any quantum mechanical observable:

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle. \quad (1.63)$$

In addition to the mean value, it is common to characterize a measurement by the standard deviation, which gives us information about the spread of measurement results about the mean. Formally, for a random variable X it is defined as

$$\Delta X = \sqrt{\langle (X - \langle X \rangle)^2 \rangle} = \sqrt{\langle X^2 \rangle - \langle X \rangle^2}. \quad (1.64)$$

Eq. 1.64 expressed in the language of operators is

$$\Delta \hat{O} = \sqrt{\langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2}, \quad (1.65)$$

where

$$\langle \hat{O}^2 \rangle = \langle \psi | \hat{O}^2 | \psi \rangle. \quad (1.66)$$

1.11 Commuting observables

The product of two operators is generally not commutative i.e. $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. To express this incompatibility of two operators we introduce a new object called a commutator:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}. \quad (1.67)$$

Two operators are said to commute if their commutator is equal to zero

$$[\hat{A}, \hat{B}] = 0 \iff \hat{A}\hat{B} = \hat{B}\hat{A}. \quad (1.68)$$

Any operator commutes with itself:

$$[\hat{A}, \hat{A}] = 0 \quad (1.69)$$

Thus, for commuting operators the order of operation does not matter, whereas it does for noncommuting operators. Now, let $|a\rangle$ be an eigenstate of the operator \hat{A} with eigenvalue a :

$$\hat{A}|a\rangle = a|a\rangle \quad (1.70)$$

If we multiply both sides of eq. 1.70 from the left by \hat{B} and suppose that \hat{A} and \hat{B} commute:

$$\hat{B}\hat{A}|a\rangle = \hat{B}a|a\rangle \rightarrow \hat{A}(\hat{B}|a\rangle) = a(\hat{B}|a\rangle), \quad (1.71)$$

then we notice, that the vector $\hat{B}|a\rangle$ is also an eigenstate of the operator \hat{A} with the same eigenvalue. Therefore, the state $\hat{B}|a\rangle$ must be some scalar multiple of the state $|a\rangle$:

$$\hat{B}|a\rangle = b|a\rangle, \quad (1.72)$$

which is just an eigenvalue equation for the operator \hat{B} . Therefore, we can conclude, that commuting operators have a common set of eigenstates. This has profound physical consequences, namely these two observables can be measured simultaneously. As an example, we may mention the commutators involving spin component operators. The complete commutation relations are

$$[S_x, S_y] = i\hbar S_z, \quad (1.73)$$

$$[S_y, S_z] = i\hbar S_x, \quad (1.74)$$

$$[S_z, S_x] = i\hbar S_y. \quad (1.75)$$

We see that spin operators do not commute and cannot be simultaneously measured.

1.12 Uncertainty Principle

An interesting application of the commutator algebra is to derive a general relation giving the uncertainties product of two operators, \hat{A} and \hat{B} . This is known as the Heisenberg's uncertainty relation. We only state the general result here:

$$\Delta\hat{A}\Delta\hat{B} \geq \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle| \quad (1.76)$$

As an example, we can lower bound the product of uncertainties for two spin component operators:

$$\Delta S_x \Delta S_y \geq \frac{1}{2}|\langle[S_x, S_y]\rangle| \geq \frac{\hbar}{2}|\langle S_z \rangle| \quad (1.77)$$

The most important uncertainty relation, which we are going to derive soon, involves the position and momentum operators:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \quad (1.78)$$

1.13 General Quantum Systems

The mathematical formalism developed so far for spin $\frac{1}{2}$ systems can be extended to higher dimensional systems. Suppose we have an observable \hat{O} for which there are n possible measurement results $o_1, o_2, o_3, \dots, o_n$. The basis ket corresponding to the result o_i is $|o_i\rangle$. The orthonormality condition then reads

$$\langle o_i | o_j \rangle = \delta_{ij}, \quad (1.79)$$

where δ_{ij} is the Kronecker delta, and an arbitrary ket $|\psi\rangle$ can be expressed as

$$|\psi\rangle = \sum_i \langle o_i | \psi \rangle |o_i\rangle. \quad (1.80)$$

The generalization of postulate 4 says that the probability of a measurement of one of the possible results o_n is

$$P_{o_n} = |\langle o_n | \psi \rangle|^2. \quad (1.81)$$

The eigenequation for \hat{O} is

$$\hat{O} |o_n\rangle = o_n |o_n\rangle. \quad (1.82)$$

In the basis formed by the eigenstates $|o_n\rangle$ the matrix representing the operator \hat{O} is diagonal

$$\hat{O} = \begin{pmatrix} o_1 & 0 & 0 & \dots \\ 0 & o_2 & 0 & \dots \\ 0 & 0 & o_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad (1.83)$$

and its size depends on the dimensionality of the system. In the same basis, the eigenstates are represented by the column vectors

$$|o_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad |o_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \quad \dots \quad (1.84)$$

The projection operator corresponding to measurement of the eigenvalue o_n is

$$\hat{P}_{o_n} = |o_n\rangle \langle o_n|, \quad (1.85)$$

and the sum of all projection operators is the identity operator

$$\sum_n \hat{P}_n = \sum_n |o_n\rangle \langle o_n| = \hat{1}. \quad (1.86)$$

1.14 Infinite Dimensional Quantum Systems

To introduce infinite dimensional systems, we need to look at classical physics. Classical mechanics is governed by Newton's law

$$\vec{F} = m\vec{a}. \quad (1.87)$$

The goal is to predict the function $r(\vec{t})$ of some body. Another method is based on energy. The total mechanical energy of a system is sum of kinetic (T) and potential (V) energies: $E = T+V$. These two methods are related by the equation

$$F_x = -\frac{dV}{dx}, \quad (1.88)$$

and hence the potential energy function is what determines the classical motion of a body.

Energy method is crucial in quantum mechanics. The last postulate says that the time evolution of a state is given by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle, \quad (1.89)$$

where the Hamiltonian operator \hat{H} represents the energy observable of the system. The prescription for finding a quantum mechanical Hamiltonian operator is to find the classical expression for the energy of the system:

$$E = \frac{p_x^2}{2m} + V(x), \quad (1.90)$$

and then replace classical momentum and position with quantum mechanical operators:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + V(\hat{x}). \quad (1.91)$$

It turns out that the action of the operator \hat{x} is represented by multiplication by x and the action of the momentum operator \hat{p} is represented by differentiation:

$$\begin{aligned} \hat{x} &\equiv x \\ \hat{p} &\equiv -i\hbar \frac{d}{dx} \end{aligned} \quad (1.92)$$

When we described spin- $\frac{1}{2}$ systems, we represented each ket (for example $|+\rangle$) as a 2×1 column vector. If we call the position eigenstates $|x_i\rangle$ then we could try to express (by analogy to spin- $\frac{1}{2}$ case) an arbitrary ket $|\psi\rangle$ as

$$|\psi\rangle \equiv \begin{pmatrix} \langle x_1 | \psi \rangle \\ \langle x_2 | \psi \rangle \\ \langle x_3 | \psi \rangle \\ \vdots \end{pmatrix} \quad (1.93)$$

where the projection $\langle x_i | \psi \rangle$ is the probability amplitude for the state $|\psi\rangle$ to be measured in the position eigenstate $|x_i\rangle$. The problem is that the position is not a quantized observable. There is a continuity of possible values of x . Hence the representation 1.93 is not adequate in this case. The natural way to represent such continuous set of numbers is a continuous function $\psi(x)$, called the wave function. The wave function expressed in Dirac notation is

$$\psi(x) = \langle x | \psi \rangle. \quad (1.94)$$

The meaning of eq. 1.94 is that $\psi(x)$ is the probability amplitude for the quantum state $|\psi\rangle$ to be measured in the position eigenstate $|x\rangle$. The probability density is equal to

$$P(x)dx = |\psi(x)|^2 dx. \quad (1.95)$$

So if we want to compute the probability that a particle is to be found in a finite interval $a < x < b$ we need to calculate the integral

$$P_{a < x < b} = \int_a^b |\psi(x)|^2 dx. \quad (1.96)$$

The normalization condition in the wave function language is expressed as

$$\langle \psi | \psi \rangle = 1 \rightarrow \int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx = 1 \quad (1.97)$$

The scalar product between two kets is defined as

$$\langle \phi | \psi \rangle = \int_{-\infty}^{\infty} \phi^*(x) \psi(x) dx. \quad (1.98)$$

The mean value of an operator is defined similarly to discrete case. For example, for position and momentum operators (using 1.92) we have:

$$\langle \hat{x} \rangle = \langle \psi | \hat{x} | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx, \quad (1.99)$$

and

$$\langle \hat{p} \rangle = \langle \psi | \hat{p} | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(-i\hbar \frac{d}{dx} \right) \psi(x) dx. \quad (1.100)$$

Later we will find that in many cases we do not have to solve the full equation 1.89, but only the energy eigenvalue equation (time-independent Schrödinger equation) $\hat{H} |E_i\rangle = E_i |E_i\rangle$, that in the wave function notation takes the form

$$\hat{H} \psi_{E_i}(x) = E_i \psi_{E_i}(x). \quad (1.101)$$

Inserting 1.91 into the above equation and using 1.92 gives

$$\hat{H} \psi_{E_i}(x) = E_i \psi_{E_i}(x) \rightarrow \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi_{E_i}(x) = E_i \psi_{E_i}(x). \quad (1.102)$$

Chapter 2

Schrödinger Time Evolution

2.1 Schrödinger Equation

One of the postulates of quantum mechanics says that the time evolution of a quantum system is governed by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t)\psi(t), \quad (2.1)$$

where the Hamiltonian \hat{H} is the operator of the total energy. The eigenvalues of \hat{H} are the allowed energies that the system can have.

In practice we do not have to solve 2.1 directly. Let's try to see why. Since the Hamiltonian \hat{H} is a Hermitian operator, its eigenstates form a complete basis, which means that we can express an arbitrary quantum state as a superposition of these eigenstates. For simplicity assume, that \hat{H} is time independent, eigenvectors of \hat{H} are orthonormal

$$\langle E_k | E_n \rangle = \delta_{kn} \quad (2.2)$$

and form a countable set. Let's expand a general state vector as

$$|\psi(t)\rangle = \sum_n c_n(t) |E_n\rangle. \quad (2.3)$$

Now we substitute 2.3 into 2.1:

$$i\hbar \frac{d}{dt} \sum_n c_n(t) |E_n\rangle = \hat{H} \sum_n c_n(t) |E_n\rangle. \quad (2.4)$$

Using the linearity of $\frac{d}{dt}$ and \hat{H} operators we can write

$$i\hbar \sum_n \frac{dc_n(t)}{dt} |E_n\rangle = \sum_n c_n(t) E_n |E_n\rangle. \quad (2.5)$$

Next step is to multiply both sides of 2.5 from the left by $\langle E_k|$ and use the orthonormality relation 2.2:

$$i\hbar \sum_n \frac{dc_n(t)}{dt} \delta_{kn} = \sum_n c_n(t) E_n \delta_{kn}, \quad (2.6)$$

which leads to

$$i\hbar \frac{dc_k(t)}{dt} = c_k(t) E_k. \quad (2.7)$$

After a small rearrangement we obtain the differential equation

$$\frac{dc_k(t)}{dt} = -i \frac{E_k}{\hbar} c_k(t), \quad (2.8)$$

whose solution is

$$c_k(t) = c_k(0) e^{-\frac{iE_k t}{\hbar}}, \quad (2.9)$$

where $c_k(0)$ is initial condition constant, which we denote simply as c_k hereafter. So if the initial state of the quantum system at time $t = 0$ is

$$|\psi(0)\rangle = \sum_n c_n |E_n\rangle, \quad (2.10)$$

then the state vector at time t is given by

$$|\psi(t)\rangle = \sum_n c_n e^{-\frac{iE_k t}{\hbar}} |E_n\rangle. \quad (2.11)$$

2.2 Stationary States and Superposition

Let's illustrate the evolution of a quantum state vector with few examples. First, consider the situation where the system is initially in one particular energy eigenstate:

$$|\psi(0)\rangle = |E_1\rangle. \quad (2.12)$$

To find its time evolution it's enough to multiply 2.12 by the phase factor $e^{-\frac{iE_1 t}{\hbar}}$:

$$|\psi(t)\rangle = e^{-\frac{iE_1 t}{\hbar}} |E_1\rangle. \quad (2.13)$$

Now, suppose we want to measure some observable \hat{O} . Then the probability of measuring a value o_j is

$$P_{o_j} = |\langle o_j | \psi(t) \rangle|^2 = |\langle o_j | e^{-\frac{iE_1 t}{\hbar}} | E_1 \rangle|^2 = |\langle o_j | E_1 \rangle|^2, \quad (2.14)$$

which is independent of time and is equal to the probability at the initial time. We call such states (energy eigenstates) stationary.

Suppose now that the state vector is a superposition of two energy eigenstates:

$$|\psi(0)\rangle = c_1 |E_1\rangle + c_2 |E_2\rangle. \quad (2.15)$$

We multiply by the corresponding phase factors:

$$|\psi(t)\rangle = c_1 e^{-\frac{iE_1 t}{\hbar}} |E_1\rangle + c_2 e^{-\frac{iE_2 t}{\hbar}} |E_2\rangle. \quad (2.16)$$

The probability of measuring the value of, say E_1 is

$$P_{E_1} = |\langle E_1 | \psi(t) \rangle|^2 = |\langle E_1 | (c_1 e^{-\frac{iE_1 t}{\hbar}} |E_1\rangle + c_2 e^{-\frac{iE_2 t}{\hbar}} |E_2\rangle) \rangle|^2 = |c_1|^2, \quad (2.17)$$

which again is time independent. Of course the same is true for E_2 . But consider the situation where we would like to measure some other observable \hat{O} . The interesting case is when \hat{O} does not commute with \hat{H} , so suppose this is the case. Then, in general the eigenstate $|o_j\rangle$ of \hat{O} corresponding to a measurement value o_j is a superposition of energy eigenstates, say:

$$|o_1\rangle = \alpha_1 |E_1\rangle + \alpha_2 |E_2\rangle. \quad (2.18)$$

The probability of measuring o_1 is then

$$\begin{aligned} P_{o_1} &= |\langle o_1 | \psi(t) \rangle|^2 \\ &= |(\alpha_1^* \langle E_1 | + \alpha_2^* \langle E_2 |)(c_1 e^{-\frac{iE_1 t}{\hbar}} |E_1\rangle + c_2 e^{-\frac{iE_2 t}{\hbar}} |E_2\rangle)|^2 \\ &= |\alpha_1^* c_1 e^{-\frac{iE_1 t}{\hbar}} + \alpha_2^* c_2 e^{-\frac{iE_2 t}{\hbar}}|^2 \\ &= |e^{-\frac{iE_1 t}{\hbar}}|^2 |\alpha_1^* c_1 + \alpha_2^* c_2 e^{-\frac{i(E_2 - E_1)t}{\hbar}}|^2 \\ &= |\alpha_1|^2 |c_1|^2 + |\alpha_2|^2 |c_2|^2 + 2\Re\left(\alpha_1 c_1^* \alpha_2^* c_2 e^{-\frac{i(E_2 - E_1)t}{\hbar}}\right), \end{aligned} \quad (2.19)$$

which is clearly time-dependent. To summarize, the following paragraph gives a recipe for solving any problem with a time-independent Hamiltonian

Given a time-independent Hamiltonian \hat{H} and an initial state $|\psi(0)\rangle$, to compute the probability that the eigenvalue o_j of an observable \hat{O} is measured at time t :

1. Diagonalize \hat{H} i.e. find the eigenvalues E_n and eigenvectors $|E_n\rangle$.
2. Write $|\psi(0)\rangle$ and $|o_j\rangle$ as a superposition of the energy eigenstates $|E_n\rangle$.
3. Multiply each eigenstate coefficient of $|\psi(0)\rangle$ by the term $e^{-\frac{iE_n t}{\hbar}}$ to get $|\psi(t)\rangle$.
4. Calculate $P_{o_j} = |\langle o_j | \psi(t) \rangle|^2$

2.3 Spin Precession

Let's try to apply the recipe from the previous section to solve a problem of spin $\frac{1}{2}$ particle interacting with a magnetic field. Consider an electron with mass m_e and charge e in magnetic field \vec{B} . The Hamiltonian of this system is

$$\hat{H} = \frac{e}{m_e} \vec{S} \cdot \vec{B}. \quad (2.20)$$

To make things simple we assume that the magnetic field is uniform and directed along the z -axis:

$$\vec{B} = B_0 \hat{z}. \quad (2.21)$$

Then the Hamiltonian \hat{H} reduces to

$$\hat{H} = \frac{eB_0}{m_e} S_z = \omega_0 S_z. \quad (2.22)$$

It is convenient to introduce a new constant

$$\omega_0 \equiv \frac{eB_0}{m_e}, \quad (2.23)$$

The Hamiltonian in matrix form is

$$\hat{H} = \frac{\hbar\omega_0}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.24)$$

Because the Hamiltonian is diagonal, there's no need to do step 1 in the above recipe. We have two eigenstates: $|+\rangle$ and $|-\rangle$:

$$|+\rangle = |E_+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = |E_-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (2.25)$$

which satisfy:

$$\hat{H} |+\rangle = \frac{\hbar\omega_0}{2} |+\rangle = E_+ |+\rangle \quad (2.26)$$

and

$$\hat{H}|- \rangle = -\frac{\hbar\omega_0}{2}|- \rangle = E_-|- \rangle. \quad (2.27)$$

There are also two possible energies:

$$E_+ = \frac{\hbar\omega_0}{2}, \quad E_- = -\frac{\hbar\omega_0}{2}. \quad (2.28)$$

Now consider a few examples. The simplest case is when the initial state is spin up along the z -axis. Then, following steps 2 and 3:

$$|\psi(0)\rangle = |+\rangle \rightarrow |\psi(t)\rangle = e^{-\frac{iE_+t}{\hbar}}|+\rangle = e^{-\frac{i\omega_0 t}{2}}|+\rangle. \quad (2.29)$$

The probability of measuring the energy E_+ (or spin "up") is thus

$$P_+ = |\langle +|\psi(t)\rangle|^2 = 1. \quad (2.30)$$

Notice, that the probability does not depend on time, as was expected based on the general discussion in the previous section.

Now let's see what happens when the initial state vector is a superposition of spin up and spin down. The most general superposition expressed in spherical coordinates and parametrized by two angles: θ and ϕ is

$$|\psi(0)\rangle = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}e^{i\phi}|-\rangle, \quad (2.31)$$

or in matrix notation:

$$|\psi(0)\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}. \quad (2.32)$$

The state vector evolves with time according to

$$|\psi(t)\rangle = \begin{pmatrix} e^{-\frac{iE_+t}{\hbar}} \cos\frac{\theta}{2} \\ e^{-\frac{iE_-t}{\hbar}} \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix} = \begin{pmatrix} e^{-\frac{i\omega_0 t}{2}} \cos\frac{\theta}{2} \\ e^{\frac{i\omega_0 t}{2}} \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix} = e^{-\frac{i\omega_0 t}{2}} \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i(\omega_0 t + \phi)} \sin\frac{\theta}{2} \end{pmatrix}. \quad (2.33)$$

The probability of measuring the energy E_+ is

$$P_+ = |\langle +|\psi(t)\rangle|^2 = \cos^2\left(\frac{\theta}{2}\right), \quad (2.34)$$

which again is independent of time. This is because the S_z commutes with \hat{H} and eigenstates of S_z are also energy eigenstates. Let's see what happens when we try to measure spin along different axis. For example, the probability for

measuring spin up along the x -axis is

$$P_{+x} = |\langle +x | \psi(t) \rangle|^2 = \frac{1}{2} (1 + \sin \theta \cos(\phi + \omega_0 t)), \quad (2.35)$$

which is time dependent, because \hat{S}_x doesn't commute with \hat{H} . The time-dependence of 2.35 is a manifestation of the spin precession around the z -axis. Let's calculate the expectation values for each of the spin components:

$$\langle S_z \rangle = \langle \psi(t) | S_z | \psi(t) \rangle = \frac{\hbar}{2} \cos \theta, \quad (2.36)$$

$$\langle S_y \rangle = \langle \psi(t) | S_y | \psi(t) \rangle = \frac{\hbar}{2} \sin \theta \sin(\phi + \omega_0 t) \quad (2.37)$$

and

$$\langle S_x \rangle = \langle \psi(t) | S_x | \psi(t) \rangle = \frac{\hbar}{2} \sin \theta \cos(\phi + \omega_0 t) \quad (2.38)$$

If we build a vector $(\langle S_x \rangle, \langle S_y \rangle, \langle S_z \rangle)$ from the expectation values we see it precess around the magnetic field direction with an angular frequency ω_0 . This precession is known as Larmor precession.

Chapter 3

Particle in a Box

3.1 Motivation

Physicists try to understand the building blocks of our Universe i.e. atoms, nuclei, molecules, solids etc. The key to understanding the structure of matter lies in the energy states that the systems are allowed to have. Each microscopic system has a unique set of energy levels (kind of a fingerprint) that uniquely identifies it, see fig. 3.1

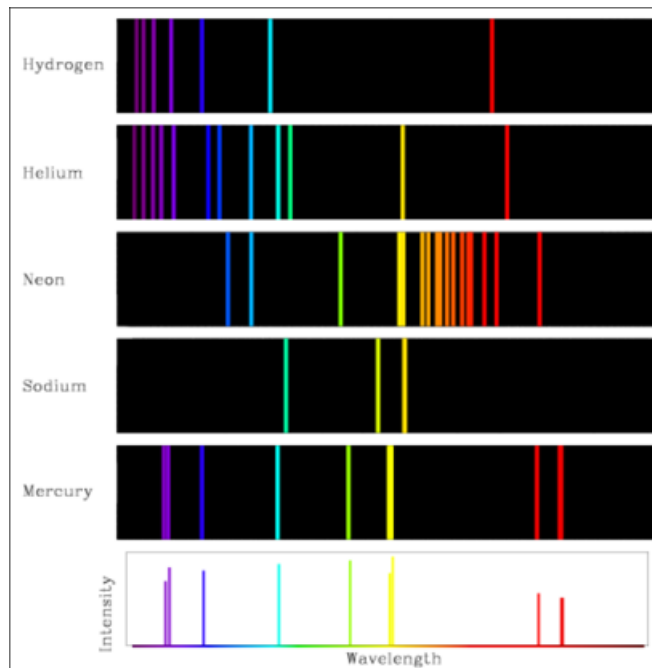


Figure 3.1: Spectra of various elements [2].

With help of quantum mechanics we can build the model for the specific system and calculate its fingerprint. Particle in a box model is simple and exhibits most of the important features shared by all microscopic systems.

3.2 Infinite Square Well

The Schrödinger equation for a single non-relativistic particle in one dimension is

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi_E(x) = E \psi_E(x). \quad (3.1)$$

In order to solve it, one must specify the potential function $V(x)$. In infinite square well model we take the potential function

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

which is schematically depicted if fig. 3.2

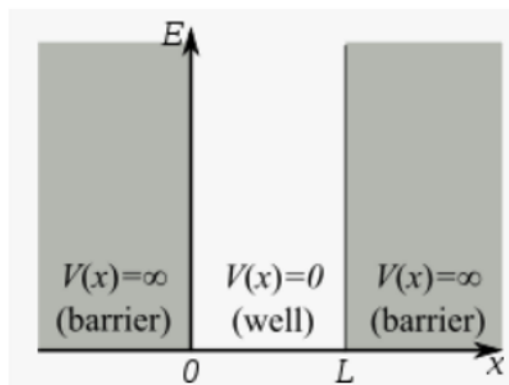


Figure 3.2: Infinite square potential energy well [3].

The potential energy is zero within the well and it is infinite outside the well, so the particle trapped inside the region $0 < x < L$.

Our goal is to solve the Schrödinger equation 3.1 for this potential function. We need to consider two cases:

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \infty \right) \psi_E(x) = E \psi_E(x), \quad \text{outside box} \quad (3.2)$$

and

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + 0\right) \psi_E(x) = E\psi_E(x), \quad \text{inside box.} \quad (3.3)$$

Since we require particle to have a finite energy, the wave function outside the well must be identically zero, so we only need to consider what happens inside the well:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_E(x) = E\psi_E(x). \quad (3.4)$$

After a little rearrangement we get

$$\frac{d^2}{dx^2} \psi_E(x) = -\frac{2mE}{\hbar^2} \psi_E(x). \quad (3.5)$$

It's profitable to define a new parameter

$$k^2 \equiv \frac{2mE}{\hbar^2}. \quad (3.6)$$

Then, equation 3.5 becomes

$$\frac{d^2}{dx^2} \psi_E(x) = -k^2 \psi_E(x). \quad (3.7)$$

Eq. 3.7 is a simple differential equation. Its solution can be expressed in terms of sine and cosine functions

$$\psi_E(x) = A \sin kx + B \cos kx, \quad (3.8)$$

for some constants A and B . The partial solution is

$$\psi_E(x) = \begin{cases} 0, & x < 0 \\ A \sin kx + B \cos kx, & 0 < x < L \\ 0, & x > L. \end{cases}$$

To reach the final solution we need to figure out what are the values of: A , B and k . We proceed by imposing boundary conditions on the wave function. We require the continuity of the wave function at the boundary of the well. This leads to two equations:

$$\psi_E(0) = A \sin(0) + B \cos(0) = 0 \quad (3.9)$$

and

$$\psi_E(L) = A \sin(kL) + B \cos(kL) = 0 \quad (3.10)$$

From 3.9 we immediately get

$$B = 0 \quad (3.11)$$

and from 3.10

$$A \sin(kL) = 0 \quad (3.12)$$

Eq. 3.12 is satisfied if $A = 0$, but this solution is not interesting. Suppose that $A \neq 0$. Then we can divide 3.12 by A to get

$$\sin(kL) = 0 \quad (3.13)$$

In order for 3.13 to be satisfied, it must be the case that

$$kL = n\pi \quad (3.14)$$

or

$$k_n = \frac{n\pi}{L}, \quad n = 1, 2, 3, \dots \quad (3.15)$$

We obtained the quantization condition. The index n is the quantum number used to label the quantized states and energies. The quantization condition transfers directly to the quantization of energy

$$E_n = \frac{\hbar^2 k_n^2}{2m} \quad (3.16)$$

or

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \dots \quad (3.17)$$

It is worth noticing that the allowed energies scale with the square of the quantum number n (see fig. 3.3).

We find A by imposing the normalization condition

$$\int_{-\infty}^{\infty} \psi_n^*(x) \psi_n(x) dx = 1. \quad (3.18)$$

After a simple integration we obtain

$$1 = \int_0^L |A|^2 \sin^2 \frac{n\pi x}{L} dx = |A|^2 \frac{L}{2}. \quad (3.19)$$

We are free to choose A to be real and positive, since the global phase factor does not matter

$$A = \sqrt{\frac{2}{L}}. \quad (3.20)$$

The complete solution is

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, \quad n = 1, 2, 3, \dots \quad (3.21)$$

If we square 3.21 we obtain the probability density function, which can be used to calculate the probability of finding the particle in some region inside the well

$$P_n(x) = |\psi_n(x)|^2 = \frac{2}{L} \sin^2 \frac{n\pi x}{L}. \quad (3.22)$$

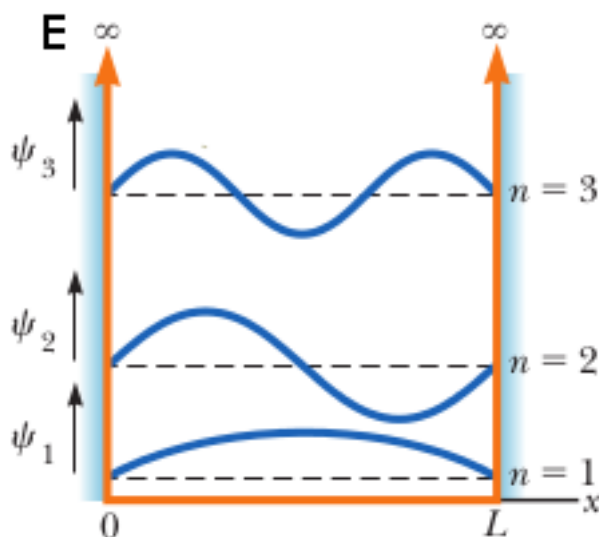


Figure 3.3: Wave functions of the first three energy eigenstates of the infinite square potential well [4].

3.3 Finite Square Well

Consider now the situation where the potential energy outside the wall is finite 3.4 and given by

$$V(x) = \begin{cases} V_0, & x < -a \\ 0, & -a < x < a \\ V_0, & x > a. \end{cases}$$

Assume that the energy E of a particle is less than V_0 . Our goal is to solve

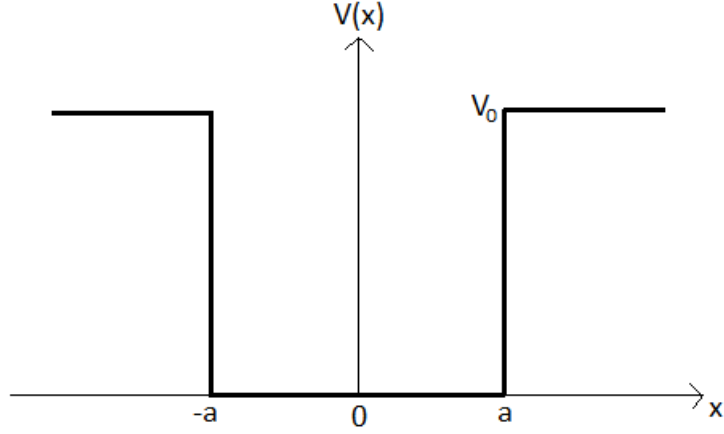


Figure 3.4: Finite square potential energy well.

the Schrödinger equation, which takes the form

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0\right) \psi_E(x) = E \psi_E(x), \quad \text{outside box.} \quad (3.23)$$

and

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + 0\right) \psi_E(x) = E \psi_E(x), \quad \text{inside box.} \quad (3.24)$$

It is useful to define two constants

$$k \equiv \sqrt{\frac{2mE}{\hbar^2}} \quad (3.25)$$

and

$$q \equiv \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}. \quad (3.26)$$

Then the above equations become:

$$\frac{d^2 \psi_E(x)}{dx^2} = -k^2 \psi_E(x), \quad \text{inside box} \quad (3.27)$$

and

$$\frac{d^2 \psi_E(x)}{dx^2} = q^2 \psi_E(x), \quad \text{outside box} \quad (3.28)$$

Notice that eq. 3.27 is identical to the one for infinite well potential, so it has the same solution. The equation outside the box 3.28 is qualitatively different, because the constant on the right hand side of 3.28 is positive. The solution outside the box is

$$\psi_E(x) = A e^{qx} + B e^{-qx}, \quad (3.29)$$

for some constants A and B . The general solution in all regions of space is

$$\psi_E(x) = \begin{cases} Ae^{qx} + Be^{-qx}, & x < -a \\ C \sin kx + D \cos kx, & -a < x < a \\ Fe^{qx} + Ge^{-qx}, & x > a. \end{cases}$$

Altogether we have six undetermined constants: A, B, C, D, F, G . However, since in the region $x < -a$ the function e^{-qx} tends to infinity with $x \rightarrow -\infty$, we must set $B = 0$. For similar reasons we must set $F = 0$. Hence our wave function must be of the form

$$\psi_E(x) = \begin{cases} \psi_I(x) = Ae^{qx}, & x < -a \\ \psi_{II}(x) = C \sin kx + D \cos kx, & -a < x < a \\ \psi_{III}(x) = Ge^{-qx}, & x > a. \end{cases}$$

Now we must impose boundary conditions. In infinite square well problem we required that the wave function must be continuous across a boundary. This is also the case for the finite potential well, but this is not enough. We must also require the derivative of the wave function to be continuous across a boundary. The complete set of conditions is

$$\psi_I(x) \Big|_{x=-a} = \psi_{II}(x) \Big|_{x=-a} \quad \text{and} \quad \frac{d\psi_I(x)}{dx} \Big|_{x=-a} = \frac{d\psi_{II}(x)}{dx} \Big|_{x=-a} \quad (3.30)$$

$$\psi_{II}(x) \Big|_{x=a} = \psi_{III}(x) \Big|_{x=a} \quad \text{and} \quad \frac{d\psi_{II}(x)}{dx} \Big|_{x=a} = \frac{d\psi_{III}(x)}{dx} \Big|_{x=a} \quad (3.31)$$

From 3.30 we get

$$Ae^{-qa} = D \cos ka - C \sin ka \quad (3.32)$$

and

$$qAe^{-qa} = kC \cos ka + kD \sin ka. \quad (3.33)$$

And from 3.31 we get

$$C \sin ka + D \cos ka = Ge^{-qa} \quad (3.34)$$

and

$$kC \cos ka - kD \sin ka = -qGe^{-qa} \quad (3.35)$$

We eliminate A from 3.32 and 3.33 and G from 3.34 and 3.35 to obtain

$$qD \cos ka - qC \sin ka = kC \cos ka + kD \sin ka \quad (3.36)$$

and

$$-qC \sin ka - qD \cos ka = kC \cos ka - kD \sin ka. \quad (3.37)$$

If we add eq. 3.36 and 3.37 we get

$$k \cot ka = -q. \quad (3.38)$$

If we subtract eq. 3.36 and 3.37 we get

$$k \tan ka = q \quad (3.39)$$

The crucial thing to notice is that the equations 3.38 and 3.39 cannot be satisfied simultaneously, because if we multiply them, we get $k^2 = -q^2$, which is a contradiction, because both k and q must be positive. Therefore the solution of the Schrödinger equation splits into two categories:

1. $D \neq 0$ and $C = 0$, which leads to $\psi_{II}(x) = D \cos kx$ - even solutions which satisfy 3.39.
2. $C \neq 0$ and $D = 0$, which leads to $\psi_{II}(x) = C \sin kx$ - odd solutions which satisfy 3.38.

Under the condition 1. equations 3.32 and 3.34 reduce to

$$Ae^{-qa} = D \cos ka \quad (3.40)$$

and

$$Ge^{-qa} = D \cos ka, \quad (3.41)$$

from which it follows that

$$\psi_{even}(x) = \begin{cases} \psi_I(x) = D \cos(ka)e^{q(x+a)}, & x < -a \\ \psi_{II}(x) = D \cos kx, & -a < x < a \\ \psi_{III}(x) = D \cos(ka)e^{q(a-x)}, & x > a. \end{cases}$$

The constant D is simply derived from the normalization condition:

$$D = \sqrt{\frac{q}{aq + 1}}. \quad (3.42)$$

Similar reasoning leads to odd solutions:

$$\psi_{odd}(x) = \begin{cases} \psi_I(x) = -C \sin(ka)e^{q(x+a)}, & x < -a \\ \psi_{II}(x) = C \sin kx, & -a < x < a \\ \psi_{III}(x) = C \sin(ka)e^{q(a-x)}, & x > a, \end{cases}$$

where

$$C = \sqrt{\frac{q}{aq+1}}. \quad (3.43)$$

Finally, we notice that eq. 3.38 and 3.39 are transcendental, so we can only hope to find numerical solutions. Graphical analysis of both equations is also helpful, but we need to do some preparations. Let's define some new dimensionless parameters:

$$z = ka = \sqrt{\frac{2mEa^2}{\hbar^2}}, \quad (3.44)$$

$$z_0 = \sqrt{\frac{2mV_0a^2}{\hbar^2}}, \quad (3.45)$$

and

$$qa = \sqrt{\frac{2m(V_0 - E)a^2}{\hbar^2}}. \quad (3.46)$$

These definitions lead to the convenient expressions

$$(ka)^2 + (qa)^2 = z_0^2 \quad (3.47)$$

and

$$(qa)^2 = z_0^2 - (ka)^2 = z_0^2 - z^2. \quad (3.48)$$

This allows us to write the transcendental equations in the form:

$$ka \tan(ka) = qa \rightarrow z \tan(z) = \sqrt{z_0^2 - z^2} \quad (3.49)$$

and

$$-ka \cot(ka) = qa \rightarrow -z \cot(z) = \sqrt{z_0^2 - z^2}. \quad (3.50)$$

These functions are plotted in fig. 3.5. The intersection points of these curves determine the allowed values of z and hence the allowed energies E_n through eq. 3.44

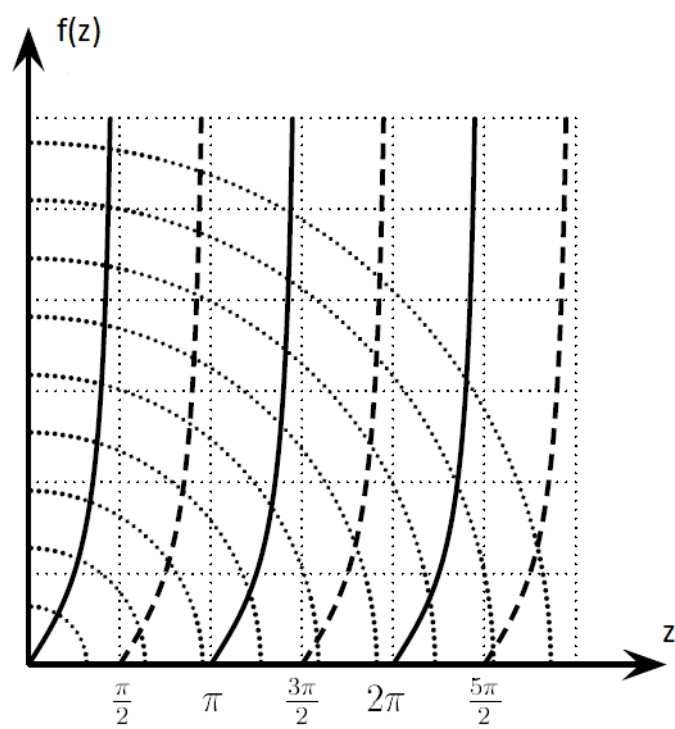


Figure 3.5: Graphical solution of the transcendental equations for the allowed energies of a finite square well [5].

Chapter 4

Quantum Harmonic Oscillator

4.1 Classically

The classical harmonic oscillator system is a mass m connected to a spring attached to a wall. The motion of a mass is governed by Hooke's law, which says that the restoring force is proportional to the displacement x of the mass from equilibrium:

$$F = -kx, \quad (4.1)$$

where k is the spring constant.

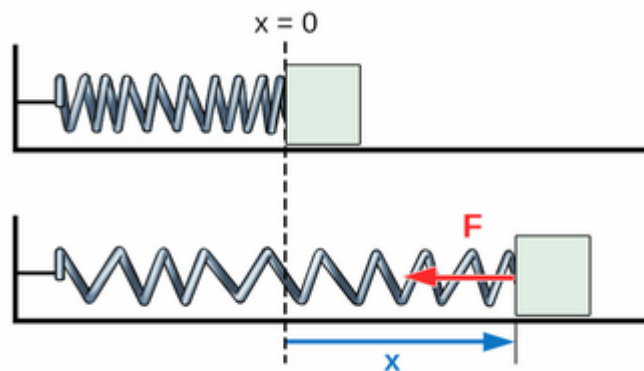


Figure 4.1: Mass on a spring [6]

When the spring is stretched or compressed a distance x , the potential energy

stored in the spring is

$$V(x) = \frac{1}{2}kx^2. \quad (4.2)$$

The mass-on-a-spring system models many other systems in nature that perform oscillatory motion. This is the case because one can expand an arbitrary potential function about the local minimum:

$$V(x - x_0) = V(x_0) + (x - x_0) \left. \frac{dV}{dx} \right|_{x=x_0} + \frac{1}{2}(x - x_0)^2 \left. \frac{d^2V}{dx^2} \right|_{x=x_0} + \dots \quad (4.3)$$

In 4.3 we can set $V(x_0) = 0$ as it depends on our choice of the reference point. In addition $\left. \frac{dV}{dx} \right|_{x=x_0} = 0$, because we are expanding about the minimum. Hence if we set $k \equiv \left. \frac{d^2V}{dx^2} \right|_{x=x_0}$ we obtain $V(x - x_0) \approx \frac{1}{2}k(x - x_0)^2$ hence the motion of the system is that of harmonic oscillator.

The solution of the classical harmonic oscillator problem starts by using Newton's second law:

$$F = ma. \quad (4.4)$$

Since $a = \frac{d^2x}{dt^2}$ we can write

$$-kx = m \frac{d^2x}{dt^2}. \quad (4.5)$$

It is convenient to introduce a new constant

$$\omega = \sqrt{\frac{k}{m}}. \quad (4.6)$$

Then 4.5 takes the form:

$$\frac{d^2x}{dt^2} = -\omega^2x. \quad (4.7)$$

The solution of 4.7 is the sinusoidal function

$$x(t) = A \cos(\omega t + \phi), \quad (4.8)$$

where A is the amplitude of motion and ϕ is the phase constant determined by the initial conditions.

4.2 Quantumly

The total energy (kinetic and potential energy) of the classical harmonic oscillator is

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2, \quad (4.9)$$

where p is the momentum.

To construct the quantum mechanical Hamiltonian, we replace p with \hat{p} and x with \hat{x}

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \quad (4.10)$$

Our goal is to solve the energy eigenvalue equation

$$\hat{H}|\psi\rangle = E|\psi\rangle \quad (4.11)$$

to find the allowed energies in the system. To do that, we first need to recall the definitions of position and momentum operators:

$$\begin{aligned} \hat{x} &= x \\ \hat{p} &= -i\hbar\frac{d}{dx} \end{aligned} \quad (4.12)$$

It is best to express the differential equation in the wave function picture:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\psi_E(x) = E\psi_E(x) \quad (4.13)$$

There are two approaches for solving 4.13. There is an analytic method, where we seek for a power series solution. The other method - algebraic in nature - is more elegant and is used in many places in physics especially in quantum field theory. Hence we concentrate on the latter.

4.2.1 Algebraic Method

The idea of the algebraic method is quite easy. It relies on the identity:

$$a^2 + b^2 = (a - ib)(a + ib). \quad (4.14)$$

The Hamiltonian 4.10 has the appropriate form to use the above identity:

$$\begin{aligned} \hat{H} &= \frac{1}{2}m\omega^2\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right) \\ &= \hbar\omega\left\{\frac{m\omega}{2\hbar}\left[\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right]\right\} \end{aligned} \quad (4.15)$$

We define two new operators:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right), \quad (4.16)$$

we call 4.16 the lowering operator or the annihilation operator and

$$\begin{aligned}\hat{a}^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}^\dagger - i\frac{\hat{p}^\dagger}{m\omega}\right) \\ &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right)\end{aligned}\tag{4.17}$$

which we call the rising operator or the creation operator. Let's take a closer look at their properties.

4.2.2 Properties of Raising and Lowering Operators

The first observation is that 4.16 and 4.17 are not Hermitian, so they do not correspond to observables, but they are quite useful. Let's try to find out what their product is:

$$\hat{a}^\dagger\hat{a} = \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right) - \frac{1}{2},\tag{4.18}$$

$$\hat{a}\hat{a}^\dagger = \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2}\right) + \frac{1}{2}.\tag{4.19}$$

From 4.18 and 4.19 we clearly see that \hat{a} and \hat{a}^\dagger do not commute. In fact, their commutator is

$$[\hat{a}, \hat{a}^\dagger] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1.\tag{4.20}$$

Now, let's calculate the commutators of \hat{a} and \hat{a}^\dagger with the Hamiltonian:

$$[\hat{H}, \hat{a}] = -\hbar\omega\hat{a},\tag{4.21}$$

$$[\hat{H}, \hat{a}^\dagger] = +\hbar\omega\hat{a}^\dagger.\tag{4.22}$$

Comparing 4.15 and 4.18 we see that the Hamiltonian written in terms of these new operators is

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right).\tag{4.23}$$

4.2.3 Energy

Now, we can explain why \hat{a} is called the lowering operator and \hat{a}^\dagger is called the rising operator. Let's see what happens when the Hamiltonian \hat{H} acts on a ket $\hat{a}|E\rangle$, where $|E\rangle$ is some energy eigenstate:

$$\hat{H}(\hat{a}|E\rangle) = \hat{H}\hat{a}|E\rangle.\tag{4.24}$$

Using the commutation relation 4.21 we can rewrite the above equation as

$$\begin{aligned}\hat{H}(\hat{a}|E\rangle) &= (\hat{a}\hat{H} - \hbar\omega\hat{a})|E\rangle \\ &= (E - \hbar\omega)(\hat{a}|E\rangle).\end{aligned}\tag{4.25}$$

The equation 4.25 says, that the ket $\hat{a}|E\rangle$ is also an eigenstate of the of the Hamiltonian, but with an energy eigenvalue $E - \hbar\omega$:

$$\hat{H}|E - \hbar\omega\rangle = (E - \hbar\omega)|E - \hbar\omega\rangle.\tag{4.26}$$

That's why we call \hat{a} the lowering or the annihilation operator. There's one problem here. We cannot say that $\hat{a}|E\rangle$ is equal to $|E - \hbar\omega\rangle$, but only that these kets are proportional. We will find this constant of proportionality soon.

Now let's repeat the above calculations for \hat{a}^\dagger .

$$\begin{aligned}\hat{H}(\hat{a}^\dagger|E\rangle) &= (\hat{a}^\dagger\hat{H} + \hbar\omega\hat{a}^\dagger)|E\rangle \\ &= (E + \hbar\omega)(\hat{a}^\dagger|E\rangle)\end{aligned}\tag{4.27}$$

The equation 4.27 says, that the ket $\hat{a}^\dagger|E\rangle$ is also an eigenstate of the of the Hamiltonian, but with an energy eigenvalue $E + \hbar\omega$:

$$\hat{H}|E + \hbar\omega\rangle = (E + \hbar\omega)|E + \hbar\omega\rangle.\tag{4.28}$$

That's why we call \hat{a}^\dagger the rising or the creation operator.

We refer to the operators \hat{a} and \hat{a}^\dagger collectively as ladder operators, because they take us up and down a ladder of energy eigenstates, as illustrated in 4.2

Even though the picture 4.2 may suggest that we could climb down the ladder arbitrarily low, it is not really the case as the total energy of a system cannot be negative. Hence, there must exist the lowest energy state $|E_{lowest}\rangle$, such that

$$\hat{a}|E_{lowest}\rangle = 0.\tag{4.29}$$

Let's act the Hamiltonian \hat{H} on this state:

$$\hat{H}|E_{lowest}\rangle = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|E_{lowest}\rangle.\tag{4.30}$$

Since we have the condition 4.29, the above expression reduces to

$$\hat{H}|E_{lowest}\rangle = \frac{1}{2}\hbar\omega|E_{lowest}\rangle.\tag{4.31}$$

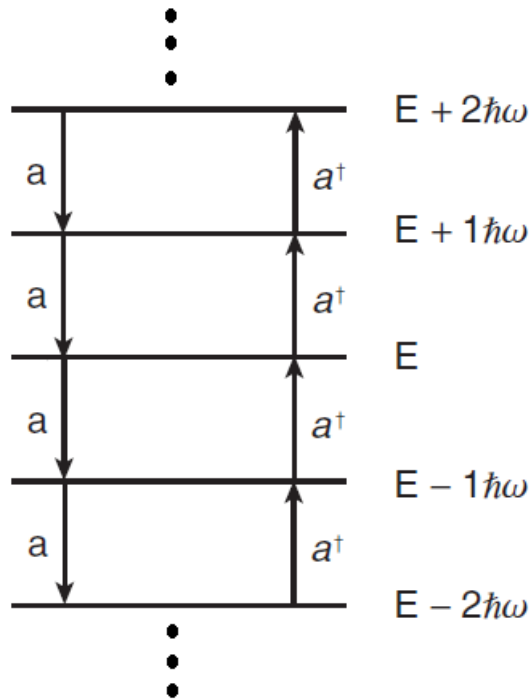


Figure 4.2: Ladder of energy eigenstates.

Therefore, the lowest possible energy of the quantum mechanical oscillator is

$$E_{lowest} = \frac{1}{2}\hbar\omega. \quad (4.32)$$

We also call it the ground state energy.

To generate next energy, we act with the raising operator on the ground state $|E_{lowest}\rangle$, which produces an eigenstate with energy increased by $\hbar\omega$. If we repeat this process, we obtain all allowed energies of the oscillator:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, 3, \dots \quad (4.33)$$

It is convenient to label the energy eigenstates as $|E_n\rangle = |n\rangle$. These states satisfy the energy eigenvalue equation

$$\hat{H}|n\rangle = E_n|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega|n\rangle, \quad (4.34)$$

are normalized (since $|E_n\rangle$'s are)

$$\langle n|n\rangle = 1, \quad (4.35)$$

and are mutually orthogonal

$$\langle m | n \rangle = \delta_{mn}. \quad (4.36)$$

If we write the Schrödinger equation using ladder operators:

$$\hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) |n\rangle = \hbar\omega \left(n + \frac{1}{2} \right) |n\rangle, \quad (4.37)$$

we can notice a very useful identity:

$$\hat{a}^\dagger \hat{a} |n\rangle = n |n\rangle. \quad (4.38)$$

The equation 4.38 suggests that we define the operator $\hat{a}^\dagger \hat{a}$ as the number operator \hat{N}

$$\hat{N} = \hat{a}^\dagger \hat{a}, \quad (4.39)$$

such that

$$\hat{N} |n\rangle = n |n\rangle. \quad (4.40)$$

The eigenvalues of the number operator are the same integers n that were used to label the energy eigenstates $|n\rangle$. Finally, we can write the Hamiltonian in terms of the number operator:

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right) \quad (4.41)$$

Now it's time to go back to the problem of normalization of ladder operators. From our previous discussion we know that kets $\hat{a}|E\rangle$ and $|E - \hbar\omega\rangle$ are proportional. Let's write the proportionality equation using developed notation:

$$\hat{a} |n\rangle = c |n-1\rangle. \quad (4.42)$$

Consider the norm of the state $\hat{a} |n\rangle$:

$$|\hat{a} |n\rangle|^2 = (\langle n | \hat{a}^\dagger) (\hat{a} |n\rangle) = \langle n | \hat{a}^\dagger \hat{a} |n\rangle. \quad (4.43)$$

As $\hat{a}^\dagger \hat{a} = \hat{N}$, we can write

$$|\hat{a} |n\rangle|^2 = \langle n | \hat{N} |n\rangle = n, \quad (4.44)$$

from which we obtain

$$|\hat{a} |n\rangle|^2 = |c |n-1\rangle|^2. \quad (4.45)$$

Hence

$$n = |c|^2 \quad (4.46)$$

and we get the normalization constant. Since an overall phase is not measurable, we can choose c to be positive and real and obtain

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle. \quad (4.47)$$

Similarly, for the raising operator we get

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \quad (4.48)$$

4.2.4 Wave Functions

If we knew one of the eigenstates, then we could use ladder operators to generate others. Luckily, we can use the ladder termination equation

$$\hat{a}|0\rangle = 0. \quad (4.49)$$

It's best to work in wave function representation, so we rewrite 4.49:

$$\hat{a}\psi_0(x) = 0. \quad (4.50)$$

Now, we use the definition of the lowering operator

$$\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right)\psi_0(x) = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{\hbar}{m\omega}\frac{d}{dx}\right)\psi_0(x) = 0. \quad (4.51)$$

A simple rearrangement of terms in 4.51 leads to

$$\frac{d}{dx}\psi_0(x) = -\frac{m\omega x}{\hbar}\psi_0(x) \quad (4.52)$$

The solution (after normalization) of 4.52 is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}, \quad (4.53)$$

which is the ground state of the quantum harmonic oscillator.

To generate states above the ground state we use eq. 4.48, which can be rewritten as

$$|n+1\rangle = \frac{1}{\sqrt{n+1}}\hat{a}^\dagger|n\rangle \quad (4.54)$$

We apply 4.54 to the ground state to obtain

$$|1\rangle = \frac{1}{\sqrt{1}} \hat{a}^\dagger |0\rangle, \quad (4.55)$$

$$|2\rangle = \frac{1}{\sqrt{2}} \hat{a}^\dagger |1\rangle = \frac{1}{\sqrt{2 \cdot 1}} (\hat{a}^\dagger)^2 |0\rangle, \quad (4.56)$$

$$|3\rangle = \frac{1}{\sqrt{3}} \hat{a}^\dagger |2\rangle = \frac{1}{\sqrt{3 \cdot 2 \cdot 1}} (\hat{a}^\dagger)^3 |0\rangle, \quad (4.57)$$

and more generally

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n |0\rangle. \quad (4.58)$$

Using the definition of \hat{a}^\dagger and substituting 4.53 for $|0\rangle$ we get

$$\psi_n(x) = \frac{1}{n!} \left[\sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{\hbar}{m\omega} \frac{d}{dx} \right) \right]^n \psi_0(x) \quad (4.59)$$

When we apply the creation operator to the Gaussian function $\psi_0(x)$ n times, we obtain the Gaussian function multiplied by a polynomial of order n . These polynomials are called Hermite polynomials. To simplify calculations it is common to define a dimensionless variable

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}} x. \quad (4.60)$$

The ground state and the general states are written as

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{\xi^2}{2}} \quad (4.61)$$

and

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\frac{\xi^2}{2}}. \quad (4.62)$$

The first few Hermite polynomials are:

$$\begin{aligned} H_0(\xi) &= 1 \\ H_1(\xi) &= 2\xi \\ H_2(\xi) &= 4\xi^2 - 2 \\ H_3(\xi) &= 8\xi^3 - 12\xi \\ H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12. \end{aligned} \quad (4.63)$$

The first seven wave functions are plotted in fig. 4.3

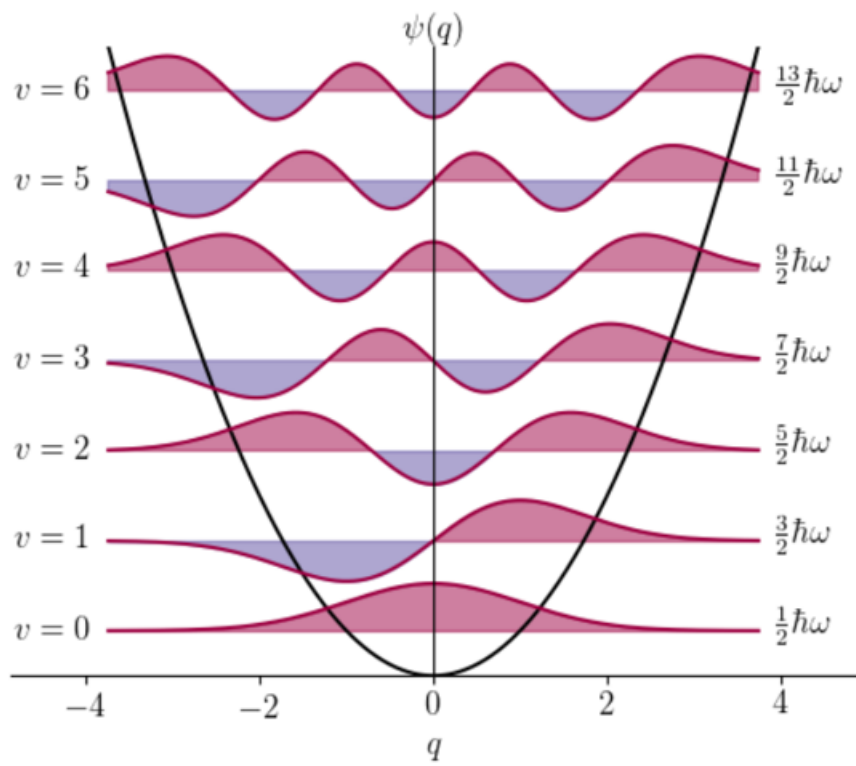


Figure 4.3: The harmonic oscillator wave functions [7]

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