Quantum Mechanics

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Summer 2000

Contents

Chapter 1

A brief reminder of linear Algebra

The fundamental principle of quantum mechanics is that an isolated physical system can be put into correspondence with a linear vector space in such a way that a definite state of the system corresponds to a vector and physical observables correspond to linear operators. For this reason the mathematics of linear vector space plays an important role in the quantum theory.

1.1 Linear vector space

A linear vector space is a set of objects (vectors) $|a>, |b>, |c> ...$ which is closed under two operations:

1. Addition, which is commutative and associative:

$$\begin{aligned} &|a> + |b> = |b> + |a> \\ &(|a> + |b>) + |c> = |a> + (|b> + |c>). \end{aligned} \tag{1.1}$$

2. Multiplication by a scalar (any complex number), which is distributive and associative, that is,

$$\begin{aligned} &\lambda(|a> + |b>) = \lambda|a> + \lambda|b> \\ &\lambda(\mu|a>) = (\lambda\mu)|a> \\ &(\lambda + \mu)|a> = \lambda|a> + \mu|a> . \end{aligned} \tag{1.2}$$

In addition, we assume a null vector —0¿ exists such that for all $|a>$

$$|a> +|0> = |a>, \tag{1.3}$$

and that for every $|a>$, a vector $-|a>$ exists such that

$$|a> +(-|a>) = |0> . \tag{1.4}$$

In the rest of the course we abbreviate $|0>$ by 0. Finally the multiplication by the scalar 1 leaves every vector unchanged:

$$1|a> = |a> . \tag{1.5}$$

A set of vectors $|a_1>, |a_2>, ..., |a_n>$ is said to be linearly independent provided

$$\lambda_1|a_1> +\lambda_2|a_2> +... + \lambda_n|a_n> = 0, \tag{1.6}$$

implies $\lambda_1 = \lambda_2 = ... = \lambda_n = 0$.

If in a particular vector space there exists n linearly independent vectors but no set of $n+1$ linearly independent ones, the space is said to be n-dimensional.

Let $|a_1>, ..., |a_n>$ be a set of n linearly independent vector in an n-dimensional vector space. Then if $|x>$ is an arbitrary vector in the space there exists an unique set of numbers $\{x_i\}$ such that

$$|x> = \sum_{i=1}^{n} x_i|a_i> . \tag{1.7}$$

The fact that an arbitrary vector $|x>$ can be written as a linear combination of the $|a_i>$ is often expressed as this: the set of "base vectors" $\{|a_i>\}$ is complete. Under a particular choice of base vectors there is an 1-1 correspondence between a vector $|x>$ and its components:

$$|x> \leftrightarrow \begin{pmatrix} x_1 \\ . \\ . \\ . \\ x_n \end{pmatrix} . \tag{1.8}$$

1.2 Linear operators and their corresponding matrices

A linear operator is a linear function of a vector, that is, a mapping which associates with every vector $|x>$ a vector $\mathbf{A}(|x>)$, in a linear way,

$$\mathbf{A}(\lambda|a>+\mu|b>) = \lambda\mathbf{A}(|a>) + \mu\mathbf{A}(|b>). \tag{1.9}$$

Due to Eq. (1.9) it is sufficient to know $\mathbf{A}(|a_i>)$ for the n base vectors $|a_i>$. Since $\mathbf{A}(|a_i>)$ is also a vector in the vector space, it can be expressed as the linear combination of $|a_j>$

$$\mathbf{A}(|a_i>) = \sum_{j=1}^{n} A_{ji}|a_j> . \tag{1.10}$$

Using Eq. (1.7) and Eq. (1.9) we can then evaluate

$$\mathbf{A}(|x>) = \mathbf{A}(\sum_i x_i|a_i>) = \sum_i x_i\mathbf{A}(|a_i>) = \sum_i\sum_j x_i A_{ji}|a_j> . \tag{1.11}$$

Consequently the component y_i of the vector $\mathbf{A}(|x>)$ can be obtained as follows

$$\mathbf{A}(|x>) \leftrightarrow \begin{pmatrix} y_1 \\ . \\ . \\ . \\ y_n \end{pmatrix} = \begin{pmatrix} A_{11} & . & . & . & A_{1n} \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ A_{n1} & . & . & . & A_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ . \\ . \\ . \\ x_n \end{pmatrix} . \tag{1.12}$$

In the above matrix product is assumed. Thus the entire information of the vector function $\mathbf{A}$ is encoded in the following matrix

$$\mathbf{A} \leftrightarrow \begin{pmatrix} A_{11} & . & . & . & A_{1n} \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ A_{n1} & . & . & . & A_{nn} \end{pmatrix} . \tag{1.13}$$

The sum and product of linear operators and the product of an operator and a scalar is defined by the following relation

$$(\mathbf{A}+\mathbf{B})(|x>) \equiv \mathbf{A}(|x>) + \mathbf{B}(|x>)$$

$$(\mathbf{AB})(|x>) \equiv \mathbf{A}(\mathbf{B}(|x>))$$
$$(\lambda\mathbf{A})(|x>) \equiv \lambda\mathbf{A}(|x>). \tag{1.14}$$

The matrices corresponding to the operators on the left hand side of Eq. (1.14) are

$$(\mathbf{A}+\mathbf{B}) \leftrightarrow A+B$$
$$(\mathbf{AB}) \leftrightarrow AB$$
$$(\lambda\mathbf{A}) \leftrightarrow \lambda A, \tag{1.15}$$

where $A+B$, AB and λA denote matrix addition, matrix multiplication and the multiplication of a matrix be a scalar respectively.

In general matrix multiplication is not commutative, i.e. AB needs not equal BA. When $AB = BA$ we say that A and B commute. The commutator of two matrices is defined as

$$[A, B] \equiv AB - BA. \tag{1.16}$$

The elements of a null matrix are all zero, and the elements of the identity matrix are

$$I_{ij} = \delta_{ij}. \tag{1.17}$$

The inverse of a matrix does not always exist. However if it exists the following condition is satisfied

$$AA^{-1} = A^{-1}A = I. \tag{1.18}$$

In order for a matrix A to have the inverse its determinant must be non-zero, in which case

$$A^{-1}_{ij} = \frac{\text{cofactor of} A_{ji}}{\det A}. \tag{1.19}$$

In the above the cofactor of the element A_{ji} equals $(-1)^{i+j}$ times the determinant of the matrix which A becomes if its jth row and the ith column are deleted.

A number of matrices closely related to a given matrix A are given in the following table.

matrix	elements
A	A_{ij}
transpose $\tilde{A}$	$\tilde{A}_{ij} = A_{ji}$
complex conjugate A^*	$A^*_{ij} = (A_{ij})^*$
hermitian conjugate A^+	$A^+_{ij} = (A_{ji})^*$

1.3 Function of an operator

A function of an operator (matrix) is defined by the power series expansion. For example:

$$e^A = \sum_{n=0}^{\infty} \frac{1}{n!} A^n. \tag{1.20}$$

1.4 Unitary space and the scalar product

A unitary space is one in which for any two vectors $|u>$ and $|v>$ the scalar product $<u|v>$ is defined as a complex number with the following properties

$$\begin{aligned} &<u|v> = <v|u>^* \\ &<u|\lambda v + \eta w> = \lambda <u|v> + \eta <u|w> \\ &<u|u> \geq 0 \ \text{ and } \ <u|u> = 0 \text{ if and only if } |u> = 0. \end{aligned} \tag{1.21}$$

The scalar product defined above obeys the following Schwartz' inequality

$$<u|u><v|v> \ \geq |<u|v>|^2. \tag{1.22}$$

Two vectors whose scalar product is zero are said to be orthogonal.

1.5 Complete orthonormal set

let $|e_1>, ..., |e_n>$ be n-linearly independent vectors in a unitary space. They are said to form a orthonormal set if and only if

$$<e_i|e_j> = \delta_{ij}. \tag{1.23}$$

Any set of linearly independent vectors $|a_1>, ..., |a_n>$ can be made orthonormal by the following Gram-Schmidt process. First we choose, say, $|a_1>$ and normalize it

$$|e_1> \equiv \frac{|a_1>}{\sqrt{<a_1|a_1>}}. \tag{1.24}$$

Next we orthogonalize $|a_2>$ with respect to $|e_1>$

$$|a_2'> \equiv |a_2> - <e_1|a_2> |e_1> . \tag{1.25}$$

Then we normalize $|a_2'>$

$$|e_2> \equiv \frac{|a_2'>}{\sqrt{<a_2'|a_2'>}}. \tag{1.26}$$

Next we orthogonalize $|a_3>$ to $|e_1>$ and $|e_2>$

$$|a_3'> \equiv |a_3> - <e_1|a_3> |e_1> - <e_2|a_3> |e_2> . \tag{1.27}$$

Afterwards we normalize $|a_3'>$

$$|e_3> \equiv \frac{|a_3'>}{\sqrt{<a_3'|a_3'>}}. \tag{1.28}$$

We repeat this process until exhaust all vectors in the set.

A set of n orthonormal vectors in a n-dimensional vector space is called a complete orthonormal set. Any vector in this vector space can be written as a linear combination of these base vectors

$$|x> = \sum_{i=1}^{n} \phi_i |e_i> . \tag{1.29}$$

The statement that $\{|e_k>\}$ form a complete orthonormal set is often stated as the following equation

$$\sum_k |e_k><e_k| = I, \tag{1.30}$$

because

$$|x>=I|x>=\sum_k |e_k><e_k|x> . \tag{1.31}$$

The scalar product of two vectors can be expressed in terms of their components with respect to an orthonormal basis

$$<y|x>=\sum_{i=1}^{n} y_i^* x_i. \tag{1.32}$$

The matrix corresponds to a linear operator under an orthonormal basis is of particular importance in quantum mechanics. A compact way to write down such a matrix is

$$A=\sum_{ij} A_{ij}|e_i><e_j|. \tag{1.33}$$

The hermitian conjugate of A is the operator given by

$$A^+=\sum_{ij} A_{ji}^*|e_i><e_j|. \tag{1.34}$$

From Eq. (1.33) and Eq. (1.34) it follows that

$$<u|A^+|v>=(<v|A|u>)^*. \tag{1.35}$$

1.6 Unitary transformation

A linear operator satisfying

$$U^+=U^{-1}, \tag{1.36}$$

is said to be unitary. If $\{|e_i>\}$ is an orthonormal basis, then

$$|e'_k>=\sum_i U_{ik}|e_i> \tag{1.37}$$

where U is a unitary matrix also form an orthonormal basis.

Substituting $|e_i>=\sum_j U_{ji}^+|e'_j>$ into Eq. (1.33) we obtain

$$A=\sum_{ij} A'_{ij}|e'_i><e'_j|, \tag{1.38}$$

where

$$A'_{ij}=\sum_{k,l} U_{ik}^+ A_{kl} U_{lj}. \tag{1.39}$$

1.7 Eigenvalue and eigenvector

Let A be a linear operator and $|v>$ be a vector. If

$$A|v>=\lambda|v>, \tag{1.40}$$

then we said that $|v>$ is an eigenvector of A and λ is the associated eigenvalue. Under an orthonormal basis Eq. (1.40) read

$$\sum_j A_{ij}v_j = \lambda v_i, \quad \forall i. \tag{1.41}$$

Since Eq. (1.41) can be rewritten as the following n simultaneous equation

$$\sum_j (A_{ij} - \lambda\delta_{ij})v_j = 0, \tag{1.42}$$

the condition for the existence of non-trivial solution $\begin{pmatrix} v_1 \\ \cdot \\ \cdot \\ v_n \end{pmatrix}$ is

$$\det\left(A_{ij} - \lambda\delta_{ij}\right) = 0. \tag{1.43}$$

Eq. (1.43) is called the secular equation of Eq. (1.40).

There are three theorems concerning the eigenvalues of a hermitian operator.

1. The eigenvalues of a hermitian operator are all real numbers.
2. The eigenvectors of a hermitian operator that correspond to different eigenvalues are orthogonal.
3. It is possible to choose the eigenvectors of a hermitian operator so that they form a complete orthonormal set.

1.8 Diagonalization of matrices via unitary transformations

Let H be the matrix corresponds to a hermitian operator. Let $e_1, ..., e_n$ be its complete orthonormal eigen (column) vectors. Then under the

unitary transformation where

$$U \equiv \begin{pmatrix} e_1 & \cdot & \cdot & \cdot & e_n \\ \downarrow & \cdot & \cdot & \cdot & \downarrow \end{pmatrix} \tag{1.44}$$

H becomes a diagonal matrix

$$U^+ HU = D = \begin{pmatrix} \lambda_1 & 0 & 0 & ... \\ 0 & \lambda_2 & 0 & ... \\ 0 & 0 & \lambda_3 & ... \\ . & . & . & ... \end{pmatrix}. \tag{1.45}$$

Two matrices A and B can be simultaneously diagonalized if and only if A commute with B.

The eigenvalues of a matrix is unaffected by a unitary transformation, i.e., H and S^+HS have the same eigenvalues. In addition to the eigenvalues the trace of a matrix (TrA) and the determinant (det A)of a matrix are also invariant under unitary transformations.

Finally we state the general condition that a matrix be diagonalizable by means of unitary transformation. Consider an arbitrary matrix M. We can write

$$M = A + iB, \tag{1.46}$$

where A and B are both hermitian, by choosing

$$\begin{aligned} A &= \frac{M + M^+}{2} \\ B &= \frac{M - M^+}{2i}. \end{aligned} \tag{1.47}$$

Now A and B can be diagonalized separately, but in order that M may be diagonalized, we must be able to diagonalize A and B simultaneously. The requirement is that A and B commute.

1.9 Spaces of infinite dimensionality

Two kinds of infinite dimensional vector spaces are encountered in quantum mechanics. One has denumerably infinite number of base

vectors. For example a complete orthonormal set in this space may read

$$|e_k > \quad ; k = 1, ..., \infty. \tag{1.48}$$

In this case aside from the fact that vectors/matrices carry infinite components/elements everything else is the same

The other is nondenumerably infinite. For example consider a particle in one dimension. The eigenstate of the position operator of a particle:

$$X|x >= x|x > . \tag{1.49}$$

Two such states obeys the following orthonormal relationship

$$< y|x >= \delta(x - y), \tag{1.50}$$

with $\delta(x - y)$ the generalization of δ_{ij}.

$\{|x >\}$ form a complete orthonormal set in the sense that any state $|\psi >$ of that particle can by expressed as linear combination of $\{|x >\}$:

$$|\psi >= \int dx\psi(x)|x > . \tag{1.51}$$

We note that $\sum_i$ is now replace by $\int dx$. The scalar $\psi(x)$ is often called the wavefunction. The above completeness can be stated as

$$\int dx|x >< x| = I. \tag{1.52}$$

Physical observable are linear operators. The matrices corresponding to these operators carries continuous labels. For example the matrix corresponds to the momentum operator

$$P(x, y) = -\frac{\hbar}{i}\delta'(x - y). \tag{1.53}$$

In component form the equation

$$|\chi >= P|\psi > \tag{1.54}$$

becomes

$$\chi(x) = \int dy[-\frac{\hbar}{i}\delta'(x - y)]\psi(y) = \frac{\hbar}{i}\frac{d\psi(x)}{dx}. \tag{1.55}$$

Chapter 2

The fundamental assumptions

2.1 The dogma

1. An isolated physical system can by put into 1-1 correspondence with a vector space (Hilbert space), so that a definite state of the system corresponds to a definite unit norm vector in the space.

2. Each physical observable of a system is associated with a hermitian operator acting on the Hilbert space. The eigenstates of each such operator form a complete orthonormal set.

3. If the system is in state $|\psi>$, then the result of a given measurement of a physical observable O is an eigenvalue λ_n of the associated hermitian operator with the probability $p = |<\phi_n|\psi>|^2$. In the above $|\phi_n>$ denotes the eigenstate of O corresponds to eigenvalue λ_n. The averaged value of a observable after large number of measurements is

$$\bar{O} =<\psi|O|\psi> . \tag{2.1}$$

4. A measurement of observable A resulting in value λ_i projects the state vector from initial value $|u>$ to final state $|\phi_i>$. The latter is the eigenstate associated with λ_i. If $|u>$ is already an

eigenstate of A, then it is not changed by the measurement. If $|u>$ is not an eigenstate of A it is projected into $|\phi_n>$ with the following probability

$$p = |<\phi_n|u>|^2. \tag{2.2}$$

The assumption of quantum mechanics has some far reaching implications. The following are two examples.

2.2 The uncertainty relation

Item (3) of the above list implies the following *uncertainty relation*. Consider two physical observables whose corresponding (hermitian) operators are A and B. If $[A, B] = ic$[1] where c is a real number, then $\Delta A \Delta B \geq \frac{c}{2}$. Thus

$$[A, B] = ic \text{ implies } \Delta A \Delta B \geq \frac{c}{2}. \tag{2.3}$$

In the above

$$\Delta A^2 \equiv <u|A^2|u> - <u|A|u>^2 = <u|(A - <u|A|u>)^2|u>, \tag{2.4}$$

where $|u>$ is the state of the system. Physically ΔA is the root-mean-square deviation of the outcome of a large number of identical measurements made on observable A. Thus Eq. (2.3) implies that in a series of experiments where A and B are simultaneously measured, the root-mean-square deviation of A and B obeys the inequality $\Delta A \Delta B \geq \frac{c}{2}$.

Proof: Let

$$\begin{aligned} O_1 &\equiv A - <u|A|u> \\ O_2 &\equiv B - <u|B|u> . \end{aligned} \tag{2.5}$$

[1] If the commutator of two hermitian operators is a c-number (scalar) then this number is necessarily pure imaginary. Proof: if $[A, B] = z$, then $[A, B]^+ = -[A, B] = z^*$. Thus $z^* = -z$ which implies that z is pure imaginary.

Since A and B are hermitian so are O_1 and O_2. In addition it is obvious that

$$[O_1, O_2] = ic \tag{2.6}$$

. Let $|v>= O_1|u>, |w>= O_2|u>$. (Consequently $< v|v>= \Delta A^2, \Delta B^2 =< w|w>$.) By Schartz' inequality

$$\begin{aligned} \Delta A^2 \Delta B^2 \quad &=< v|v >< w|w >\geq | < v|w > |^2 = | < u|O_1 O_2|u > |^2 \\ &= \frac{1}{4}| < u|[O_1, O_2] + \{O_1, O_2\}|u > |^2. \end{aligned} \tag{2.7}$$

In the above

$$\{O_1, O_2\} \equiv O_1 O_2 + O_2 O_1, \tag{2.8}$$

is the anti-commutator of O_1 and O_2. Since both O_1 and O_2 are hermitian, so is $\{O_1, O_2\}$. As a result

$$< u|\{O_1, O_2\}|u >= \alpha = \text{a real number.} \tag{2.9}$$

Substitute Eq. (2.6) and Eq. (2.9) into Eq. (2.7) we obtain

$$\Delta A^2 \Delta B^2 \geq \frac{1}{4}|\alpha + ic|^2 = \frac{1}{4}(\alpha^2 + c^2) \geq \frac{1}{4}c^2. \tag{2.10}$$

As the result Eq. (2.3) holds.

A commonly cited example of Eq. (2.3) is the position-momentum uncertainty relation

$$\Delta x \Delta y \geq \frac{\hbar}{2}. \tag{2.11}$$

2.3 A reminder of the spin 1/2 algebra

In the second example we discuss the implication of item (4) of the dogma - i.e. a measurement "collapses" the system into an eigenstate of the observable that is been measured.

Let us consider two spin 1/2 particles. As the reader probably remember for a spin 1/2 particle the projection of its spin angular momentum along any direction is of either $+\hbar/2$ or $-\hbar/2$. We shall revisit the spin angular momentum later, at this time let me just remind the readers of some facts of the spin 1/2 problem.

The state space of a single spin 1/2 is two dimensional because there are two othonormal state $|+\hat{z}>$ and $|-\hat{z}>$ correspond to $\pm\hbar/2$ spin angular momentum along the z-axis respectively. The matrices that correspond to the spin operator in x,y,z directions are

$$\begin{aligned} S_x &\leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ S_y &\leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ S_z &\leftrightarrow \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \tag{2.12}$$

The state that corresponds to $\pm\hbar/2$ spin angular momentum along the z-axis are

$$\begin{aligned} |+\hat{z}> &\leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |-\hat{z}> &\leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \end{aligned} \tag{2.13}$$

The state above satisfies the following eigen equations

$$\begin{aligned} S_z|+\hat{z}> &= \frac{\hbar}{2}|+\hat{z}> \\ S_z|-\hat{z}> &= -\frac{\hbar}{2}|-\hat{z}>. \end{aligned} \tag{2.14}$$

Similarly we can show that the state that satisfies

$$\begin{aligned} S_x|+\hat{x}> &= \frac{\hbar}{2}|+\hat{x}> \\ S_x|-\hat{x}> &= -\frac{\hbar}{2}|-\hat{x}> \end{aligned} \tag{2.15}$$

are given by

$$\begin{aligned} |+\hat{x}> &\leftrightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|+\hat{z}>+|-\hat{z}>) \\ |-\hat{x}> &\leftrightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|+\hat{z}>-|-\hat{z}>). \end{aligned} \tag{2.16}$$

Similarly it can be shown that the state that satisfy

$$\begin{aligned} \hat{a}\cdot\mathbf{S}|+\hat{a}>&=\frac{\hbar}{2}|+\hat{a}> \\ \hat{a}\cdot\mathbf{S}|-\hat{a}>&=\frac{\hbar}{2}|-\hat{a}>, \end{aligned} \tag{2.17}$$

where $\hat{a}=(\sin 2\phi_a, 0, \cos 2\phi_a)$ is

$$\begin{aligned} |+\hat{a}> &= (\cos\phi_a|+>+\sin\phi_a|->) \\ |-\hat{a}> &= (-\sin\phi_a|+>+\cos\phi_a|->)\,. \end{aligned} \tag{2.18}$$

In the above $2\phi_a$ is the angle made by $\hat{a}$ and the z-axis.

For two particles the state space is 4-dimensional since there are four possible orthonormal states $|+\hat{z},+\hat{z}>, |+\hat{z},-\hat{z}>, |-\hat{z},+\hat{z}>$, $|-\hat{z},-\hat{z}>$. Out of the four possible states above we can construct a very special state

$$|S>=\frac{1}{\sqrt{2}}(|+\hat{z},-\hat{z}>-|-\hat{z},+\hat{z}>\,. \tag{2.19}$$

This state has the property that the total spin angular momentum is zero. In other words

$$(S_{1z}+S_{2z})|S>=(S_{1x}+S_{2x})|S>=(S_{1y}+S_{2y})|S>=0. \tag{2.20}$$

Imagine that the two particles are initially close together and are in the singlet state Now imagine the particles fly apart in a way that their total spin angular momentum is conserved. Let there be two observers A and B who intercept these particles.

If B measures the spin of the particle (say 2) he/she intercepts while observer A does nothing. The outcome of B's experiment is that there is equal probability for spin up ($+\hat{z}$) and spin down ($-\hat{z}$).

Now consider A first measures the spin of particle 1 then B measures the spin of particle 2. In this case if A sees spin up then there is a 100% probability that B will see spin down. Likewise if A sees spin down B for sure will see spin up. (Of course there is equal chances for the above

two scenario to occur.)[2]

Thus one might say that what A does affect the outcome of B's measurement. One might say that this is nothing unusual. Imagine two billiard balls colliding with equal and opposite velocities. After the collision the direction of ball 2's velocity is totally random. However if one measures the velocity of ball 1, then due to the conservation of momentum ball 2's velocity will for sure be opposite to that.

Of course in the billiard ball's case the fact that the final velocity of ball 1 appears random is because our imperfect knowledge about the initial condition such as impact parameter ... etc. In principle if we have such information, the final velocities should be completely predictable. The situation is entirely different in the spin 1/2 case. This time the probabilistic outcome of a measurement on particle 1's spin is not due to imperfect information. According to quantum mechanics this probabilistic feature exists at the most fundamental level of nature.

[2]According to the assumption of quantum mechanics the probability that B observes spin up/down while A does not make any measurement is given by

$$\begin{aligned} P_u &= |<+\hat{z},+\hat{z}|S>|^2 + |<+\hat{z},-\hat{z}|S>|^2 = \frac{1}{2} \\ P_d &= |<-\hat{z},+\hat{z}|S>|^2 + |<-\hat{z},-\hat{z}|S>|^2 = \frac{1}{2}. \end{aligned} \tag{2.21}$$

However once A has measured that particle 1 has spin, say, $-\hat{z}$, then the singlet state is "collapsed" to

$$|S> \rightarrow -|-\hat{z},+\hat{z}>, \tag{2.22}$$

Thus the probability that a subsequent measurement of B will yield spin up/down is given by

$$\begin{aligned} P_u &= |-<+\hat{z},-\hat{z}|-\hat{z},+\hat{z}>|^2 = 1 \\ P_d &= |-<-\hat{z},-\hat{z}|-\hat{z},+\hat{z}>|^2 = 0. \end{aligned} \tag{2.23}$$

Similarly if A has measured $+\hat{z}$ for particle 1's spin, the probability for the outcome of B's measurement are

$$\begin{aligned} P_u &= |<+\hat{z},+\hat{z}|+\hat{z},-\hat{z}>|^2 = 0 \\ P_d &= |<-\hat{z},+\hat{z}|+\hat{z},-\hat{z}>|^2 = 1. \end{aligned} \tag{2.24}$$

The billiard ball example is a special case of the "hidden variable theory".

2.4 The hidden variable theory

In this theory it is argued that the fact that the behavior at the microscopic level appears probabilistic is only because some yet unknown variables have not been specified. For example when a hidden variable h falls in the range of R_{++} the spins of particle 1 and 2 are $+1/2, +1/2$, ... etc. If particle 1's spin is not measured the range of h that is consistent with particle 2 having spin up/down is $R_{++} \bigcup R_{-+}/R_{+-} \bigcup R_{--}$. Thus if $R_{++} \bigcup R_{-+}$ and $R_{+-} \bigcup R_{--}$ occupy the same "volume" in the h-space, there is equal probability for particle 2 to have spin up and down. If particle 1's spin is measured to be $+/-$ that fixes the range of h to $R_{++} \bigcup R_{+-}/R_{-+} \bigcup R_{--}$. Now if R_{++}/R_{--} has zero volume, then the subsequent measurement of particle 2's spin must yield the value $-/+$. The above is summarized in the following table

Range	probability	Particle 1	Particle 2
R_{+-}	$p_1 = 1/2$	$+\hat{z}$	$-\hat{z}$
R_{-+}	$p_2 = 1/2$	$-\hat{z}$	$+\hat{z}$

The way that hidden variable theory works is to design the h-space until the quantum mechanical prediction is met. For sometime it is felt that it is always possible to design the h-space so that it will be consistent with quantum mechanics.

For example, let us consider observer A and B measure the z as well as the x components of the spin. According to the assumption of quantum mechanics there are the following possibilities:

1. If A measures S_z and B measures S_x, there is a completely random correlation between the two measurements.

2. If A measures S_x and B measures S_x, there is a 100% correlation between the two measurements.

3. If A makes no measurement, B's measurement show random results.

The proof that quantum mechanics yield the above prediction is left as a homework problem.

The way that hidden variable theory cope with the above result is to designs the space of the hidden variables as follows:

Range	Probability	Particle 1	Particle 2
$R^{(+\hat{z},-\hat{x})}_{(-\hat{z},+\hat{x})}$	1/4	$(+\hat{z},-\hat{x})$	$(-\hat{z},+\hat{x})$
$R^{(+\hat{z},+\hat{x})}_{(-\hat{z},-\hat{x})}$	1/4	$(+\hat{z},+\hat{x})$	$(-\hat{z},-\hat{x})$
$R^{(-\hat{z},+\hat{x})}_{(+\hat{z},-\hat{x})}$	1/4	$(-\hat{z},+\hat{x})$	$(+\hat{z},-\hat{x})$
$R^{(-\hat{z},-\hat{x})}_{(+\hat{z},+\hat{x})}$	1/4	$(-\hat{z},-\hat{x})$	$(+\hat{z},+\hat{x})$

In the above by $(+\hat{z},-\hat{x})$ we mean a state where if one measures S_z one will get $+\hbar/2$ with certainty, while if one measures S_x instead one will get $-\hbar/2$ with certainty. It should be emphasized that we are not saying that one can simultaneously measure S_z and S_x to be $+\hbar/2$ and $-\hbar/2$. When we measure S_z we do not measure S_x and vice versa. We are assigning definite values of spin components in more than one direction with the understanding that only one or the other of the components can actually be measured.

2.5 Bell's inequality

For a long time it is believed that the hidden variable theory can always be concocted in such a way that they would give no predictions other than the usual quantum mechanical one. It is until in 1964 J.S. Bell (see, e.g., J.S. Bell Rev. Mod. Phys. **38**, 447 (1966)) pointed out that the hidden variable theory has an experimentally-testable prediction that disagrees with the prediction of quantum mechanics.

Let us consider three directions $\hat{a}$, $\hat{b}$, $\hat{c}$ in the $z-x$ plane which are, in general, not mutually orthogonal. Since the singlet state has total spin angular momentum zero, the projection of particle 1 and particle 2's spin along $\hat{a}$, $\hat{b}$ or $\hat{c}$ must sum to zero.

In order to be consistent with the above the hidden variable theory designs a table like the following.

Range	Probability	Particle 1	Particle 2
$R^{(+\hat{a},+\hat{b},+\hat{c})}_{(-\hat{a},-\hat{b},-\hat{c})}$	p_1	$(+\hat{a},+\hat{b},+\hat{c})$	$(-\hat{a},-\hat{b},-\hat{c})$
$R^{(+\hat{a},+\hat{b},-\hat{c})}_{(-\hat{a},-\hat{b},+\hat{c})}$	p_2	$(+\hat{a},+\hat{b},-\hat{c})$	$(-\hat{a},-\hat{b},+\hat{c})$
$R^{(+\hat{a},-\hat{b},+\hat{c})}_{(-\hat{a},+\hat{b},-\hat{c})}$	p_3	$(+\hat{a},-\hat{b},+\hat{c})$	$(-\hat{a},+\hat{b},-\hat{c})$
$R^{(+\hat{a},-\hat{b},-\hat{c})}_{(-\hat{a},+\hat{b},+\hat{c})}$	p_4	$(+\hat{a},-\hat{b},-\hat{c})$	$(-\hat{a},+\hat{b},+\hat{c})$
$R^{(-\hat{a},+\hat{b},+\hat{c})}_{(+\hat{a},-\hat{b},-\hat{c})}$	p_5	$(-\hat{a},+\hat{b},+\hat{c})$	$(+\hat{a},-\hat{b},-\hat{c})$
$R^{(-\hat{a},+\hat{b},-\hat{c})}_{(+\hat{a},-\hat{b},+\hat{c})}$	p_6	$(-\hat{a},+\hat{b},-\hat{c})$	$(+\hat{a},-\hat{b},+\hat{c})$
$R^{(-\hat{a},-\hat{b},+\hat{c})}_{(+\hat{a},+\hat{b},-\hat{c})}$	p_7	$(-\hat{a},-\hat{b},+\hat{c})$	$(+\hat{a},+\hat{b},-\hat{c})$
$R^{(-\hat{a},-\hat{b},-\hat{c})}_{(+\hat{a},+\hat{b},+\hat{c})}$	p_8	$(-\hat{a},-\hat{b},-\hat{c})$	$(+\hat{a},+\hat{b},+\hat{c})$

According to this table

$$\begin{aligned} P^{+\hat{a}}_{+\hat{b}} &= p_3 + p_4 \\ P^{+\hat{a}}_{+\hat{c}} &= p_2 + p_4 \\ P^{+\hat{c}}_{+\hat{b}} &= p_3 + p_7. \end{aligned} \tag{2.25}$$

Since $p_i \geq 0$, we conclude

$$P^{+\hat{a}}_{+\hat{b}} \leq P^{+\hat{a}}_{+\hat{c}} + P^{+\hat{c}}_{+\hat{b}}. \tag{2.26}$$

This is called the Bell inequality.

Now let us ask what is the quantum mechanical prediction. According to Eq. (2.18) the spin state that satisfy

$$\hat{a} \cdot \mathbf{S}| + \hat{a} >= +\frac{\hbar}{2}| + \hat{a} >, \tag{2.27}$$

is

$$| + \hat{a} >= (\cos\phi_a|+ > + \sin\phi_a|- >)\,. \tag{2.28}$$

In the above $2\phi_a$ is the angle made by $\hat{a}$ and the z-axis.

Using Eq. (2.28) we obtain

$$\begin{aligned} &< S| + \hat{a}, +\hat{b} > \\ &= \frac{1}{\sqrt{2}}\left[< - + | \; - \;\; < + - |\right]\left[\cos\phi_a \cos\phi_b| + + >\right. \end{aligned}$$

$$
\begin{aligned}
&+\cos\phi_a \sin\phi_b|+->+\sin\phi_a\cos\phi_b|-+> \\
&+\sin\phi_a\sin\phi_b|-->] \\
&=\frac{1}{\sqrt{2}}[\cos\phi_a\sin\phi_b-\sin\phi_a\cos\phi_b] \\
&=\frac{1}{\sqrt{2}}\sin(\phi_b-\phi_a). \qquad (2.29)
\end{aligned}
$$

As the result

$$P^{+\hat{a}}_{+\hat{b}} = |<S|+\hat{a},+\hat{b}>|^2 = \frac{1}{2}\sin^2(\phi_b-\phi_a). \qquad (2.30)$$

Similarly we have

$$
\begin{aligned}
P^{+\hat{c}}_{+\hat{b}} &= \frac{1}{2}\sin^2(\phi_b-\phi_c) \\
P^{+\hat{a}}_{+\hat{c}} &= \frac{1}{2}\sin^2(\phi_c-\phi_a) \qquad (2.31)
\end{aligned}
$$

Thus according to quantum mechanics we have

$$
\begin{aligned}
P^{+\hat{a}}_{+\hat{b}} &= \frac{1}{2}\sin^2(\phi_b-\phi_a) \\
P^{+\hat{a}}_{+\hat{c}} + P^{+\hat{c}}_{+\hat{b}} &= \frac{1}{2}\sin^2(\phi_c-\phi_a)+\frac{1}{2}\sin^2(\phi_b-\phi_c). \qquad (2.32)
\end{aligned}
$$

Thus in order for the Bell inequality to be satisfied we require

$$\sin^2(\phi_b-\phi_a) \le \sin^2(\phi_c-\phi_a)+\sin^2(\phi_b-\phi_c). \qquad (2.33)$$

There are clearly choice of ϕ's so that the above equation is violated. Example are such as $\phi_a = 0, \phi_c = \theta, \phi_b = 2\theta$. The Bell inequality requires

$$\sin^2 2\theta = (1-2\sin^2\theta)^2 \le 2\sin^2\theta. \qquad (2.34)$$

Thus if we choose θ so that

$$\sin^2\theta > \frac{3-\sqrt{5}}{4}, \qquad (2.35)$$

(or $\theta \ge 25.9$ degrees) the Bell inequality is violated. The first experimental demonstration of the violation of Bell's inequality is achieved at Berkeley by Freedman *et al* (Phys. Rev. Lett. **28**, 938 (1972).) using the photon analog of the spin 1/2 problem.

Chapter 3

Quantum dynamics

So far we have not discussed how physical systems change with time. This section is devoted to the dynamic evolution of states and observables.

The first important point we should keep in mind is that time is just a parameter in quantum mechanics, *not* an operator. In particular time is not an observable in the language of the previous sections. It is incorrect to talk about the time operator in the same sense as we talk about the position operator.

3.1 The Hamiltonian and time evolution operator

The basic question is, how does a state change with time. To answer this question it is sufficient to describe how does a physical state change after infinitesimal time increment from t to $t + dt$. The answer is that suppose the system is in state $|\phi>$ at time t, then after dt the system is in the state

$$|\chi>=[I - i\frac{dt}{\hbar}H(t)]|\phi> . \tag{3.1}$$

In the above $H(t)$ is a hermitian operator that in general depends on t. This operator is commonly referred to as the Hamiltonian (energy operator) of the system.

Because $H(t)$ is hermitian Eq. (3.1) implies that

$$< \chi|\chi >=< \phi|\phi > +O(dt^2). \tag{3.2}$$

Thus the time evolution dictated by Eq. (3.1) conserves the norm of the state vector. Eq. (3.1) can be integrated to yield the evolution of a state after finite time Δt elapse. The answer is that

$$|\eta >= [I-i\frac{\epsilon}{\hbar}H(t+(N-1)\epsilon)]...[I-i\frac{\epsilon}{\hbar}H(t+\epsilon)][I-i\frac{\epsilon}{\hbar}H(t)]|\phi > . \tag{3.3}$$

In the above we have divided the total time evolution into N infinitesimal pieces, i.e.

$$\epsilon = \frac{\Delta t}{N}. \tag{3.4}$$

Eq. (3.3) is equivalent to

$$|\eta >= T_>\{e^{-\frac{i}{\hbar}\int_t^{t+\Delta t} dtH(t)}\}|\phi >, \tag{3.5}$$

where $T_>$ is the time ordering operator. To be more specific,

$$T_>[H(t_1)H(t_2)...H(t_N)] = H(t_{latest})...H(t_{earliest}). \tag{3.6}$$

But what happen if Δt is negative. In that case the time evolution from $|\eta >$ to $|\phi >$ is given by Eq. (3.5) or

$$|\phi >= T_>\{e^{-\frac{i}{\hbar}\int_{t+\Delta t}^{t} dtH(t)}\}|\eta >, \tag{3.7}$$

As the result

$$\begin{aligned} |\eta > \quad &= \{T_>e^{-\frac{i}{\hbar}\int_{t+\Delta t}^{t} dtH(t)}\}^{-1}|\phi >= T_<e^{\frac{i}{\hbar}\int_{t+\Delta t}^{t} dtH(t)}|\phi > \\ &= T_<e^{-\frac{i}{\hbar}\int_{t}^{t+\Delta t} dtH(t)}|\phi > . \end{aligned} \tag{3.8}$$

In the above $T_<$ is the anti time ordering operator i.e.

$$T_<[H(t_1)H(t_2)...H(t_N)] = H(t_{earliest})...H(t_{latest}). \tag{3.9}$$

The operator that evolves a state from time t_1 to t_2 is called the time evolution operator

$$\mathcal{U}(t_2;t_1) \equiv T_{t_2-t_1}\{e^{-\frac{i}{\hbar}\int_{t_1}^{t_2} dtH(t)}\}, \tag{3.10}$$

where

$$\begin{aligned} T_{t_2-t_1} &= T_>, \quad t_2 > t_1 \\ &= T_<, \quad t_2 < t_1. \end{aligned} \tag{3.11}$$

Two immediate implications of Eq. (3.10) are that

$$\mathcal{U}(t_1;t_2) = \mathcal{U}^+(t_2;t_1), \tag{3.12}$$

and

$$\mathcal{U}(t+\delta t;t_0) = e^{-\frac{i}{\hbar}\delta t H(t)}\mathcal{U}(t;t_0). \tag{3.13}$$

The consequence of Eq. (3.12) is that if

$$|\psi_2> = \mathcal{U}(t_2;t_1)|\psi_1>, \tag{3.14}$$

then

$$|\psi_1> = \mathcal{U}(t_2:t_1)^+|\psi_2> = \mathcal{U}(t_1;t_2)|\psi_2> . \tag{3.15}$$

Thus the hermitian conjugate of the time evolution operator does the backward time evolution. The consequence of Eq. (3.13) is that

$$\begin{aligned} i\hbar\frac{d\mathcal{U}(t;t_0)}{dt} &= H(t)\mathcal{U}(t;t_0) \\ -i\hbar\frac{d\mathcal{U}^+(t;t_0)}{dt} &= \mathcal{U}^+(t;t_0)H(t) \end{aligned} \tag{3.16}$$

3.2 The Schrödinger equation

A state that evolves by the time evolution operator $|\psi(t)> = \mathcal{U}(t;t_0)|\psi_0>$ obeys the following differential equation - the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)> = H(t)|\psi(t)> . \tag{3.17}$$

In the case where the Hamiltonian is time independent Eq. (3.10) becomes

$$\mathcal{U}(t_2;t_1) = e^{-\frac{i}{\hbar}(t_2-t_1)H}. \tag{3.18}$$

If at $t = 0$ a system is in the eigenstate of a time-independent Hamiltonian $H|n> = E_n|n>$ then the state at time t is

$$|\psi(t)> = e^{-\frac{i}{\hbar}tH}|n> = e^{-\frac{i}{\hbar}E_n t}|n> . \tag{3.19}$$

3.3 The Heisenberg equation

Let $\{|e_n>\}$ be an orthonormal basis, and A be a linear operator corresponds to a physical observable. The matrix corresponds to A is given by

$$A_{nm} =< e_n|A|e_m > . \tag{3.20}$$

Upon time evolution each of the basis state becomes

$$\mathcal{U}(t;0)|e_n > . \tag{3.21}$$

The matrix element of A then evolves to

$$< e_n|\mathcal{U}(t;0)^+ A\mathcal{U}(t;0)|e_m > . \tag{3.22}$$

As far as the matrix elements is concerned we can regard the state as static while the operator is evolving:

$$A_H(t) = \mathcal{U}(t;0)^+ A\mathcal{U}(t;0). \tag{3.23}$$

This point of view is called the "Heisenberg picture". In the following we contrast the Heisenberg picture with the Schrödinger one.

	States	Operators
Schrödinger	time dependent	time independent
Heisenberg	time independent	time dependent

According to the Heisenberg picture the physical observables evolves according to the following differential equation

$$\frac{dA_H}{dt} = \frac{i}{\hbar}[H_H, A_H] + \left(\frac{\partial A}{\partial t}\right)_H . \tag{3.24}$$

Due to the fact that $\mathcal{U}(t;0)^+\mathcal{U}(t;0) = I$,

$$[H_H, A_H] = \mathcal{U}(t;0)^+[H(t), A]\mathcal{U}(t;0) \tag{3.25}$$

. The last term of the above equation arises from the explicit time dependence of the operator itself.

3.4 Two-state problem

The two-state problem has the simplest state-space – there are only two linearly independent vectors. Let us call them $|u>$ and $|d>$.[1] They form a orthonormal set, i.e.,

$$|u><u| + |d><d| = I. \tag{3.26}$$

Any hermitian matrix in this space can be written as

$$M = \begin{pmatrix} a & b - ic \\ b + ic & d \end{pmatrix}, \tag{3.27}$$

where a, b, c, d are real. A matrix of the form Eq. (3.27) can be expressed as a linear combination of the identity and three Pauli matrices:

$$M = \left(\frac{a+d}{2}\right) I + b\sigma_x + c\sigma_y + \left(\frac{a-d}{2}\right)\sigma_z. \tag{3.28}$$

In the above

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.29}$$

are the three Pauli matrices. Some important properties of the Pauli matrices are

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I, \tag{3.30}$$

and

$$\begin{aligned} \sigma_x\sigma_y &= i\sigma_z \\ \sigma_y\sigma_z &= i\sigma_x \\ \sigma_z\sigma_x &= i\sigma_y. \end{aligned} \tag{3.31}$$

Eq. (3.31) implies the following commutation relation

$$[\sigma_\alpha, \sigma_\beta] = 2i \sum_\gamma \epsilon_{\alpha\beta\gamma}\sigma_\gamma, \tag{3.32}$$

[1] A physical realization of the two-state problem is the spin state of a spin 1/2 particle.

and anticommutation relation

$$\{\sigma_\alpha, \sigma_\beta\} = 0. \tag{3.33}$$

In Eq. (3.32) $\epsilon_{xyz} = \epsilon_{yzx} = \epsilon_{zxy} = -\epsilon_{yxz} = -\epsilon_{zyx} = -\epsilon_{xzy} = 1$, and all other combination of α, β, γ give zero.

A simple example of Hamiltonian in this two-state space is

$$H = -B\sigma_x. \tag{3.34}$$

The eigenstates of this Hamiltonian is

$$\begin{aligned} &\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \quad \text{eigenenergy } = -B \\ &\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \quad \text{eigenenergy } = B. \end{aligned} \tag{3.35}$$

The unitary matrix which transforms H into diagonal form is

$$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}, \tag{3.36}$$

and

$$U^+ H U = \begin{pmatrix} -B & 0 \\ 0 & B \end{pmatrix}. \tag{3.37}$$

If the system starts in the up state ($\begin{pmatrix}1\\0\end{pmatrix}$) after time t it becomes

$$\begin{aligned} &e^{-\frac{i}{\hbar}tH}\begin{pmatrix}1\\0\end{pmatrix} = e^{\frac{i}{\hbar}tB\sigma_x}\begin{pmatrix}1\\0\end{pmatrix} \\ &= [\cos\left(\frac{Bt}{\hbar}\right) + i\sin\left(\frac{Bt}{\hbar}\right)\sigma_x]\begin{pmatrix}1\\0\end{pmatrix} \\ &= \cos\left(\frac{Bt}{\hbar}\right)\begin{pmatrix}1\\0\end{pmatrix} + i\sin\left(\frac{Bt}{\hbar}\right)\begin{pmatrix}0\\1\end{pmatrix}. \end{aligned} \tag{3.38}$$

Thus the system oscillates between the spin up and spin down states with frequency

$$\Omega = \frac{B}{\hbar}. \tag{3.39}$$

In Heisenberg picture the time-dependent operator evolves from σ_x, σ_y and σ_z are

$$
\begin{aligned}
& e^{\frac{i}{\hbar}tH}\sigma_x e^{-\frac{i}{\hbar}tH} = \sigma_x \\
& e^{\frac{i}{\hbar}tH}\sigma_y e^{-\frac{i}{\hbar}tH} \\
&= \begin{pmatrix} \cos\left(\frac{Bt}{\hbar}\right) & -i\sin\left(\frac{Bt}{\hbar}\right) \\ -i\sin\left(\frac{Bt}{\hbar}\right) & \cos\left(\frac{Bt}{\hbar}\right) \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \cos\left(\frac{Bt}{\hbar}\right) & i\sin\left(\frac{Bt}{\hbar}\right) \\ i\sin\left(\frac{Bt}{\hbar}\right) & \cos\left(\frac{Bt}{\hbar}\right) \end{pmatrix} \\
&= \begin{pmatrix} \sin\left(\frac{2Bt}{\hbar}\right) & -i\cos\left(\frac{2Bt}{\hbar}\right) \\ i\cos\left(\frac{2Bt}{\hbar}\right) & -\sin\left(\frac{2Bt}{\hbar}\right) \end{pmatrix} = \sin\left(\frac{2Bt}{\hbar}\right)\sigma_z + \cos\left(\frac{2Bt}{\hbar}\right)\sigma_y \\
& e^{\frac{i}{\hbar}tH}\sigma_z e^{-\frac{i}{\hbar}tH} \\
&= \begin{pmatrix} \cos\left(\frac{Bt}{\hbar}\right) & -i\sin\left(\frac{Bt}{\hbar}\right) \\ -i\sin\left(\frac{Bt}{\hbar}\right) & \cos\left(\frac{Bt}{\hbar}\right) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos\left(\frac{Bt}{\hbar}\right) & i\sin\left(\frac{Bt}{\hbar}\right) \\ i\sin\left(\frac{Bt}{\hbar}\right) & \cos\left(\frac{Bt}{\hbar}\right) \end{pmatrix} \\
&= \begin{pmatrix} \cos\left(\frac{2Bt}{\hbar}\right) & i\sin\left(\frac{2Bt}{\hbar}\right) \\ -i\sin\left(\frac{2Bt}{\hbar}\right) & -\cos\left(\frac{2Bt}{\hbar}\right) \end{pmatrix} = \cos\left(\frac{2Bt}{\hbar}\right)\sigma_z - \sin\left(\frac{2Bt}{\hbar}\right)\sigma_y
\end{aligned} \tag{3.40}
$$

Thus

$$\dot{\vec{\sigma}}_H = \frac{2B}{\hbar}\hat{x} \times \vec{\sigma}_H. \tag{3.41}$$

Eq. (3.41) is very important in studying the precession of the electron spin in magnetic field. The matrix corresponds to the spin of an electron is given by

$$\mathbf{S} = \frac{\hbar}{2}\vec{\sigma}. \tag{3.42}$$

The Hamiltonian that governs such a spin in external magnetic field is

$$H = -\frac{e}{m_e c}\mathbf{B} \cdot \mathbf{S}. \tag{3.43}$$

Here $\frac{e}{m_e c}\mathbf{S}$ is the magnetic moment of an electron. Putting Eq. (3.42),Eq. (3.41),Eq. (3.43) and Eq. (3.34) together we conclude that

$$\dot{\mathbf{S}}_H = \Omega\hat{B} \times \mathbf{S}_H, \tag{3.44}$$

where

$$\hbar\Omega = \frac{eB}{m_e c}. \tag{3.45}$$

Eq. (3.44) implies that the electron spin precesses at the frequency Ω.

3.5 The Berry's phase in two-state systems

Let us consider the following Hamiltonian parametrized by $\mathbf{R} = (X, Y)$

$$H(\mathbf{R}) = X\sigma_z + Y\sigma_x = \mathbf{R} \cdot \vec{\sigma}. \tag{3.46}$$

The eigenvalues of $H(\mathbf{R})$ are $\pm\sqrt{X^2 + Y^2} = \pm|\mathbf{R}|$. Thus at $\mathbf{R} = 0$ H is degenerate.

M. Berry (Proc. R. Soc. Lond. A **392**, 45 (1984)) discovered a deep theorem concerning the eigenstates of this type of Hamiltonian. Let us imagine $\mathbf{R}$ in Eq. (3.46) changes with time. We say that the change in $\mathbf{R}$ is "adiabatic" if $\dot{\mathbf{R}}(t)$ is very small. Of course a slowly varying $\mathbf{R}$ induces a slowly varying $H(\mathbf{R}(t))$. Let $|\psi_\pm(\mathbf{R}(t)) >$ be the instantaneous eigenstate of $H(\mathbf{R}(t))$ with eigen energy $E_\pm(\mathbf{R}(t)) = \pm|\mathbf{R}(t)|$. It can be shown that if we start off in the state $|\psi_\pm(\mathbf{R}(0)) >$ and change $\mathbf{R}(t)$ adiabatically, then the state at time t is given by

$$|\psi_\pm(t) >= e^{-\frac{i}{\hbar}\int_0^t E_\pm(\mathbf{R}(\tau))d\tau} e^{-i\gamma_\pm(t)} |\psi_\pm(\mathbf{R}(t)) > . \tag{3.47}$$

The first exponential factor is the usual phase factor which an energy-eigen state acquires upon time evolution. The only difference is that in the present case the Hamiltonian is time-dependent, and this phase factor is the product of infinitely many phase factors each corresponds to an infinitesimal time evolution with the instantaneous energy eigenvalues appear in the exponent. The second phase factor is commonly referred to as the Berry's phase. Berry showed that

$$\gamma_\pm(t) \quad = \int_0^t d\tau < \psi_\pm(\mathbf{R}(\tau))| i\frac{\partial}{\partial t} |\psi_\pm(\mathbf{R}(\tau)) > . \tag{3.48}$$

Some discussions are in order regarding the above equation. Eq. (3.48) assumes that the instantaneous eigenstate $|\psi_\pm(\mathbf{R}(\tau)) >$ is differentiable with respect to t. Since eigenstates are only defined up to a phase factor,[2] we can certainly choose the phase factors (e.g. make them change abruptly from one instant of time to the next) so that

[2] i.e. if $|\psi_\pm(\mathbf{R}) >$ are eigenstates of $H(\mathbf{R})$ so are $e^{i\phi_\pm}|\psi_\pm(\mathbf{R}) >$

$\frac{\partial}{\partial t}|\psi_\pm(\mathbf{R}(\tau))>$ does not exist. Eq. (3.48) implicitly assumes that we choose the phase factors so that $|\psi_\pm(\mathbf{R}(t))>$ are *differentiable* over the time period considered.

Now imagine during the time interval $[0,T]$ the $\mathbf{R}(t)$ slowly changed in a full circuit C.[3] Berry showed that the integral

$$\begin{aligned}\gamma_\pm(T) &= \int_0^T d\tau < \psi_\pm(\mathbf{R}(\tau))|i\frac{\partial}{\partial t}|\psi_\pm(\mathbf{R}(\tau))> \\ &= \oint_C d\mathbf{R}\cdot[<\psi_\pm(\mathbf{R})|\frac{\nabla_\mathbf{R}}{i}|\psi_\pm(\mathbf{R})>] = \pi Q_c \end{aligned} \tag{3.49}$$

where $Q_c = 0(mod 2)$ or $1(mod 2)$ depending on whether C encloses the point $\mathbf{R}=0$ where the Hamiltonian is degenerate.

Obviously if $|\psi_\pm(\mathbf{R}))>$ is differentiable and single-valued as $\mathbf{R}$ sweeps through a full circuit so does $e^{i\theta_\pm(\mathbf{R})}|\psi_\pm(\mathbf{R}))>$, assuming $e^{i\theta_\pm(\mathbf{R})}$ is differentiable and single-valued. Upon this phase-transformation

$$\gamma_\pm(T) \to \gamma_\pm(T) + \oint d\mathbf{R}\cdot\nabla_\mathbf{R}\theta_\pm(\mathbf{R}). \tag{3.50}$$

The second term on the right is the integral of a total differential, hence it vanishes upon the loop integration.

Let us demonstrate Berry's theorem by using Eq. (3.46) as an example. As we discussed before the instantaneous eigenstates of Eq. (3.46) are

$$\begin{aligned}|\psi_+(\mathbf{R})> &= \left(\cos\frac{\phi}{2}|u> + \sin\frac{\phi}{2}|d>\right) \\ |\psi_-(\mathbf{R})> &= \left(-\sin\frac{\phi}{2}|u> + \cos\frac{\phi}{2}|d>\right), \end{aligned} \tag{3.51}$$

where $\cos\phi = \frac{X}{\sqrt{X^2+Y^2}}$ and $\sin\phi = \frac{Y}{\sqrt{X^2+Y^2}}$. Although Eq. (3.51) are legitimate eigenstates of Eq. (3.46), they are not single valued, for example, on the unit circle enclosing $\mathbf{R}=0$. To make the eigenstates single valued, we take advantage of the freedom of multiplying them by

[3] If $\mathbf{R}(t)$ sweeps through a full circuit, we need to choose the phase factors so that $|\psi_\pm(\mathbf{R}(t))>$ are not only differentiable but also single valued.

a phase factor. For example

$$\begin{aligned} |\psi_+(\mathbf{R}(t))> &= e^{i\phi(t)/2}\left(\cos\frac{\phi(t)}{2}|u> + \sin\frac{\phi(t)}{2}|d>\right) \\ |\psi_-(\mathbf{R}(t))> &= e^{i\phi(t)/2}\left(-\sin\frac{\phi(t)}{2}|u> + \cos\frac{\phi(t)}{2}|d>\right). \end{aligned} \tag{3.52}$$

are single-valued. Now it is simple to show that

$$\begin{aligned} <\psi_+(\mathbf{R}(t))|\frac{\nabla_{\mathbf{R}}}{i}|\psi_+(\mathbf{R}(t))> &= \frac{1}{2}\nabla_{\mathbf{R}}\phi(t) \\ <\psi_-(\mathbf{R}(t))|\frac{\nabla_{\mathbf{R}}}{i}|\psi_-(\mathbf{R}(t))> &= \frac{1}{2}\nabla_{\mathbf{R}}\phi(t). \end{aligned} \tag{3.53}$$

As the result

$$\begin{aligned} \oint_{\mathcal{C}} d\mathbf{R}\cdot[<\psi_+(\mathbf{R}(t))|\frac{\nabla_{\mathbf{R}}}{i}|\psi_+(\mathbf{R}(t))>] &= \pi \quad or \quad 0 \\ \oint_{\mathcal{C}} d\mathbf{R}\cdot[<\psi_-(\mathbf{R}(t))|\frac{\nabla_{\mathbf{R}}}{i}|\psi_-(\mathbf{R}(t))>] &= \pi \quad or \quad 0 \end{aligned} \tag{3.54}$$

depending on whether ϕ went through a 2π loop.

In the above we stated Berry's theorem without proof. The proof of it will be presented in chapter 5, after we have discussed the perturbation theory.

Although we demonstrate Berry's theorem using a simple 2-state problem as example, it turns out that we have actually covered the most general case. This is because any real symmetric matrix can be written as

$$M = \lambda_u|u><u| + \lambda_d|d><d| + \text{ rest.} \tag{3.55}$$

Since it is the first two terms that becomes "singular" at the degeneracy point, we can simply concentrate on them.

3.6 A few words on the many spin problem

In the above we have seen the Hamiltonian of a single electron spin in external magnetic field. In reality such an electron also have orbital degrees of freedom, i.e., the electron also moves around. However

in condensed-matter physics there exists a insulating electronic state where each electron localizes within a crystalline unit cell so that the electron spin is the only dynamic freedom. A famous example is the host compound of high-temperature superconductivity La_2CuO_4. A caricature of this system is square lattices stacked in the third direction where on each lattice site sits an electron carrying a spin. It turns out that the coupling between adjacent planes turns is very weak so that we can think of one plane at a time. The Hamiltonian governing such a system is given by the so-called Heisenberg model

$$H = J \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{3.56}$$

Here i and j labels sites of a square lattice. The question is what is the ground state of such Hamiltonian, and what are its properties.

Until today this problem has not been exactly solved. The difficulty of solving such a problem lies in the size of the Hilbert space. Since each spins can be in either the "up" or "down" states, and since there is a spin on each lattice site, the dimension of the Hilbert space is 2^N where N is the number of lattice sites. Thus to exactly solved the problem we need to find the lowest eigenvector of a $2^N \times 2^N$ matrix. Remember that $2^10 \sim 10^3$, it is not surprising that we have not been able to diagonalize such a Hamiltonian with N much greater than that. In reality, of course, $N \sim 10^{23}$.

The above simple example illustrate the difficulty of many-body problems – they have exponentially large Hilbert spaces.

3.7 A spinless particle moving in external potential

As we learned in elementary quantum mechanics the Hilbert space of a spinless single particle is spanned by $\{|\mathbf{x}>\}$ where $\mathbf{x}$ is the position of the particle. Such basis set is constructed out of the eigenstates of the position operator $\mathbf{X}$. Indeed,

$$\mathbf{X}|\mathbf{x}>=\mathbf{x}|\mathbf{x}> . \tag{3.57}$$

Under this basis the matrix correspond to the position operator is

$$\mathbf{X} \leftrightarrow X(\mathbf{x}, \mathbf{x}') = \mathbf{x}\delta(\mathbf{x} - \mathbf{x}'). \tag{3.58}$$

The momentum operator $\mathbf{P}$ of the particle does not commute with the position operator:

$$[X_\alpha, P_\beta] = i\hbar\delta_{\alpha\beta}. \tag{3.59}$$

Sandwich the above equation between $< \mathbf{x}'|$ and $|\mathbf{x} >$ we obtain

$$(x'_\alpha - x_\alpha) < \mathbf{x}'|P_\beta|\mathbf{x} >= i\hbar\delta_{\alpha\beta} < \mathbf{x}'|\mathbf{x} >= i\hbar\delta_{\alpha\beta}\delta(\mathbf{x}' - \mathbf{x}). \tag{3.60}$$

As the result[4]

$$< \mathbf{x}'|P_\beta|\mathbf{x} >= \frac{i\hbar\delta(\mathbf{x}' - \mathbf{x})}{x'_\beta - x_\beta} = \frac{\hbar}{i}\frac{\partial}{\partial x_\beta}\delta(\mathbf{x}' - \mathbf{x}). \tag{3.61}$$

Thus under the basis $\{|\mathbf{x} >\}$

$$\begin{aligned} X_\alpha &= x_\alpha \\ P_\beta &= \frac{\hbar}{i}\frac{\partial}{\partial x_\beta}. \end{aligned} \tag{3.62}$$

Like $\{|\mathbf{x} >\}$ an equally good basis set is the momentum eigenstates $\{|\mathbf{k} >\}$. Each $|\mathbf{k} >$ satisfies

$$\mathbf{P}|\mathbf{k} >= \hbar\mathbf{k}|\mathbf{k} > . \tag{3.63}$$

Such a state can be expressed as linear combination of the position eigenstates as

$$|\mathbf{k} >= \int d^3x\phi_{\mathbf{k}}(\mathbf{x})|\mathbf{x} > . \tag{3.64}$$

here

$$|\phi_{\mathbf{k}}(\mathbf{x}) >=< \mathbf{x}|\mathbf{k} >, \tag{3.65}$$

satisfies

$$\frac{\hbar}{i}\nabla\phi_{\mathbf{k}}(\mathbf{x}) = \hbar\mathbf{k}\phi_{\mathbf{k}}(\mathbf{x}). \tag{3.66}$$

[4] $\lim_{\delta\to 0}\frac{1}{x}\frac{1}{\pi}\frac{\delta}{x^2+\delta^2} = \delta'(x)$.

The solution of the above equation is

$$\phi_{\mathbf{k}}(\mathbf{x}) \sim e^{i\mathbf{k}\cdot\mathbf{x}}. \tag{3.67}$$

Such wavefunction is commonly referred to as a "plane wave". It is normalizable assuming we impose the "periodic box boundary condition". In that case the normalization factor is the volume L^3 of the box, and the momentum eigenvalue become quantized

$$\mathbf{k} = \frac{2\pi}{L}(n_x, n_y, n_z). \tag{3.68}$$

It is worth noting that in the limit of infinite volume

$$\frac{1}{L^3}\sum_{n_x,n_y,n_z} = \int \frac{d^3k}{(2\pi)^3}. \tag{3.69}$$

The Hamiltonian for a particle moving in external potential is

$$H = \frac{P^2}{2m} + U(\mathbf{X}). \tag{3.70}$$

Under the basis $\{|\mathbf{x}>\}$ it reads

$$H = -\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{x}). \tag{3.71}$$

3.8 Simple harmonic oscillator

The potential of a simple harmonic oscillator is

$$U(\mathbf{x}) = \frac{K}{2}|\mathbf{x}|^2. \tag{3.72}$$

In component for the Hamiltonian of such a system read

$$H = \sum_{\alpha=1}^{3}[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_\alpha^2} + \frac{K}{2}x_\alpha^2]. \tag{3.73}$$

Since Eq. (3.73) is the sum of three independent one-dimensional simple harmonic oscillator Hamiltonian, it is sufficient to concentrate on such a problem

$$H_{1d} = \frac{P^2}{2m} + \frac{K}{2}x^2. \tag{3.74}$$

In the above $P = \frac{\hbar}{i}\frac{\partial}{\partial x}$.

It is instructive to factorize H as follow

$$H = \left(\frac{P}{\sqrt{2m}} + i\sqrt{\frac{K}{2}}x\right)\left(\frac{P}{\sqrt{2m}} - i\sqrt{\frac{K}{2}}x\right) + \frac{i}{2}\sqrt{\frac{K}{m}}[P, x]. \tag{3.75}$$

Since $[P, x] = -i\hbar$ the above reduces to

$$H = \left(\frac{P}{\sqrt{2m}} + i\sqrt{\frac{K}{2}}x\right)\left(\frac{P}{\sqrt{2m}} - i\sqrt{\frac{K}{2}}x\right) + \frac{\hbar}{2}\sqrt{\frac{K}{m}}. \tag{3.76}$$

Let us look at the operators $\left(\frac{P}{\sqrt{2m}} + i\sqrt{\frac{K}{2}}x\right)$ and $\left(\frac{P}{\sqrt{2m}} - i\sqrt{\frac{K}{2}}x\right)$. First we notice that they are the hermitian conjugate of each other. Second let us see whether they commute

$$[\left(\frac{P}{\sqrt{2m}} - i\sqrt{\frac{K}{2}}x\right), \left(\frac{P}{\sqrt{2m}} + i\sqrt{\frac{K}{2}}x\right)] = i\sqrt{\frac{K}{m}}[P, x] = \hbar\sqrt{\frac{K}{m}}. \tag{3.77}$$

Thus if we define

$$\begin{aligned} a &\equiv \left(\hbar\sqrt{\frac{K}{m}}\right)^{-1/2}\left(\frac{P}{\sqrt{2m}} - i\sqrt{\frac{K}{2}}x\right) \\ a^+ &\equiv \left(\hbar\sqrt{\frac{K}{m}}\right)^{-1/2}\left(\frac{P}{\sqrt{2m}} + i\sqrt{\frac{K}{2}}x\right) \end{aligned} \tag{3.78}$$

we have

$$[a, a^+] = 1, \tag{3.79}$$

and

$$H = \hbar\Omega[a^+a + \frac{1}{2}]. \tag{3.80}$$

In the above

$$\Omega \equiv \sqrt{\frac{K}{m}} \tag{3.81}$$

is the classical vibrational frequency of the oscillator.

Thus in order to diagonalize H we have to find all eigenstates of a^+a. First we prove that all eigenvalues of this operator are greater or equal to zero. Let $|\lambda>$ be an eigenstate of a^+a with eigenvalue λ, thus

$$\lambda =< \lambda|a^+a|\lambda >=< \phi|\phi > \quad \geq 0 \quad \text{where} \quad |\phi >= a|\lambda > . \tag{3.82}$$

Next using Eq. (3.79) it is simple to prove that given a eigenstate $|\lambda>$ with eigenvalue λ, $a^+|\lambda>$ is an eigenstate with eigenvalue $\lambda+1$ and $a|\lambda>$ is an eigenstate with eigenvalue $\lambda-1$. In this way we can "raise" and "lower" the eigenvalues as we wish. If the lowering process can be continued without end, then negative eigenvalues will be generated eventually, which violates Eq. (3.82). As the result there must exist an eigenstate $|0>$ which upon acting by a vanishes

$$a|0 >= 0. \tag{3.83}$$

By Eq. (3.83) such state satisfies

$$a^+a|0 >= 0|0 > . \tag{3.84}$$

which means that it is a state of zero eigenvalue.

The above arguments prove that the eigenvalues of a^+a are all non-negative integers and a tower of eigenstates can be generated by operating a^+ on each states satisfying Eq. (3.83).

Next we show that there is only one state satisfying Eq. (3.83) and explicitly find it. Let us expand $|0>$ in terms of the basis set $\{|x>\}$

$$|0 >= \int dx\phi_0(x)|x > . \tag{3.85}$$

In the above $\phi_0(x) =< x|0 >$ is what we call the wavefunction associated with $|0>$. By taking the scalar product of Eq. (3.83) with $< x|$ we find

$$\int dx' < x|a|x >< x'|0 >= 0, \tag{3.86}$$

or

$$\left(\hbar\sqrt{\frac{K}{m}}\right)^{-1/2}\left(\frac{1}{\sqrt{2m}}\frac{\hbar}{i}\frac{\partial}{\partial x} - i\sqrt{\frac{K}{2}}x\right)\phi_0(x) = 0, \tag{3.87}$$

or

$$\left(\frac{\partial}{\partial x}+\frac{\sqrt{mK}}{\hbar}x\right)\phi_0(x)=0. \tag{3.88}$$

Eq. (3.88) has a unique normalizable solution

$$\phi_0(x)=\frac{1}{\sqrt{\mathcal{N}}}e^{-\frac{x^2}{2l_0^2}}, \tag{3.89}$$

where $\frac{1}{l_0^2}\equiv\frac{\sqrt{mK}}{\hbar}$, and $\mathcal{N}$ is the normalization factor. By requiring $\int dx|\phi_0(x)|^2=1$ we find $\mathcal{N}=\sqrt{\pi}l_0$, thus

$$\phi_0(x)=\frac{1}{\sqrt{\sqrt{\pi}l_0}}e^{-\frac{x^2}{2l_0^2}}. \tag{3.90}$$

The eigenfunctions of a^+a with larger eigenvalues can all be generated from $\phi_0(x)$ as follow

$$\phi_n(x)\sim\left(\frac{1}{\sqrt{2m}}\frac{\hbar}{i}\frac{\partial}{\partial x}+i\sqrt{\frac{K}{2}}x\right)^n\phi_0(x). \tag{3.91}$$

Thus from $|0>$ we can generate a tower of eigenstates of Eq. (3.80), namely

$$H(a^+)^n|0>=(n+\frac{1}{2})\hbar\Omega(a^+)^n|0>. \tag{3.92}$$

However it is important to note that the norm of $(a^+)^n|0>$ is not one. In fa ct let $|n>$ be the normalized nth state of H, then

$$\begin{aligned}|n+1>&=\frac{1}{\sqrt{n+1}}a^+|n>\\ |n-1>&=\frac{1}{\sqrt{n}}a|n>.\end{aligned} \tag{3.93}$$

Thus the normalized eigenstates are

$$|0>,\ a^+|0>,\ \frac{1}{\sqrt{2!}}(a^+)^2|0>,\ \frac{1}{\sqrt{3!}}(a^+)^3|0>,\ \text{etc.} \tag{3.94}$$

Physically a^+ and a "creates" and "annihilates" the excitation quanta of the simple harmonic oscillator, and a^+a counts them. From this point of view the ground state $|0>$ is the vacuum of the oscillation quantum. Let me summarize the above discussion in the following table

	coordinate space	oscillation quanta
Hamiltonian	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{K}{2}x^2$	$\hbar\Omega(a^+a+\frac{1}{2})$
Ground state	$\sim e^{-\frac{x^2}{2l_0^2}}$	$\|0>$
Excited state	$\sim\left(\frac{1}{\sqrt{2m}}\frac{\hbar}{i}\frac{\partial}{\partial x}+i\sqrt{\frac{K}{2}}x\right)^n e^{-\frac{x^2}{2l_0^2}}$	$\sim (a^+)^n\|0>$

After we understood the one-dimensional simple harmonic oscillator it is trivial to understand the three-dimensional one. The Hamiltonian is given by

$$H=\hbar\Omega(a_x^+a_x+a_y^+a_y+a_z^+a_z+\frac{3}{2}), \tag{3.95}$$

and the eigenstates are now labeled by three integers ($|n_x,n_y,n_z>$) correspond to the number of oscillation quanta in x,y,z direction respectively.

3.9 The coherent state

The peculiar state

$$|\phi>\equiv e^{\phi a^+}|0>, \tag{3.96}$$

where ϕ is a complex scalar is the eigenstate of a, and

$$a|\phi>=\phi|\phi>. \tag{3.97}$$

To prove the above equation we note that

$$[a,f(a^+)]=f'(a^+), \tag{3.98}$$

and that $f(a^+)a|0>=0$. The state in Eq. (3.96) is called the coherent state. Physically it correspond to the state in which the oscillation quanta (Bose particles) of the harmonic oscillator have condensed. It is simple to show that the norm of Eq. (3.96) is $e^{|\phi|^2}$, and

$$<\phi'|\phi>=e^{\phi'^*\phi}. \tag{3.99}$$

Moreover

$$\int \frac{d\phi}{\pi} e^{-|\phi|^2} |\phi >< \phi| = I. \tag{3.100}$$

3.10 The hydrogen atom

The central triumph of early quantum mechanics is the ability to solve the hydrogen atom problem exactly. The hydrogen atom consists of two particles, a proton and an electron. The Hamiltonian for this problem is given by

$$H = -\frac{\hbar^2}{2M}\nabla_X^2 - \frac{\hbar^2}{2m}\nabla_x^2 - \frac{e^2}{|\mathbf{X}-\mathbf{x}|}. \tag{3.101}$$

In the above M and m are the proton and electron mass respectively, and $\mathbf{X}$ and $\mathbf{x}$ are the proton and electron coordinate.

Due to the fact that the center of mass experiences no force we make the following coordinate transformation

$$\mathbf{x}, \quad \mathbf{X} \to \mathbf{R} \equiv \frac{m}{m+M}\mathbf{x} + \frac{M}{m+M}\mathbf{X}, \quad \mathbf{r} \equiv \mathbf{x} - \mathbf{X}. \tag{3.102}$$

In terms of the new coordinate the Hamiltonian read

$$H = -\frac{\hbar^2}{2(M+m)}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{r}. \tag{3.103}$$

The eigen wavefunction of Eq. (3.103) is obviously of the form

$$e^{\mathbf{k}} \cdot \mathbf{R}\psi(\mathbf{r}). \tag{3.104}$$

The eigen energy is the sum of $\frac{\hbar^2 k^2}{2(M+m)}$ and E where

$$\left[-\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{r}\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{3.105}$$

(Here $\mu = \frac{Mm}{M+m}$)

To solve Eq. (3.105) we relies on the symmetry reduction. Since the Hamiltonian in Eq. (3.105) is invariant under the spatial rotation, the

eigen function can be chosen as eigen functions of the angular momentum operator L^2 and L_z, i.e.

$$\begin{aligned} L^2\psi(r,\theta,\phi) &= \hbar^2 l(l+1)\psi(r,\theta,\phi) \\ L_z\psi(r,\theta,\phi) &= m\hbar\psi(r,\theta,\phi). \end{aligned} \tag{3.106}$$

Since in general we can write

$$\psi_{Elm}(r,\theta,\phi) = \sum_{l'} \sum_{m'=-l'}^{l'} R_{El'm'}(r) Y_{l'm'}(\theta,\phi), \tag{3.107}$$

the above symmetry argument suggests that $R_{Elm} \neq 0$ for only $l' = l$ and $m' = m$.

Thus without loosing any generality we can write

$$\psi_{E,l,m}(\mathbf{r}) = R_{Elm}(r) Y_{lm}(\theta,\phi). \tag{3.108}$$

Recall Eq. (4.54) and the fact that

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2}, \tag{3.109}$$

we have, by Eq. (3.106)

$$\left[-\frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{e^2}{r}\right] R_{Elm}(r) = E R_{Elm}(r). \tag{3.110}$$

Since the left hand side of Eq. (3.110) does not depend on m we conclude

$$R_{Elm}(r) \to R_{El}(r). \tag{3.111}$$

Eq. (3.110) can be solved by brute force power series techniques under the boundary condition that R is finite at $r = 0$ and $\int 4\pi r^2 R^2(r) dr = finite$.[5] Here we review the solution. First we let

$$\begin{aligned} E &\to E\frac{me^4}{2\hbar^2} \\ r &\to \frac{\hbar^2}{me^2} r. \end{aligned} \tag{3.112}$$

[5]This boundary condition limits us to finding the bound state solution.

In terms of the new E and r the equation read

$$\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{l(l+1)}{r^2}-\frac{2}{r}\right]R_{Elm}(r)=E'R_{Elm}(r). \tag{3.113}$$

Let

$$R_{El}(r)\equiv\frac{u_{El}(r)}{r}. \tag{3.114}$$

The boundary condition requires that $u_{El}(r)\to 0$ for both $r\to 0$ and $r\to\infty$.

The differential equation that u_{El} satisfies is

$$\frac{d^2u_{El}}{dr^2}+\left[E+\frac{2}{r}-\frac{l(l+1)}{r^2}\right]u_{El}=0. \tag{3.115}$$

In the limit of large r the above equation reduces to

$$\frac{d^2u_{El}}{dr^2}+Eu_{El}=0. \tag{3.116}$$

As the result

$$u_{El}(r)\to e^{\pm\sqrt{|E|}r}\quad as\quad r\to\infty. \tag{3.117}$$

In the above $+$ applies to the case of $E>0$ and $-$ to $E<0$. As the result the asymptotic equation has decaying solutions only when $E<0$. For $r\to 0$ Eq. (3.115) approaches

$$\frac{d^2u_{El}}{dr^2}-\frac{l(l+1)}{r^2}u_{El}=0. \tag{3.118}$$

As the result we expect

$$u_{El}(r)\to r^{l+1}\quad as\quad r\to 0. \tag{3.119}$$

Thus we write

$$u(r)=w(r)e^{-\sqrt{|E|}r}, \tag{3.120}$$

and expect $w(r)\to r^{l+1}$ as $r\to 0$. The Equation that w satisfies is

$$w''-2\sqrt{|E|}w'+\left(\frac{2}{r}-\frac{l(l+1)}{r^2}\right)w=0. \tag{3.121}$$

Eq. (3.121) can be solved by means of a power series in r, beginning with a term in r^{l+1}, thus

$$w(r) = \sum_{k=l+1}^{\infty} c_k r^k. \tag{3.122}$$

Substitute Eq. (3.122) into Eq. (3.121) we obtain the recursion relation

$$c_{k+1} = 2\left[\frac{k\sqrt{|E|-1}}{k(k+1)-l(l+1)}\right] c_k. \tag{3.123}$$

The above recursion relation dictates that as $k \to \infty$

$$\frac{c_{k+1}}{c_k} \to 2\frac{\sqrt{|E|}}{(k+1)}. \tag{3.124}$$

If this ratio holds then w behaves, for large r, as $e^{2\sqrt{|E|}r}$. In that case u is not bounded. Exception occurs when the series Eq. (3.123) is broken off at some value of k. This means that

$$\sqrt{|E|} = \frac{1}{k}, \quad or \quad E = -\frac{1}{k^2}, \tag{3.125}$$

which in original unit means that

$$E = -\frac{\mu e^4}{2\hbar^2 k^2}, \quad k = l+1, ... \tag{3.126}$$

3.11 Feynman path integrals

In this section we focus on a particle moving in one-dimension under potential $U(x)$. At the end of the section we will generalize the result to three dimensions.

Suppose the particle is in the position eigenstate $|x>$ at $t = 0$, according to the Schrödinger equation it should be in the state

$$e^{-\frac{i}{\hbar}tH}|x>, \tag{3.127}$$

at time t. Thus the probability amplitude that such particle will be in the position eigenstate $|x'>$ is

$$G(x',t;x,0) =< x'|e^{-\frac{i}{\hbar}tH}|x> . \tag{3.128}$$

Following Feynman, in the following we develop a means to compute such quantity.

Let us split the time elapse into N infinitesimal pieces

$$e^{-\frac{i}{\hbar}tH} = e^{-\frac{i}{\hbar}\epsilon H}...e^{-\frac{i}{\hbar}\epsilon H}. \tag{3.129}$$

In the above $\epsilon = t/N$. Thus Eq. (3.128) becomes

$$G(x',t;x,0) =< x'|e^{-\frac{i}{\hbar}\epsilon H}...e^{-\frac{i}{\hbar}\epsilon H}|x> . \tag{3.130}$$

Next we insert the identity operator

$$I = \int dy|y >< y| \tag{3.131}$$

between two adjacent time evolution operator to get

$$G(x',t;x,0) = \int \prod_{i=1}^{N-1} dy_i < x'|e^{-\frac{i}{\hbar}\epsilon H}|y_{N-1} >< y_{N-1}|...|y_1 >< y_1|e^{-\frac{i}{\hbar}\epsilon H}|x> . \tag{3.132}$$

Next we compute

$$< y_{i+1}|e^{-\frac{i}{\hbar}\epsilon H}|y_i >=< y_{i+1}|e^{-\frac{i}{\hbar}\epsilon\frac{P^2}{2m}}e^{-\frac{i}{\hbar}\epsilon U(x)}|y_i> . \tag{3.133}$$

A word of caution should be given here. In general

$$e^{A+B} \neq e^A e^B. \tag{3.134}$$

The equality holds when $[A,B] = 0$. Since $[\epsilon\frac{P^2}{2m}, \epsilon U(x)] = O(\epsilon^2)$ they can be regarded as commutative as $\epsilon \to 0$. Since $|y_i>$ are the eigenstate of the position operator Eq. (3.133) becomes

$$< y_{i+1}|e^{-\frac{i}{\hbar}\epsilon H}|y_i >=< y_{i+1}|e^{-\frac{i}{\hbar}\epsilon\frac{P^2}{2m}}|y_i > e^{-\frac{i}{\hbar}\epsilon U(y_i)}. \tag{3.135}$$

Now

$$\begin{aligned} < y_{i+1}|e^{-\frac{i}{\hbar}\epsilon\frac{P^2}{2m}}|y_i > \quad &= \int \frac{dp}{(2\pi)} < y_{i+1}|p > e^{-\frac{i}{\hbar}\epsilon\frac{\hbar^2p^2}{2m}} < p|y_i > \\ &= \int \frac{dp}{(2\pi)} e^{ip(y_{i+1}-y_i)} e^{-\frac{i}{\hbar}\epsilon\frac{\hbar^2p^2}{2m}} \\ &= \int \frac{dp}{(2\pi)} e^{-\frac{i}{\hbar}\epsilon\frac{\hbar^2}{2m}(p-m\frac{y_{i+1}-y_i}{\epsilon\hbar})^2} e^{\frac{i}{\hbar}\epsilon\frac{m}{2}\left(\frac{y_{i+1}-y_i}{\epsilon}\right)^2} \\ &\propto e^{\frac{i}{\hbar}\epsilon\frac{m}{2}\left(\frac{y_{i+1}-y_i}{\epsilon}\right)^2}. \end{aligned} \tag{3.136}$$

Thus

$$< y_{i+1}|e^{-\frac{i}{\hbar}\epsilon H}|y_i > \propto e^{\frac{i}{\hbar}\epsilon\frac{m}{2}\left(\frac{y_{i+1}-y_i}{\epsilon}\right)^2} e^{-\frac{i}{\hbar}\epsilon U(y_i)}. \tag{3.137}$$

Thus

$$G(x',x;t,0) \propto \int_{y_0=x;y_N=x'} \prod_{i=0}^{N} dy_i e^{\frac{i}{\hbar}\epsilon[\frac{m}{2}\left(\frac{y_{i+1}-y_i}{\epsilon}\right)^2 - U(y_i)]}. \tag{3.138}$$

In the limit $\epsilon \to 0$ we have

$$\begin{aligned} G(x',x;t,0) &\propto \int_{y(0)=x;y(t)=x'} D[y(\tau)] e^{\frac{i}{\hbar}S[y(\tau)]} \\ S[y(\tau)] &= \int_0^t d\tau [\frac{m}{2}\dot{y(\tau)}^2 - U(y(\tau))]. \end{aligned} \tag{3.139}$$

Physically Eq. (3.139) depicts a sum over all possible "path" of the particle leading from $y = x$ at $\tau = 0$ to $y = x'$ at $\tau = t$ where each path is weighted by the phase factor $e^{\frac{i}{\hbar}S[y(\tau)]}$.

Eq. (3.139) can easily be generalized to three-dimension

$$\begin{aligned} G(\mathbf{x}',\mathbf{x};t,0) &\propto \int_{\mathbf{y}(0)=\mathbf{x};\mathbf{y}(t)=\mathbf{x}'} D[\mathbf{y}(\tau)] e^{\frac{i}{\hbar}S[\mathbf{y}(\tau)]} \\ S[\mathbf{y}(\tau)] &= \int_0^t d\tau [\frac{m}{2}|\dot{\mathbf{y}}(\tau)|^2 - U(\mathbf{y}(\tau))]. \end{aligned} \tag{3.140}$$

3.12 Classical approximation

In the limit $\hbar \to 0$, the contribution to $G(\mathbf{x}', t; \mathbf{x}, 0)$ entirely comes from the stationary path $\mathbf{y}_c(\tau)$ which satisfies

$$\frac{\delta S[\mathbf{y}(\tau)]}{\delta \mathbf{y}(\tau)} = 0, \tag{3.141}$$

and

$$\mathbf{y}_c(0) = \mathbf{x}, \quad \mathbf{y}_c(t) = \mathbf{x}'. \tag{3.142}$$

The left hand side of Eq. (3.141) is called the "functional derivative" of S. One way to perform such derivative it is best to imagine discretize $\mathbf{y}(\tau)$ into $\mathbf{y}_j = \mathbf{y}(j\epsilon)$ and simply perform the ordinary partial differentiation. After that is done take the $\epsilon \to 0$ limit of the result. Another way is to imagine deform the path

$$\mathbf{y}(\tau) \to \mathbf{y}(\tau) + \delta\mathbf{y}(\tau). \tag{3.143}$$

(In order to fulfill Eq. (3.142) we must have $\delta\mathbf{y}(0) = \delta\mathbf{y}(t) = 0$.) To linear order in $\delta\mathbf{y}(\tau)$ the change in action due to such deformation is

$$\begin{aligned} \delta S &= \int_0^t d\tau [m\dot{\mathbf{y}}(\tau) \cdot \delta\dot{\mathbf{y}}(\tau) - \nabla U(\mathbf{y}(\tau)) \cdot \delta\mathbf{y}(\tau)] \\ &= \int_0^t d\tau \delta\mathbf{y}(\tau) \cdot [-m\ddot{\mathbf{y}}(\tau) - \nabla U(\mathbf{y}(\tau))] \end{aligned} \tag{3.144}$$

$\frac{\delta S[\mathbf{y}(\tau)]}{\delta \mathbf{y}(\tau)}$ is defined as

$$\frac{\delta S[\mathbf{y}(\tau)]}{\delta \mathbf{y}(\tau)} = -m\ddot{\mathbf{y}}(\tau) - \nabla U(\mathbf{y}(\tau)). \tag{3.145}$$

Thus Eq. (3.141) implies

$$m\ddot{\mathbf{y}} = -\nabla U(\mathbf{y}), \tag{3.146}$$

which is the Newton equation. Thus $\mathbf{y}_c(\tau)$ is the solution of Newton equation under the condition $\mathbf{y}_c(0) = \mathbf{x}$ and $\mathbf{y}_c(t) = \mathbf{x}'$.

It is quite satisfactory that in the limit of vanishing $\hbar$ the contribution to the path integral in Eq. (3.139) entirely comes from the classical path.

Once we obtained $G(\mathbf{x}', t; \mathbf{x}, 0)$ we can obtain the time-dependent wavefunction easily. Assume that the system is initially in state $|\psi>$, upon time evolution it becomes

$$|\psi(t)>= e^{-\frac{i}{\hbar}tH}|\psi>=\int d^3x' e^{-\frac{i}{\hbar}tH}|\mathbf{x}'><\mathbf{x}'|\psi> . \tag{3.147}$$

Thus

$$\psi(\mathbf{x}, t) = \int d^3x' G(\mathbf{x}, t; \mathbf{x}'0)\psi(\mathbf{x}'). \tag{3.148}$$

3.13 Quantum statistical mechanics as Feynman path integrals in imaginary time

Like in classical statistical mechanics the partition function

$$\mathcal{Z} = \sum_a < a|e^{-\beta H}|a >, \tag{3.149}$$

is of central importance in quantum statistical mechanics. In the above $\{|a>\}$ is any orthonormal basis. In the special case of single particle moving external potential we can take $|a>$ as the position eigenstates. Thus

$$\mathcal{Z} = \int d^3x < \mathbf{x}|e^{-\beta H}|\mathbf{x} > . \tag{3.150}$$

Compare with Eq. (3.139) we can view the partition function as the integral over the imaginary time Feynman amplitude:

$$\mathcal{Z} \sim \int d^3x G(x, i\hbar\beta; x, 0). \tag{3.151}$$

3.14 From classical to quantum mechanics

3.14.1 Route I

The above exercise suggest the following passage from classical to quantum mechanics:

	Classical	Quantum
Action	$S = \int dt L[q_j(\tau), \dot{q}_j(\tau)]$	$S = \int dt L[q_j(\tau), \dot{q}_j(\tau)]$
Dynamics	$\delta S[q_j(\tau)]/\delta q_k(\tau) = 0$ + initial and final condition $\rightarrow$ classical path	Probability amplitude $\propto \int_{q_j(0)=q_j; q_j(t)=q'_j} D[q_j(\tau)]$ $e^{\frac{i}{\hbar}S[q_j(\tau)]}$

3.14.2 Route II

This alternative route to quantum mechanics is referred to as the "canonical quantization procedure".

	Classical	Quantum
Action	$S = \int dt L[q_j(\tau), \dot{q}_j(\tau)]$	$S = \int dt L[q_j(\tau), \dot{q}_j(\tau)]$
Hamiltonian	$H(p_j, q_j) = \sum_j p_j \dot{q}_j - L(q_j, \dot{q}_j)$ where $\dot{q}_j$ is substituted by p's via $p_k = \partial L[q_j, \dot{q}_j]/\partial \dot{q}_k$	same expression $H(p_j, q_j)$ plus the commutation relation $[q_j, p_k] = i\hbar\delta_{jk}$
Dynamics	$\dot{q}_k = \partial H/\partial p_k$ $\dot{p}_k = -\partial H/\partial q_k$	$e^{-\frac{i}{\hbar}tH}$ is the time-evolution operator

We will omit the proof but it is straightforward to show that these two routes are equivalent. With route II it is possible to write down the quantum Hamiltonian knowing the classical one.

3.15 Quantum dynamics in the presence of electromagnetic field

Electromagnetic field affects the dynamics of a charged particles. let A_0 and $\mathbf{A}$ be the scalar and vector potential, i.e.

$$\begin{aligned} \mathbf{E} &= -\nabla A_0 - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} \\ \mathbf{B} &= \nabla \times \mathbf{A}. \end{aligned} \tag{3.152}$$

The time-dependent Schrödinger equation that the coordinate-space wavefunction of a charge-q particle satisfies is

$$(i\hbar\frac{\partial}{\partial t} - qA_0)\psi(\mathbf{x}, t) = \frac{1}{2m}(\frac{\hbar}{i}\nabla - \frac{q}{c}\mathbf{A})^2\psi(\mathbf{x}, t). \tag{3.153}$$

Compare with the free Schrödinger equation of neutral particle we find the following substitution

$$\begin{aligned}
&\frac{\hbar}{i}\frac{\partial}{\partial t} \to (\frac{\hbar}{i}\frac{\partial}{\partial t} + qA_0) \\
&\frac{\hbar}{i}\nabla \to \frac{\hbar}{i}\nabla - \frac{q}{c}\mathbf{A}.
\end{aligned} \tag{3.154}$$

3.16 Gauge invariance

Eq. (3.153) is invariant under the following transformation

$$\begin{aligned}
&A_0 \to A_0 - \frac{1}{c}\partial_t \Lambda \\
&\mathbf{A} \to \mathbf{A} + \nabla\Lambda \\
&\psi(\mathbf{x}, t) \to e^{i\frac{q}{\hbar c}\Lambda}\psi(x, t).
\end{aligned} \tag{3.155}$$

Eq. (3.155) is called the gauge transformation.

Eq. (3.153) implies that the Hamiltonian of a charged particle is

$$H(t) = \frac{1}{2m}(\frac{\hbar}{i}\nabla - \frac{q}{c}\mathbf{A}(\mathbf{x}, t))^2 + qA_0(\mathbf{x}, t). \tag{3.156}$$

Repeating the derivation of the Feynman propagator

$$G(\mathbf{x}', t; \mathbf{x}, 0) = \int_{\mathbf{y}(0)=\mathbf{x};\mathbf{y}(t)=\mathbf{x}'} D[\mathbf{y}(\tau)]e^{\frac{i}{\hbar}S}, \tag{3.157}$$

where

$$S[\mathbf{y}(\tau)] = \int_0^t d\tau\{\frac{m}{2}|\dot{\mathbf{y}}|^2 - qA_0(\mathbf{y}(\tau)) + \frac{q}{c}\dot{\mathbf{y}}\cdot\mathbf{A}(\mathbf{y}(\tau))\}. \tag{3.158}$$

Eq. (3.158) is the action for a charged particle interacting with the electromagnetic field. The classical equation of motion is

$$\frac{\delta S[\mathbf{y}(\tau)]}{\delta y_\alpha(\tau)} = 0. \tag{3.159}$$

Actual calculation of the left hand side of the above equation gives

$$-m\ddot{y}_\alpha - q\partial_\alpha A_0 - \frac{q}{c}\dot{A}_\alpha + \frac{q}{c}\dot{y}_\beta(\partial_\alpha A_\beta - \partial_\beta A_\alpha) = 0. \tag{3.160}$$

Since

$$\partial_\alpha A_\beta - \partial_\beta A_\alpha = \epsilon_{\alpha\beta\gamma} B_\gamma, \tag{3.161}$$

and

$$E_\alpha = -\partial_\alpha A_0 - \frac{1}{c}\dot{A}_\alpha, \tag{3.162}$$

we have

$$m\ddot{y}_\alpha = -qE_\alpha + \frac{q}{c}\epsilon_{\alpha\beta\gamma}\dot{y}_\beta B_\gamma. \tag{3.163}$$

Restore to the vector form we recover the Lorentz force law

$$m\ddot{\mathbf{y}} = q\mathbf{E} + \frac{q}{c}\dot{\mathbf{y}} \times \mathbf{B}. \tag{3.164}$$

Using Eq. (3.156) as the Hamiltonian we can define the time evolution operator (Eq. (3.10)) $\mathcal{U}(t;0)$ and hence define

$$\begin{aligned} \mathbf{X}_H &= \mathcal{U}(t;0)^+ \mathbf{X} \mathcal{U}(t;0) \mathcal{U}(t;0) \\ \mathbf{P}_H &= \mathcal{U}(t;0)^+ \mathbf{P} \mathcal{U}(t;0) \mathcal{U}(t;0). \end{aligned} \tag{3.165}$$

According to the Heisenberg equation of motion

$$\begin{aligned} \dot{\mathbf{X}}_H &= \frac{i}{\hbar}[H(t)_H, \mathbf{X}_H] = \frac{i}{\hbar}\mathcal{U}(t;0)^+[H(t), \mathbf{X}]\mathcal{U}(t;0) \\ \dot{\mathbf{P}}_H &= \frac{i}{\hbar}[H(t)_H, \mathbf{P}_H] = \frac{i}{\hbar}\mathcal{U}(t;0)^+[H(t), \mathbf{P}]\mathcal{U}(t;0). \end{aligned} \tag{3.166}$$

Let us now compute $[H(t), \mathbf{X}]$,

$$.[H(t), \mathbf{X}] = -\frac{i\hbar}{m}[\mathbf{P} - \frac{q}{c}\mathbf{A}(\mathbf{X}, t)]. \tag{3.167}$$

As the result

$$\dot{\mathbf{X}}_H = \frac{1}{m}[\mathbf{P}_H - \frac{q}{c}\mathbf{A}(\mathbf{X}_H, t)]. \tag{3.168}$$

Next we compute $[H(t), \mathbf{P} - \frac{q}{c}\mathbf{A}(\mathbf{X}, t)]$.

$$\begin{aligned} [H(t), P_\alpha - \frac{q}{c}A_\alpha(\mathbf{X}, t)] \quad &= i\hbar q \partial_\alpha A_0 - i\hbar \frac{q}{2mc}\epsilon_{\alpha\beta\gamma}\{(P_\beta - \frac{q}{c}A_\beta)B_\gamma \\ &\quad + B_\gamma(P_\beta - \frac{q}{c}A_\beta)\}. \end{aligned} \tag{3.169}$$

In the above

$$B_\alpha \equiv \epsilon_{\alpha\beta\gamma}\partial_\beta A_\gamma, \tag{3.170}$$

is an operator itself. Thus

$$m\ddot{X}_{\alpha H} = -q\partial_\alpha A_{0H} - \frac{q}{c}\partial_t A_{\alpha H} + \frac{q}{2c}\epsilon_{\alpha\beta\gamma}(\dot{X}_{\beta H}B_{\gamma H} + B_{\gamma H}\dot{X}_{\beta H}). \tag{3.171}$$

We note that the second term on the righthand side of the above equation is due to the fact that the operator whose time derivative is computed has explicit time dependence. Eq. (3.171) is the quantum version of the Lorentz force law.

3.17 Current conservation

In the Heisenberg picture the operators corresponds to charge density is

$$\rho_H(\mathbf{x}, t) = q\delta(\mathbf{x} - \mathbf{X}_H(t)). \tag{3.172}$$

Note that in the above equation $\mathbf{x}$ is a c-number vector. According to the Heisenberg equation

$$\dot{\rho}_H = \frac{i}{\hbar}[H_H, q\delta(\mathbf{x} - \mathbf{X}_H(t))]. \tag{3.173}$$

Let us compute $[H, q\delta(\mathbf{x} - \mathbf{X})]$.

$$[H, q\delta(\mathbf{x}-\mathbf{X})] = -\frac{q\hbar}{2mi}[(\mathbf{P}-\frac{q}{c}\mathbf{A})\cdot\nabla_x\delta(\mathbf{x}-\mathbf{X})+\nabla_x\delta(\mathbf{x}-\mathbf{X})\cdot(\mathbf{P}-\frac{q}{c}\mathbf{A})]. \tag{3.174}$$

Thus

$$\dot{\rho}_H + \frac{q}{2m}\nabla_x\cdot\{(\mathbf{P}_H - \frac{q}{c}\mathbf{A}_H)\delta(\mathbf{x} - \mathbf{X}_H) + \delta(\mathbf{x} - \mathbf{X}_H)(\mathbf{P}_H - \frac{q}{c}\mathbf{A}_H)\} = 0, \tag{3.175}$$

or

$$\dot{\rho}_H + \frac{q}{2}\nabla_x\cdot\{\dot{\mathbf{X}}_H\delta(\mathbf{x} - \mathbf{X}_H) + \delta(\mathbf{x} - \mathbf{X}_H)\dot{\mathbf{X}}_H\} = 0. \tag{3.176}$$

This suggest that the current operator is given by

$$\mathbf{j}_H(\mathbf{x}, t) = \frac{q}{2}\{\dot{\mathbf{X}}_H\delta(\mathbf{x} - \mathbf{X}_H) + \delta(\mathbf{x} - \mathbf{X}_H)\dot{\mathbf{X}}_H\}. \tag{3.177}$$

3.18 The Aharonov-Bohm effect

To simplify the situation let us consider the case where the space dimension is two. Consider a source of electrons and a pair of slits. On the opposite side of the slits there is a detector screen. In the region between the slits and the screen there is an idea solenoid which confines a magnetic flux Φ perpendicular to the plane.

Let us consider the Feynman amplitude $G(x', t; x, 0)$ given by Eq. (3.157) and Eq. (3.158). The probability that an electron leaving the source $\mathbf{x} = 0$ at $t = 0$ arriving at a spot $\mathbf{x}$ on the screen at time t is given by

$$P(x't; x, 0) = G^*(x', t; x, 0)G(x', t; x, 0)$$
$$\int_{y_1(0)=y_2(0)=x}^{y_1(t)=y_2(t)=x'} D[y_1]D[y_2]e^{\frac{i}{\hbar}\{S[y_1(\tau)]-S[y_2(\tau)]\}}. \tag{3.178}$$

In the above

$$S[y(\tau)] = \int_0^t d\tau\{\frac{m}{2}|\dot{y}|^2 + \frac{q}{c}\dot{y}\cdot A(y(\tau))\}. \tag{3.179}$$

The collection of all possible pairs of path $(y_1(\tau), y_2(\tau))$ can be separated into two categories. For the first type the path $y_1(\tau)$ and the time reversed path $y_2(\tau)$ enclose the solenoid, and for the second type they don't. Let us concentrate on the contribution of the second term to the action

$$\begin{aligned}
&\frac{q}{c}\int_0^2 [\dot{y_1}\cdot A(y_1) - \dot{y_2}\cdot A(y_2)]d\tau \\
&= \frac{q}{c}[\int_{path_1} dy_1\cdot A(y_1) - \int_{path_2} dy_2\cdot A(y_2)] \\
&= \frac{q}{\hbar c}\oint_{\mathcal{C}} d\mathbf{y}\cdot\mathbf{A} \\
&= \frac{q}{\hbar c}\int\int d\mathbf{a}\cdot\nabla\times\mathbf{A} \\
&= \frac{q}{\hbar c}\phi.
\end{aligned} \tag{3.180}$$

In the above $\mathcal{C}$ is the oriented closed curve corresponds to $P_1 - P_2$, and $d\mathbf{a}$ is the oriented area element (using the right-handed rule) of

the surface enclosed by $\mathcal{C}$, and ϕ is magnetic flux passing through the surface.

Thus if (P_1, P_2) belongs to the first category, $\phi = \pm\Phi$ and if (P_1, P_2) belongs to the second category $\phi = 0$. In order to calculate the contribution of the two family of pairs of path we define a pair reference paths P and P'. First we choose P_a and P_b so that (P_a, P_b) is a pair in the first category.

Now let us calculate the contribution of the second category to the probability. It is apparent that this contribution is of the form

$$[\sum_{P,(P,P_a)\in 2nd\ cat} e^{i\theta_P}][\sum_{P',(P',P_a)\in 2nd\ cat} e^{-i\theta_{P'}}] + [\sum_{P,(P,P_b)\in 2nd\ cat} e^{i\theta_P}][\sum_{P',(P',P_b)\in 2nd\ cat} e^{-i\theta_{P'}}]$$
$$= |A|^2 + |B|^2. \tag{3.181}$$

As to the first category

$$\int_{1st\ category} D[y_1, y_2] e^{\frac{i}{\hbar}(S[y_1]-S[y_2])} = \left(\sum e^{i\theta_{12}}\right) e^{i\frac{q}{\hbar c}\Phi} + c.c. = 2|C|^2 \cos\left(\delta + \frac{q}{\hbar c}\Phi\right) \tag{3.182}$$

Thus

$$P(x', t; x, 0) \sim |A|^2 + |B|^2 + 2|C|^2 \cos\left(\delta + \frac{q}{\hbar c}\Phi\right). \tag{3.183}$$

Thus every time

$$\Phi = n\frac{hc}{q} \tag{3.184}$$

the interference pattern repeats.

3.19 Magnetic monopole

In ordinary electricity and magnetism there are free electric charges (electric monopoles) but no free magnetic charges (magnetic monopole). There is no physical principle that prohibit the existence of magnetic monopole. However they simply do not occur - no one has ever made an observation of a magnetic monopole. Despite of this, interest in magnetic monopoles has appeared and reappeared over the years. If the magnetic monopole exist then the following modification of the Maxwell equation is necessary

$$\nabla \cdot \mathbf{E} = 4\pi\rho_e$$
$$\nabla \cdot \mathbf{B} = 4\pi\rho_m$$
$$\nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = -\frac{4\pi}{c}\mathbf{j}_m$$
$$\nabla \times \mathbf{B} - \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} = \frac{4\pi}{c}\mathbf{j}_e. \tag{3.185}$$

In the above $\rho_e, \mathbf{j}_e$ and $\rho_m, \mathbf{j}_m$ are the density and current of electric charge and magnetic monopole respectively.

One immediate consequence of the existence of monopole is that the vector potential can not be defined everywhere. This is because if $\mathbf{B} = \nabla \times \mathbf{A}$ necessitate the equality $\nabla \cdot \mathbf{B} = 0$.

In the following we look more closely at the situation where a magnetic monopole of strength Q_m sits at the origin, i.e.,

$$\nabla \cdot \mathbf{B} = 4\pi Q_m \delta(\mathbf{x}). \tag{3.186}$$

Let Γ be the space with the origin excluded. In Γ we have $\nabla \cdot \mathbf{B} = 0$, hence it is still possible to write $\mathbf{B} = \nabla \times \mathbf{A}$. In the following we prove that despite the above it is not possible to define a $\mathbf{A}$ that is non-singular and differentiable through out Γ. To prove that let us consider a sphere S in Γ that encloses the origin. Let us draw a oriented close curve $\mathcal{C}$ (say the equator) on the sphere. Such curve divide the sphere into two parts S_1 (the northern hemisphere) and S_2 (the southern hemisphere). Let us consider $\oint_{\mathcal{C}} d\mathbf{x} \cdot \mathbf{A}$. According to the Stokes theorem

$$\oint_{\mathcal{C}} d\mathbf{x} \cdot \mathbf{A} = \int\int_{S_1} d\mathbf{a} \cdot \nabla \times \mathbf{A} = -\int\int_{S_2} d\mathbf{a} \cdot \nabla \times \mathbf{A}. \tag{3.187}$$

In the above we have assumed that the oriented surface S_1 has the same orientation (according to the right-hand rule) as $\mathcal{C}$ while S_2 has the opposite orientation. As the result

$$\int\int_{S_1} d\mathbf{a} \cdot \mathbf{B} + \int\int_{S_2} d\mathbf{a} \cdot \mathbf{B} = 0. \tag{3.188}$$

However according to the divergence theorem the left-hand-side of the above equation is equal to $4\pi Q_m$. This establishes the fact that it is

impossible to define a non-singular and differentiable vector potential throughout Γ.

However the very concept of gauge transformation allow us to define the vector potential in different region of space using different gauges. Thus as long as we can vector potentials $\mathbf{A}_1$ and $\mathbf{A}_2$ where $\mathbf{A}_1$ is non-singular in $S_1' \subset S$ (say the upper hemisphere) and $\mathbf{A}_2$ is non-singular in $S_2' \subset S$ (say the lower hemisphere), and that $S_1' \bigcup S_2' \supset S$, and $\mathbf{A}_1 - \mathbf{A}_2 = \nabla\chi$ in $S_1' \bigcap S_2'$ (say a strip around the equator), we have a legitimate vector potential defined over S.

In classical physics the strength of the magnetic monopole (Q_m) can be arbitrary. In particular it is unrelated to the fundamental unit of charge e. However in quantum mechanics internal consistency imposes a constraint on Q_m. Furthermore this constraint relate Q_m to the fundamental electric charge. This incredible relation is discovered by P.A.M. Dirac.

Let us imagine a charge e particle confined to S. Let us consider Feynman's amplitude (Eq. (3.139)) between two points on the equator of S . In computing the path integral we encounter two paths along the equator which links the two points. The relative phase factor due to the vector potential is

$$e^{\frac{ie}{\hbar c}\oint_C d\mathbf{x}\cdot\mathbf{A}} = e^{\frac{ie}{\hbar c}\int\int_{S_1} d\mathbf{a}\cdot\nabla\times\mathbf{A}_1} = e^{-\frac{ie}{\hbar c}\int\int_{S_2} d\mathbf{a}\cdot\nabla\times\mathbf{A}_2}. \tag{3.189}$$

As the result

$$e^{\frac{ie}{\hbar c}[\int\int_{S_1} d\mathbf{a}\cdot\nabla\times\mathbf{A}_1 + \int\int_{S_2} d\mathbf{a}\cdot\nabla\times\mathbf{A}_2]} = e^{\frac{ie}{\hbar c}\int\int_S d\mathbf{a}\cdot\mathbf{B}} = e^{\frac{ie}{\hbar c}4\pi Q_m} = 1. \tag{3.190}$$

As the result

$$\frac{e}{\hbar c}4\pi Q_m = 2\pi n, \tag{3.191}$$

or

$$Q_m e = \frac{n}{2}\frac{\hbar c}{e} = \frac{n}{4\pi}\Phi_0. \tag{3.192}$$

Thus the internal consistency of quantum mechanics quantize the charge of magnetic monopoles!

Chapter 4

Symmetry in quantum mechanics

4.1 General discussions

In quantum mechanics most symmetry operation (with time reversal an exception) are implemented by unitary operators. Symmetry group is a set of such operators which has group structure.

There are two types of symmetry group: discrete and continuous. A discrete group contains finite number of elements. For example the space inversion and identity operator form a 2-element discrete group $\{I, P\}$. An example of the continuous group is the group of rotation around an fixed, say $\hat{z}$, axis. A group element g is labeled by a parameter θ - the angle of rotation. The element corresponds to $\theta = 0$ is the identity, and elements correspond to $\theta \approx 0$ is "very close" to identity. To be more specific

$$g(\epsilon) = I - \epsilon O. \tag{4.1}$$

Since $g^+ = g^{-1}$ we require $O^+ = -O$. Thus we write $O = iQ$ where Q is hermitian. As the result

$$g(\epsilon) = I - i\epsilon Q. \tag{4.2}$$

Q is called the "generator" of the group.

When we say a physical system is invariant under a symmetry group

G, what we mean is

$$g^{-1}Hg = H \quad \forall \quad g \in G, \tag{4.3}$$

where H is the Hamiltonian.[1] Eq. (4.3) is equivalent to

$$Hg = gH \quad or \quad [H, g] = 0. \tag{4.4}$$

Thus the elements of a symmetry group all commute with the Hamiltonian.

It is simple to show that the validity of Eq. (4.3) for all elements of a continuous group requires that the generator(s) must commute with the Hamiltonian, i.e.,

$$[H, Q] = 0. \tag{4.5}$$

A consequence of Eq. (4.5) is that

$$Q_H = \mathcal{U}^+(t;0)Q\mathcal{U}(t;0) \tag{4.6}$$

is a conserved quantity. This is simple to prove because according to the Heisenberg equation

$$\frac{dQ_H}{dt} = \frac{i}{\hbar}[H_H, Q_H] = \frac{i}{\hbar}\mathcal{U}^+(t;0)[H, Q]\mathcal{U}(t;0) = 0. \tag{4.7}$$

Another important usage of a symmetry group is that it helps us to diagonalize the Hamiltonian. Let us suppose that Eq. (4.3) is true, and $|n>$ is an eigenstate of H with eigenvalue E_n. Then $g|n>$ is also an eigenstate of H with the same eigenenergy, because

$$Hg|n>= gH|n>= E_n g|n> . \tag{4.8}$$

Suppose $|n>$ and $|n'>= g|n>$ represent different states. Then these are two states with the same energy, i.e., they are degenerate. We can repeat the same procedure over and over until we generate a set of states $\{|n>, |n'>, |n''>, ...\}$ so that when any element of the symmetry group acts on any of the above states the outcome is a state that can be expressed as linear combination of states that are already in the list. When that happens we say that $\{|n>, |n'>, ...\}$ form an invariant

[1] If H is time dependent we must require that Eq. (4.3) is valid at all time.

space of the symmetry group. Thus the degenerate eigenstates of the Hamiltonian form an invariant space of the symmetry group.

A invariant space of a symmetry group G is said to be *irreducible* if it is impossible to find a subspace of it which is also invariant under G. Let $\{|n>\}$ be an orthonormal basis spanning an irreducible representation space $\mathcal{V}$. If H is invariant under G then

1. $|n'>\equiv \frac{H|n>}{\sqrt{<n|H^+H|n>}}$ are a orthonormal set.
2. $\{|n'>\}$ also spanned an irreducible invariant space $\mathcal{V}'$ of G.
3. The representation carried by $\mathcal{V}$ and $\mathcal{V}'$ are identical.

Proof:

1. Although in general $H|n>$ does not have to stay in $\mathcal{V}$, $H^+H|n>$ does.
2. H^+H can be diagonalized in $\mathcal{V}$, i.e., $H^+H=\sum_n \lambda_n |e_n><e_n|$.
3. Since $[H^+H,g]=0$ for all $g\in G$ we have $<e_n|[H^+H,g]|e_m>=(\lambda_n-\lambda_m)<e_n|g|e_m>=0$. Thus if $\lambda_n\neq\lambda_m$, $<e_n|g|e_m>=0$ for all g. In other words the degenerate subspace of H^+H further divide $\mathcal{V}$ into subspaces that are invariant under G. This contradict the statement that $\mathcal{V}$ is irreducible.
4. Thus the entire $\mathcal{V}$ is a degenerate space of H^+H.
5. As the result $<n|H^+H|m>=\lambda\delta_{nm}$, and $<n'|m'>=\delta_{nm}$.
6. Let $g|n>=\sum_m g_{mn}|m>$. Thus the matrix that represent g in $\mathcal{V}$ is g_{mn}. Since H commutes with all g we have $g|n'>=gH\frac{|n>}{\sqrt{\lambda}}=Hg\frac{|n>}{\sqrt{\lambda}}=\frac{1}{\sqrt{\lambda}}\sum_m g_{mn}|m>=\sum_m g_{mn}|m'>$.

Because of the above theorem to diagonalize H we should i) collect all equivalent irreducible invariant space of the symmetry group G of H, ii) Choose the basis set in each space so that the matrices that represent the element of G are identical in all spaces, iii) to find an eigenstate of H linearly combine the corresponding basis vector in all spaces, i.e., $a_1|n>+a_2|n'>+a_3|n''>+....$

4.2 Translation

The group of space translation is a continuous group. The element of this group displaces the physical system under study by a fixed amount **a**. Under such operation the state of a particle changes according to

$$|\psi > \rightarrow T(\mathbf{a})|\psi > . \tag{4.9}$$

The translation group is "Abelian" because

$$T(\mathbf{a})T(\mathbf{b}) = T(\mathbf{b})T(\mathbf{a}) = T(\mathbf{a}+\mathbf{b}). \tag{4.10}$$

In the following we find the representation of the translation group in the space spanned by the position eigenstates of a spinless particle. Let $|\mathbf{x}>$ be such a state

$$T(\mathbf{a})|\mathbf{x} >= |\mathbf{x}+\mathbf{a} > . \tag{4.11}$$

To find out the effect of $T(\mathbf{a})$ on a general state $|\psi >$. Let us expand $|\psi >$ as linear combination of $\{|\mathbf{x} >\}$

$$|\psi >= \int d^3x g(\mathbf{x})|\mathbf{x} > . \tag{4.12}$$

The translated state $T(\mathbf{a})|\psi >$ is given by

$$T(\mathbf{a})|\psi >= \int d^3x g(\mathbf{x})|\mathbf{x}+\mathbf{a} > . \tag{4.13}$$

Thus

$$< \mathbf{x}|T(\mathbf{a})|\psi >=< \mathbf{x}-\mathbf{a}|\psi >, \tag{4.14}$$

or

$$\psi_T(\mathbf{x}) = \psi(\mathbf{x}-\mathbf{a}). \tag{4.15}$$

Any operation of space translation can be achieved by consecutive infinitesimal displacements, i.e.

$$T(\mathbf{a}) = [T(\epsilon\hat{a})]^N, \tag{4.16}$$

where $N\epsilon = a$. The effect of an infinitesimal displacement is

$$\begin{aligned} \psi_T(\mathbf{x}) \quad &= \psi(\mathbf{x}-\epsilon\hat{a}) = \psi(\mathbf{x}) - \epsilon\hat{a}\cdot\nabla\psi(\mathbf{x}) = [I-\epsilon\hat{a}\cdot\nabla]\psi(\mathbf{x}) \\ &= [I - i\hbar\epsilon\hat{a}\cdot\mathbf{P}]\psi(\mathbf{x}). \end{aligned} \tag{4.17}$$

In the above we have used the fact that under the position eigenbasis

$$\mathbf{P} = \frac{\hbar}{i}\nabla. \tag{4.18}$$

Consequently

$$T(\epsilon\hat{a}) = I - \frac{i}{\hbar}\epsilon\hat{a}\cdot\mathbf{P} = e^{-\frac{i}{\hbar}\epsilon\hat{a}\cdot\mathbf{P}}. \tag{4.19}$$

Substitute Eq. (4.19) into Eq. (4.16) we obtain

$$T(\mathbf{a}) = \left(e^{-\frac{i}{\hbar}\epsilon\hat{a}\cdot\mathbf{P}}\right)^N = e^{-\frac{i}{\hbar}\mathbf{a}\cdot\mathbf{P}}. \tag{4.20}$$

Due to this equation the three components of the momentum operator are called the "generators" of space translations.

Due to Eq. (4.20) the momentum eigenstates are also the eigenstates of the translation operators, i.e.,

$$T(\mathbf{a})|\mathbf{k}>= e^{-\frac{i}{\hbar}\hbar\mathbf{k}\cdot\mathbf{a}}|\mathbf{k}>= e^{-i\mathbf{k}\cdot\mathbf{a}}|\mathbf{k}> . \tag{4.21}$$

Phrased in terms of the wavefunction since

$$\psi(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{4.22}$$

we have

$$\psi_T(\mathbf{x}) = \psi(\mathbf{x}-\mathbf{a}) = e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{a})} = e^{-i\mathbf{k}\cdot\mathbf{a}}\psi(\mathbf{x}). \tag{4.23}$$

Thus each of the momentum eigenstate $|k>$ span an invariant space of the translation group. The matrix representing $T(\mathbf{a})$ is the scalar $e^{-i\mathbf{k}\cdot\mathbf{a}}$. These representations are obviously irreducible.

4.3 Rotation

4.3.1 General discussions

Let us first concentrate on the effect of space rotation on the states of a spinless particle. Upon space rotation

$$|\psi>\rightarrow R|\psi> . \tag{4.24}$$

The space rotations are characterized by a vector $\vec{\theta}$, where $\hat{\theta}$ is the axis around which the rotation is performed and θ is the angle of rotation. The effect of space rotation on the position eigenbasis is

$$R(\vec{\theta})|\mathbf{x}>=|\mathbf{x}_R>, \tag{4.25}$$

where $\mathbf{x}_R = \mathcal{R}(\vec{\theta})\mathbf{x}$ is the rotated position. The effect of space rotation on a general state $|\psi>=\int d^3x g(\mathbf{x})|\mathbf{x}>$ is

$$|\psi_R>=\int d^3x g(\mathbf{x})|\mathcal{R}(\vec{\theta})\mathbf{x}>, \tag{4.26}$$

or

$$\psi_R(\mathbf{x}) = \psi(\mathcal{R}^{-1}(\vec{\theta})\mathbf{x}). \tag{4.27}$$

As translations, space rotation can be achieved by consecutive infinitesimal rations, i.e.,

$$R(\vec{\theta}) = [R(\epsilon\hat{\theta})]^N. \tag{4.28}$$

The effect of $R(\epsilon\hat{\theta})$ on the wavefunction is

$$\psi_R(\mathbf{x}) = \psi(\mathcal{R}^{-1}(\epsilon\hat{\theta})\mathbf{x}). \tag{4.29}$$

To figure out what is the new position $\mathbf{x}' = \mathcal{R}^{-1}(\epsilon\hat{\theta})\mathbf{x}$ let us choose the coordinate axis so that $\hat{\theta}$ coincide with $\hat{z}$. In that case

$$\begin{aligned}\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} &= \begin{pmatrix} \cos\epsilon & \sin\epsilon & 0 \\ -\sin\epsilon & \cos\epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \\ &= \begin{pmatrix} 1 & \epsilon & 0 \\ -\epsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.\end{aligned} \tag{4.30}$$

Thus

$$\begin{aligned}\psi_R(x,y,z) &= \psi(x+\epsilon y, -\epsilon x + y, z) \\ &= \psi(x,y,z) + \epsilon\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)\psi(x,y,z) \\ &= \left[I + \frac{i}{\hbar}\epsilon(yP_x - xP_y)\right]\psi(x,y,z) \\ &= \left[I - \frac{i}{\hbar}\epsilon L_z\right]\psi(x,y,z)\end{aligned} \tag{4.31}$$

In the above

$$L_z \equiv (\mathbf{x} \times \mathbf{P})_z, \tag{4.32}$$

is the angular momentum operator. Thus

$$R(\epsilon\hat{z}) = I - \frac{i}{\hbar} L_z = e^{-\frac{i}{\hbar}\epsilon L_z}, \tag{4.33}$$

and

$$R(\theta\hat{z}) = e^{-\frac{i}{\hbar}\theta L_z}. \tag{4.34}$$

Now if we restore the general coordinate choice

$$R(\vec{\theta}) = e^{-\frac{i}{\hbar}\vec{\theta}\cdot\mathbf{L}}. \tag{4.35}$$

Thus the angular momentum operator is the generator of space rotation. Unlike space translation the rotation group is not Abelian. This is because different component of the momentum operator do not commute. Indeed explicit calculation of the commutation relation using $[x_\alpha, P_\beta] = i\hbar\delta_{\alpha\beta}$ and $\mathbf{L} = \mathbf{x} \times \mathbf{P}$ gives

$$[L_\alpha, L_\beta] = i\hbar\epsilon_{\alpha\beta\gamma} L_\gamma. \tag{4.36}$$

L_α are called the "generator" of the rotation group. Due to the fact that the generators do not commute the rotation group is "non-Abelian".

What are the irreducible representation of the rotation group? Obviously any invariant space of the rotation group must also be invariant under the action of its three generators. In such a space each of the three generators will be represented by a matrix, and the commutation relation in Eq. (4.36) is satisfied by these matrices.

It is straightforward to show that according to Eq. (4.36) the operator

$$L^2 \equiv L_x^2 + L_y^2 + L_z^2, \tag{4.37}$$

commute with all components of $\mathbf{L}$, i.e.

$$[L^2, L_\alpha] = 0 \quad \forall \quad \alpha. \tag{4.38}$$

Due to Eq. (4.36) it is not possible to find state that are the simultaneous eigenstate of the three components of the angular momentum

operator. However we can do the next best thing, namely, finding the smallest state space in which the rotation operator is fully contained.

Since L^2 commutes with all three components of $\mathbf{L}$, we can simultaneously diagonalize, for example, L^2 and L_z. Let $|l, m>$ be a state satisfying

$$\begin{aligned} L^2|\lambda, \eta>&= \lambda|\lambda, \eta> \\ L_z|\lambda, \eta>&= \eta|\lambda, \eta> . \end{aligned} \tag{4.39}$$

Then $L^+|\lambda, \eta>$ and $L^-|\lambda, \eta>$ are eigenstates of L^2 with eigenvalue λ and eigenstates of L_z with eigenvalues $\eta + \hbar$ and $\eta - \hbar$ respectively. In the above

$$\begin{aligned} L^+ &= L_x + iL_y \\ L^- &= L_x - iL_y. \end{aligned} \tag{4.40}$$

To prove the above statement we note that

$$\begin{aligned} [L_z, L^+] &= \hbar(iL_y + L_x) = \hbar L^+ \\ [L_z, L^-] &= \hbar(iL_y - L_x) = -\hbar L^-. \end{aligned} \tag{4.41}$$

As the result

$$\begin{aligned} L_z L^+|\lambda, \eta>&= L^+ L_z|\lambda, \eta> + \hbar L^+|\lambda, \eta>= (\eta + \hbar)L^+|\lambda, \eta> \\ L_z L^-|\lambda, \eta>&= L^- L_z|\lambda, \eta> - \hbar L^+|\lambda, \eta>= (\eta - \hbar)L^-|\lambda, \eta> \end{aligned} \tag{4.42}$$

The norm of $L^+|\lambda, \eta>$ is

$$\begin{aligned} &< \lambda, \eta|L^- L^+|\lambda, \eta>=< \lambda, \eta|L_x^2 + L_y^2 - i[L_y, L_x]|\lambda, \eta> \\ &=< \lambda, \eta|L^2 - L_z^2 - \hbar L_z|\lambda, \eta>= (\lambda - \eta^2 - \hbar\eta). \end{aligned} \tag{4.43}$$

Similarly the norm of $L^-|\lambda, \eta>$ is

$$< \lambda, \eta|L^+ L^-|\lambda, \eta>= (\lambda - \eta^2 + \hbar\eta). \tag{4.44}$$

Thus in order for the space that contains the rotation group to be finite dimensional we must require

$$(\lambda - \eta_{max}^2 - \hbar\eta_{max}) = 0 \tag{4.45}$$

for certain maximum η and

$$(\lambda - \eta_{min}^2 + \hbar\eta_{min}) = 0 \tag{4.46}$$

for certain minimum η. Moreover due to Eq. (4.42)

$$\eta_{max} = \eta_{min} + k\hbar, \tag{4.47}$$

where k is a positive integer. Substituting Eq. (4.47) into Eq. (4.45) we obtain

$$\eta_{min} = -\frac{k}{2}\hbar. \tag{4.48}$$

Similarly substituting Eq. (4.47) into Eq. (4.46) we obtain

$$\eta_{max} = \frac{k}{2}\hbar. \tag{4.49}$$

Now substituting Eq. (4.48) into Eq. (4.46) we obtain

$$\lambda = \hbar^2\left(\frac{k^2}{4} + \frac{k}{2}\right) = \frac{k}{2}\left(\frac{k}{2} + 1\right)\hbar^2. \tag{4.50}$$

We will from now on label the state $|\lambda, \eta>$ by $|l, l_z>$ where

$$l \equiv \frac{k}{2} \tag{4.51}$$

and $-\frac{k}{2} \leq l_z \leq \frac{k}{2}$, and

$$\begin{aligned}
&L^2|l, l_z> = \hbar^2 l(l+1)|l, l_z> \\
&L_z|l, l_z> = \hbar l_z|l, l_z> \\
&L^+|l, l_z> = \hbar\sqrt{l(l+1) - l_z(l_z+1)}|l, l_z+1> \\
&= \hbar\sqrt{(l-m)(l+m+1)}|l, l_z+1> \\
&L^-|l, l_z> = \hbar\sqrt{l(l+1) - l_z(l_z-1)}|l, l_z-1> \\
&= \hbar\sqrt{(l+m)(l-m+1)}|l, l_z-1> .
\end{aligned} \tag{4.52}$$

Thus the irreducible invariant spaces of the rotation group are labeled by l which is generally referred as the angular momentum quantum number. According to Eq. (4.51) l is either integer or half-integer.

4.3.2 Integer angular momentum

The $l = integer$ irreducible invariant space of the rotation group is spanned by the states $|l, m>$ where $l = integer$ and $-l \leq m \leq l$. It is possible to find such states in the Hilbert space of a spinless particle. Using the spherical coordinate

$$\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta, \end{aligned} \tag{4.53}$$

and $\mathbf{L} = \mathbf{x} \times \frac{\hbar}{i}\nabla$ we obtain

$$\begin{aligned} L^2 &= -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right] \\ L_x &= \frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right) \\ L_y &= \frac{\hbar}{i}\left(\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right) \\ L_z &= \frac{\hbar}{i}\frac{\partial}{\partial\phi} \\ L^+ &= \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right) \\ L^- &= -\hbar e^{-i\phi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi}\right). \end{aligned} \tag{4.54}$$

First we note that none of the angular momentum operator acts on the radial coordinate. Thus

$$< \mathbf{x}|l, m >= R(r)Y_{lm}(\theta, \phi) \tag{4.55}$$

where $R(r)$ can be any function of r and $Y_{lm}(\theta, \phi)$ satisfies

$$\begin{aligned} &-\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right]Y_{lm}(\theta, \phi) \\ &= \hbar^2 l(l+1)Y_{lm}(\theta, \phi) \\ &\frac{\hbar}{i}\frac{\partial}{\partial\phi}Y_{lm}(\theta, \phi) = \hbar m Y_{lm}(\theta, \phi). \end{aligned} \tag{4.56}$$

The solution of the above equation is the spherical harmonics[2]

$$Y_{lm}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}(-1)^m e^{im\phi} P_{lm}(\cos\theta)$$
$$P_{lm}(\xi) = \frac{(-1)^m (l+m)!}{2^l l!(l-m)!}(1-\xi^2)^{-m/2}\frac{d^{l-m}}{d\xi^{l-m}}(\xi^2-1)^l. \quad (4.57)$$

The normalization is chosen so that

$$\int d\theta d\phi Y_{l'm'}(\theta,\phi) Y_{lm}(\theta,\phi) = \delta_{ll'}\delta_{mm'}. \quad (4.58)$$

4.3.3 Half-integer angular momentum

The smallest half-integer angular momentum is 1/2. In the following we work out the matrices correspond to L_x, L_y and L_z in this space. The two possible states are $|\frac{1}{2},\frac{1}{2}>$ and $|\frac{1}{2},-\frac{1}{2}>$. Thus

$$L_z \to S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4.59)$$

Similarly

$$L_x \to S_x = \frac{1}{2}(L^+ + L^-) \to \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (4.60)$$

and

$$L_y \to S_y = \frac{1}{2i}(L^+ - L^-) \to \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (4.61)$$

These are exactly the spin 1/2 matrices we learned in elementary quantum mechanics.

For a particle with spin 1/2 the states are direct product of the "orbital" and "spin" states, i.e.

$$|state> = |orbital> \otimes |spin> . \quad (4.62)$$

The corresponding wavefunction is of the form

$$\psi(\mathbf{x};\sigma) = \phi(\mathbf{x})\chi(\sigma). \quad (4.63)$$

[2]For details see, e.g., "Quantum Mechanics" by Merzbacher, 2nd edition, page 178-190

Rotation acts simultaneously in the orbital and spin spaces. The generator of the orbital rotation is commonly denoted by $\mathbf{L}$ and the generator of the spin rotation is commonly denoted by $\mathbf{S}$. The generator of the physical rotation is the sum

$$\mathbf{J} = \mathbf{L} \otimes I + I \otimes \mathbf{S}. \tag{4.64}$$

In the above $\mathbf{L} \otimes I$ means that the operator acts on the product space, however it only affect the orbital states. Similarly $I \otimes \mathbf{S}$ means that it only affect the spin state. In the literature Eq. (4.64) is abbreviated as $\mathbf{J} = \mathbf{L} + \mathbf{S}$. It is important to note that $\mathbf{J}$ satisfies the commutation relation Eq. (4.36). Therefore everything we said between Eq. (4.36) and Eq. (4.52) holds true for $\mathbf{J}$.

It is of particular interest to note that

$$e^{-\frac{i}{\hbar}2\pi\hat{n}\cdot\mathbf{S}} = -I, \tag{4.65}$$

while for integer angular momentum representation

$$e^{-\frac{i}{\hbar}2\pi\hat{n}\cdot\mathbf{L}} = I. \tag{4.66}$$

It is thus important to remember that for particle with half-integer spin rotation around an axis by 2π is not the identify.

4.4 Euler's rotations

A rotation around an axis $\hat{n}$ by χ can be achieved by the following three steps. Let $\hat{n}$ be characterized by $(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. From the fixed reference frame (x, y, z) we shall generate two new frames (x', y', z') and (x'', y'', z''). The frame (x', y', z') is generated from (x, y, z) by rotating ϕ around the z-axis. The frame (x'', y'', z'') is generated from (x', y', z') by rotating θ around the y' axis.[3] Finally we rotate around the z'' axis by χ. The first two rotations achieve in bringing z'' to $\hat{n}$, and the last rotation achieves the actual rotation around $\hat{n}$. Thus

$$R_{\hat{n}}(\chi) = R_{z''}(\chi)R_{y'}(\theta)R_z(\phi). \tag{4.67}$$

[3]In the above the sense of rotation is always counterclockwise with the "right-handed rule".

In the above the rotations are expressed in reference to new frames (x', y', z') and (x'', y'', z''). How do we express them in reference to the fixed axis (x', y', z'). First we prove that rotation around the y' axis by θ, i.e. $R_{y'}(\theta)$ can be expressed as rotation around the fixed axis as

$$R_{y'}(\theta) = R_z(\phi) R_y(\theta) R_z^{-1}(\phi). \tag{4.68}$$

Proof. Let

$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} \tag{4.69}$$

by the components of a vector in the (x', y', z') frame. Rotation around y' by θ brings

$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} \to \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} \equiv R_y(\theta) \begin{pmatrix} a' \\ b' \\ c' \end{pmatrix}. \tag{4.70}$$

However the components of a vector in the (x', y', z') frame is related the the components of the vector in the (x, y, z) frame by

$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \equiv R_z^{-1}(\phi) \begin{pmatrix} a \\ b \\ c \end{pmatrix}. \tag{4.71}$$

As the result when Eq. (4.70) is viewed in (x, y, z) we have

$$R_z^{-1}(\phi) \begin{pmatrix} a \\ b \\ c \end{pmatrix} \to R_y(\theta) R_z^{-1}(\phi) \begin{pmatrix} a \\ b \\ c \end{pmatrix}, \tag{4.72}$$

or

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} \to R_z(\phi) R_y(\theta) R_z^{-1}(\phi) \begin{pmatrix} a \\ b \\ c \end{pmatrix}, \tag{4.73}$$

which is the meaning of Eq. (4.68).

Similarly we have

$$R_{z''}(\chi) = R_{y'}(\theta) R_z(\chi) R_{y'}^{-1}(\theta). \tag{4.74}$$

Substituting Eq. (4.68) and Eq. (4.74) into Eq. (4.67) we obtain

$$\begin{aligned} R_{\hat{n}}(\chi) &= R_{z''}(\chi)R_{y'}(\theta)R_z(\phi) \\ &= R_{y'}(\theta)R_z(\chi)R_{y'}^{-1}(\theta)R_{y'}(\theta)R_z(\phi) \\ &= R_{y'}(\theta)R_z(\chi)R_z(\phi) \\ &= R_z(\phi)R_y(\theta)R_z^{-1}(\phi)R_z(\chi)R_z(\phi) \\ &= R_z(\phi)R_y(\theta)R_z(\chi). \end{aligned} \tag{4.75}$$

In the above we have used the fact that $R_z(\chi)R_z(\phi) = R_z(\phi)R_z(\chi)$.

This can be generalized to show that

$$e^{-\frac{i}{\hbar}\chi\hat{n}\cdot\mathbf{J}} = e^{-\frac{i}{\hbar}\phi J_z}e^{-\frac{i}{\hbar}\theta J_y}e^{-\frac{i}{\hbar}\chi J_z}. \tag{4.76}$$

4.5 The Clebsch-Gordan Coefficient

Suppose we have two particles one in angular momentum state $|j_1, m_1>$ and the other in angular momentum state $|j_2, m_1>$, what is the angular momentum state of the combined system? Since the two particle states are the direct product of the single particle ones, i.e.,

$$|\text{two particle}> = |\text{particle 1}> \otimes |\text{particle2}> . \tag{4.77}$$

As the result the operator that rotates the system around $\hat{n}$ by angle θ is

$$U = e^{-\frac{i}{\hbar}\theta\hat{n}\cdot(\mathbf{J}_1\otimes I)}e^{-\frac{i}{\hbar}\theta\hat{n}\cdot(I\otimes\mathbf{J}_2)}. \tag{4.78}$$

In the above $\mathbf{J}_1\otimes I/I\otimes\mathbf{J}_2$ acts on the two particle state but only affects the state of particle 1/particle 2. Since $\mathbf{J}_1\otimes I$ and $I\otimes\mathbf{J}_2$ act on different particles they commute. As the result

$$U = e^{-\frac{i}{\hbar}\theta\hat{n}\cdot(I\otimes\mathbf{J}_1+\mathbf{J}_2\otimes I)}. \tag{4.79}$$

Therefore the total angular momentum operator of two particles is

$$\mathbf{J} = \mathbf{J}_1\otimes I + I\otimes\mathbf{J}_2, \tag{4.80}$$

which is more commonly written as

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2. \tag{4.81}$$

The total space spanned by $|j_1, m_1 > \otimes |j_2, m_2 >$ is $(2j_1+1)(2j_2+1)$ dimensional. In general $|j_1, m_1 > \otimes |j_2, m_2 >$ is not an eigen state of J^2 and J_z. However since the direct product space is a invariant space of $\mathbf{J}$ we can express such eigenstate as linear combination of $|j_1, m_1 > \otimes |j_2, m_2 >$

$$|jm >= \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} < j_1, m_1; j_2, m_2|jm > |j_1, m_1; j_2, m_2 > . \quad (4.82)$$

Here we have abbreviated $|j_1, m_1 > \otimes |j_2, m_2 >$ by $|j_1, m_1; j_2, m_2 >$. The linear combination coefficient is called the Clebsch-Gordan coefficient. Since $J_z|jm >= m\hbar|j, m >$ and since $(J_{1z} + J_{2z})|j_1, m_1; j_2, m_2 >= (m_1 + m_2)\hbar|j_1, m_1; j_2, m_2 >$ we conclude that

$$< j_1, m_1; j_2, m_2|jm >= 0, \quad \text{if } m \neq m_1 + m_2. \quad (4.83)$$

But how many different $|jm >$ multiplet[4] can be formed in the direct product space?

Since the maximum value of $m_1 + m_2$ is $j_1 + j_2$, so is the maximum value of m. The j value corresponds to $m = j_1 + j_2$ is $j = j_1 + j_2$. In the following we shall prove that the state

$$\begin{aligned} J^2|j_1, j_1; j_2, j_2 >&= \hbar^2(j_1 + j_2)(j_1 + j_2 + 1)|j_1, j_1; j_2, j_2 > \\ J_z|j_1, j_1; j_2, j_2 >&= \hbar(j_1 + j_2)|j_1, j_1; j_2, j_2 > . \end{aligned} \quad (4.84)$$

The second of the above equations is obvious hence we will focus on the first one. Use the fact that

$$J^2 = J_1^2 + J_2^2 + 2\mathbf{J}_1 \cdot \mathbf{J}_2 = J_1^2 + J_2^2 + J_1^+ J_2^- + J_1^- J_2^+, \quad (4.85)$$

and the fact that

$$J_1^+|j_1, j_1; j_2, j_2 >= J_2^+|j_1, j_1; j_2, j_2 >= 0, \quad (4.86)$$

the first equation follows trivially. Thus

$$|j_1 + j_2, j_1 + j_2 >= |j_1, j_1; j_2, j_2 > . \quad (4.87)$$

[4]The collection of $\{|j, m >; m = -j... + j\}$ is called a multiplet

By successively applying $J^- = J_1^- + J_2^-$ to Eq. (4.87) we generate the multiplet $\{|j_1+j_2, m>\}$. The dimension of this multiplet is $2(j_1+j_2)+1$. For example

$$J^-|j_1+j_2, j_1+j_2> = (J_1^- + J_2^-)|j_1, j_1; j_2, j_2> . \tag{4.88}$$

The righthand side of the above equation is $\sqrt{2(j_1+j_2)}|j_1+j_2, j_1+j_2-1>$ and the lefthand side of the above equation is $\sqrt{2j_1}|j_1, j_1-1; j_2, j_2> + \sqrt{2j_2}|j_1, j_1; j_2, j_2-1>$, thus

$$\begin{aligned} |j_1+j_2, j_1+j_2-1> \quad &= \sqrt{\frac{j_1}{j_1+j_2}}|j_1, j_1-1; j_2, j_2> \\ &+\sqrt{\frac{j_2}{j_1+j_2}}|j_1, j_1; j_2, j_2-1> . \end{aligned} \tag{4.89}$$

In the total space spanned by $\{|j_1, m_1; j_2, m_2>$ there are only two independent states can have $m = j_1+j_2-1$. They are two different linear combinations of $|j_1, j_1-1; j_2, j_2>$ and $|j_1, j_1; j_2, j_2-1>$. The state given by Eq. (4.89) already exhausts one of them. The other one can be obtained by requiring the state to be orthogonal to that in Eq. (4.89). The result is

$$\sqrt{\frac{j_2}{j_1+j_2}}|j_1, j_1-1; j_2, j_2> - \sqrt{\frac{j_1}{j_1+j_2}}|j_1, j_1; j_2, j_2-1> . \tag{4.90}$$

It is simple to show that the above state is the eigen state of J^2 and J_z both with eigenvalues j_1+j_2-1. Thus

$$\begin{aligned} |j_1+j_2-1, j_1+j_2-1> \quad &= \sqrt{\frac{j_2}{j_1+j_2}}|j_1, j_1-1; j_2, j_2> \\ &-\sqrt{\frac{j_1}{j_1+j_2}}|j_1, j_1; j_2, j_2-1> . \end{aligned} \tag{4.91}$$

We can now apply the lowering operator on Eq. (4.91) successively to generate the new multiplet $\{|j_1+j_2-1, m> \ , m = -(j_1+j_2-1)..., (j_1+j_2-1)\}$. The dimension of the multiplet is $2(j_1+j_2-1)+1$. By applying the lowering operator once we generate the state $|j_1+j_2-1, j_1+j_2-1>$.

Now we have two out of the three possible independent states having $m = j_1 + j_2 - 2$. by orthogonalizing to the two states we get the states $|j_1+j_2-2, j_1+j_2-2>$. We repeat this process until the total dimension $(2j_1 + 1)(2j_2 + 1)$ is exhausted. The end result is that we can generate multiplet with

$$|j_1 - j_2| \leq j \leq j_1 + j_2. \tag{4.92}$$

Now we demonstrate that the sum of the dimension of these multiplet is exactly $(2j_1 + 1)(2j_2 + 1)$. Without loosing generality let us assume $j_1 > j_1$. The total dimension of the generated multiplets is

$$\sum_{j=j_1-j_2}^{j_1+j_2} (2j+1) = 2\frac{(2j_1)(2j_1+1)}{2} + 2j_2 + 1 = (2j_1+1)(2j_2+1). \tag{4.93}$$

The above discussion also point out how to generate the Clebsch-Gordan coefficient.

4.6 Selection rules

4.6.1 Scalar operators

As we shall discuss in later part of the course, when an new terms is added to a Hamiltonian

$$H = H_0 + \delta H, \tag{4.94}$$

transition between the eigenstates of H_0 will be induced. In elementary quantum mechanics we have learned a rule (Fermi's golden rule) that the transition rate is given by

$$W_{fi} = \frac{2\pi}{\hbar}| < f|\delta H|i > |^2 \delta(E_f - E_i). \tag{4.95}$$

In the above $|i >$ and $|f >$ are eigenstates of H_0 with energy E_i and E_f. Thus computing the matrix element $< f|\delta H|i >$ is central to the prediction of the transition rate.

If δH is invariant under a group G, and $|i >$ and $|f >$ belongs to different irreducible invariant space of G, then $< f|\delta H|i >= 0$.

Indeed due to the theorem we proved at the beginning of this section $\delta H|i>$ falls in an irreducible invariant subspace that carries the same representation as the space where $|i>$ belong. Two states in different invariant subspace must have zero inner product.[5]

In the following we shall generalize the situation to include the case where δH is not invariant under G but transforms in certain specified fashion. For this discussion we shall concentrate on the rotation group as the symmetry group.

4.6.2 Tensor operators, the Wigner-Eckart theorem

Suppose there is a set of operators $\{T_{kq}\}$ that transform like the multiplet $|k,q>$ under rotation, i.e.

$$\begin{aligned} R^+ T_{kq} R &= \sum_{q'=-k}^{k} \mathcal{R}^k_{qq'} T_{kq'} \\ R|k,q> &= \sum_{q'=-k}^{k} \mathcal{R}^k_{qq'} |kq'>, \end{aligned} \tag{4.96}$$

then we say that T_{kq} is a spherical tensor operator of rank k. A necessary condition for the above equation is that

$$\begin{aligned} [J_z, T_{kq}] &= \hbar q T_{kq} \\ [J^{\pm}, T_{kq}] &= \hbar\sqrt{(k \mp q)(k \pm q + 1)}\, T_{kq\pm 1}. \end{aligned} \tag{4.97}$$

To prove the above equation we take

$$R = I - \epsilon \frac{i}{\hbar} \hat{n} \cdot \mathbf{J}, \tag{4.98}$$

and substitute into Eq. (4.96). We obtain

$$[\hat{n} \cdot \mathbf{J}, T_{kq}] = \sum_{q'=-k}^{k} < kq'|\hat{n} \cdot \mathbf{J}|kq > T_{kq'}. \tag{4.99}$$

[5]This is because irreducible invariant space divides the Hilbert space into disadjointing parts.

By taking $\hat{n} = \hat{z}, \hat{x} \pm i\hat{y}$ we obtain Eq. (4.96).

The Wigner-Eckart Theorem. The matrix elements of tensor operators with respect to angular momentum eigenstates satisfy

$$< \alpha' j' m' | T_{kq} | \alpha j m >= M(\alpha', j', \alpha, j, k) < j, m; k, q | j' m' > . \quad (4.100)$$

In the above α and α' denote other quantum numbers. Proof: by applying $J^{\pm} = J_1^{\pm} + J_2^{\pm}$ to both side of Eq. (4.82) we obtain the following recursion relation for the Clebsch-Gordan coefficient. The result is

$$\begin{aligned} &\sqrt{(j \mp m)(j \pm m + 1)} < j_1, m_1; j_2, m_2 | j, m \pm 1 > \\ &= \sqrt{(j_1 \mp m_1 + 1)(j_1 \pm m_1)} < j_1, m_1 \mp 1; j_2, m_2 | j m > \\ &+ \sqrt{(j_2 \mp m_2 + 1)(j_2 \pm m_2)} < j_1, m_1; j_2, m_2 \mp 1 | j m > \quad (4.101) \end{aligned}$$

Similarly using Eq. (4.96) we can compute the matrix element

$$\begin{aligned} &< \alpha', j', m' | [J^{\pm}, T_{kq} | \alpha, j, m > \\ &= \hbar \sqrt{(k \mp q)(k \pm q + 1)} < \alpha', j', m' | T_{kq \pm 1} | \alpha, j, m > . \quad (4.102) \end{aligned}$$

On the other hand we can compute the lefthand side by acting $J^{\pm}$ to the bra or the ket. The result is

$$\begin{aligned} &\sqrt{(j' \pm m')(j' \mp m' + 1)} < \alpha', j', m' \mp 1 | T_{kq} | \alpha, j, m > \\ &- \sqrt{(j \mp m)(j \pm m + 1)} < \alpha', j', m' | T_{kq} | \alpha, j, m \pm 1 > \\ &= \sqrt{(k \mp q)(k \pm q + 1)} < \alpha', j', m' | T_{kq \pm 1} | \alpha, j, m > . \quad (4.103) \end{aligned}$$

Comparing Eq. (4.101) with Eq. (4.103) we notice that the striking similarity if we identify

$$\begin{aligned} j' &\leftrightarrow j \\ m' &\leftrightarrow m \\ j &\leftrightarrow j_1 \\ m &\leftrightarrow m_1 \\ k &\leftrightarrow j_2 \\ q &\leftrightarrow m_2 \\ < \alpha', j', m' | T_{kq} | \alpha, j, m > &\leftrightarrow < j_1, m_1; j_2, m_2 | j m > . \quad (4.104) \end{aligned}$$

Thus Both recursion relations are of the form

$$\sum_j a_{ij} x_j = 0. \tag{4.105}$$

Whenever we have

$$\sum_j a_{ij} x_j = \sum_j a_{ij} y_j = 0 \tag{4.106}$$

we can conclude that

$$x_j = c y_j \tag{4.107}$$

where c is a universal proportionality factor. Thus we have

$$< \alpha', j', m' | T_{kq} | \alpha, j, m >= \text{constant} \times < j, m; k, q | j' m' > . \tag{4.108}$$

A consequence of the Wigner-Eckart theorem is

1. $< \alpha', j', m' | T_{kq} | \alpha, j, m >= 0$ if $m' \neq m + q$.
2. $< \alpha', j', m' | T_{kq} | \alpha, j, m >= 0$ if j' does not lie in the range $|j-k| \leq j' \leq j + k$.

4.7 Time reversal

The discussion in this subsection follows closely that in chapter 4 of "Modern Quantum Mechanics" by Sakurai.

Let us first look at classical mechanics. Let us imagine a particle falling down under the influence of gravity. If we record the trajectory of the particle and running the motion picture backward we will not be able to tell which is the correct sequence. In one case we see the particle moving accelerating downward and in the other we see the particle decelerating upward. Both are in accord with Newton's law. More formally if $\mathbf{x}(t)$ is a solution to Newton's equation

$$m \ddot{\mathbf{x}} = -\nabla V(\mathbf{x}), \tag{4.109}$$

so will $\mathbf{x}(-t)$.

Let us now look at quantum mechanics where Newton's equation is replaced by the Schrödinger equation:

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})\right]\psi(\mathbf{x},t). \tag{4.110}$$

In this case suppose $\psi(\mathbf{x},t)$ is a solution we can easily verify that $\psi(\mathbf{x},-t)$ is not a solution. This is due to the appearance of the first-order time derivative. However $\psi^*(\mathbf{x},-t)$ is a solution as you may verify by complex-conjugation of Eq. (4.110). Thus we conjecture that in quantum mechanics time reversal must have something to do with complex conjugation. If at $t=0$ the wavefunction is given by $\psi(\mathbf{x})=<\mathbf{x}|\psi>$, then the wavefunction for the corresponding time reversed state is given by $<\mathbf{x}|\psi>^*$ at $t=0$.

Before we begin a systematic treatment of the time-reversal operator, some general remarks on symmetry operations are in order. Consider a symmetry operation

$$|\alpha>\rightarrow|\alpha'> \quad |\beta>\rightarrow|\beta'>. \tag{4.111}$$

One should require that the probability to be preserved, i.e.,

$$|<\beta'|\alpha'>|^2=|<\beta|\alpha>|^2. \tag{4.112}$$

For symmetry operations we encounter so far such as rotation, translation, this is indeed the case. In addition for these symmetry transformation not only the modulus but also the phase of the inner products are preserved, i.e.,

$$<\beta'|\alpha'>=<\beta|\alpha>. \tag{4.113}$$

Formally this so because the corresponding symmetry operator is unitary, i.e.,

$$<\beta'|\alpha'>=<\beta|U^+U|\alpha>=<\beta|\alpha>. \tag{4.114}$$

However it turns out that time reversal preserves Eq. (4.112) by having

$$<\alpha'|\beta'>=<\beta|\alpha>^*. \tag{4.115}$$

Definition. The transformation

$$|\alpha>\rightarrow|\alpha'>=\theta|\alpha>, \quad ,|\beta>\rightarrow|\beta'>=\theta|\beta> \tag{4.116}$$

is said to be antiunitary if

$$< \beta' | \alpha' > = < \beta | \alpha >^*$$
$$\theta[c_1|\alpha > + c_2|\beta >] = c_1^* \theta|\alpha > + c_2^* \theta|\beta > . \tag{4.117}$$

The corresponding operator θ is an antiunitary operator.

Under a fixed basis set $|e_n >$ an antiunitary operator can be written as

$$\theta = UK, \tag{4.118}$$

where K is the complex conjugation operator so that for $|\psi > = \sum_n c_n |e_n >$

$$K|\psi > = K[\sum_n c_n |e_n >] = \sum_n c_n^* |e_n > . \tag{4.119}$$

The U in Eq. (4.118) is a unitary operator that transform the orthonormal basis $|e_n >$ to another orthonormal basis $|e'_n >$. Here we emphasize that the definition of K is in reference to a specific basis set. Now we check that Eq. (4.115) is indeed satisfied. Let

$$|\alpha > = \sum_n \alpha_n |e_n >$$
$$|\beta > = \sum_n \beta_n |e_n >, \tag{4.120}$$

acting Eq. (4.118) on these two states we have

$$|\alpha' > = \sum_n \alpha_n^* U |e_n >$$
$$|\beta' > = \sum_N \beta_n^* U |e_n > . \tag{4.121}$$

As the result

$$< \beta' | \alpha' > = \sum_{n,m} \beta_m \alpha_n^* < e_m | U^+ U | e_n > = \sum_n \beta_n \alpha_n^*$$
$$= (\sum_n \beta_n^* \alpha_n)^* = < \beta | \alpha >^* . \tag{4.122}$$

We are now in position to present a formal theory of time reversal. Let us denote the time reversal operator by Θ which is antiunitary. We now deduce the fundamental property of Θ by looking at the time

evolution of the time reversed state. Consider a physical system in state $|\alpha>$ at $t = 0$. Then at a slightly later time $t = \delta t$ the system is found in

$$\left(I - \frac{i}{\hbar}\delta t H\right)|\alpha> . \tag{4.123}$$

Now let us apply the time reversal at $t = 0$ and then let the time-reversed state evolve under the *same* Hamiltonian H, we then have at δt

$$\left(I - \frac{i}{\hbar}\delta t H\right)\Theta|\alpha> . \tag{4.124}$$

If the dynamics obeys symmetry under time reversal we expect the preceding state to be the same as

$$\Theta\left(I - \frac{i}{\hbar}(-\delta t) H\right)|\alpha> . \tag{4.125}$$

Thus

$$\Theta\left(I + \frac{i}{\hbar}\delta t H\right)|\alpha> = \left(I - \frac{i}{\hbar}\delta t H\right)\Theta|\alpha>, \tag{4.126}$$

or

$$-iH\Theta|\alpha> = \Theta iH|\alpha> \quad \forall|\alpha> . \tag{4.127}$$

We now argue that Θ can not be unitary if the notion of time reversal is to make sense. Suppose Θ were unitary. it would then be legitimate to cancel the i's in Eq. (4.127), and we would have the operator equation

$$-H\Theta = \Theta H \quad \text{or} \quad \Theta^{-1}H\Theta = -H. \tag{4.128}$$

Consider an energy eigenstate $|n>$ with eigenenergy E_n. The corresponding time-reversed state would have $-E_n$ as the energy eigenvalue because

$$H\Theta|n> = -\Theta H|n> = -E_n\Theta|n> . \tag{4.129}$$

This is nonsensical even in the simplest case of a free particle. We know that the energy spectrum of the free particle ranges from 0 to ∞. there is no state having energy lower than zero. Indeed since we expect the momentum to change sign under time reversal and since the kinetic energy is quadratic in momentum we expect

$$\Theta^{-1}\frac{p^2}{2m}\Theta = \frac{p^2}{2m}, \tag{4.130}$$

which clearly contradicts Eq. (4.128).

If Θ is antiunitary instead we have

$$\Theta iH|\alpha >= -i\Theta H|\alpha >, \tag{4.131}$$

then Eq. (4.127) implies that

$$\Theta H = H\Theta, \tag{4.132}$$

which makes sense.

Now let us discuss the behavior of operators upon time reversal. Let $|\alpha' >= \Theta|\alpha >$ and $|\beta' >= \Theta|\beta >$, we shall prove that

$$< \beta|A|\alpha >=< \alpha'|\Theta A^{+}\Theta^{-1}|\beta' > . \tag{4.133}$$

Proof. Let $|\gamma >= A^{+}|\beta >$, then $< \gamma| =< \beta|A$. Thus

$$\begin{aligned} < \beta|A|\alpha > \quad &=< \gamma|\alpha >=< \gamma'|\alpha' >^{*}=< \alpha'|\gamma' > \\ &=< \alpha'|\Theta|\gamma >=< \alpha'|\Theta A^{+}|\beta > \\ &=< \alpha'|\Theta A^{+}\Theta^{-1}\Theta|\beta > \\ &=< \alpha'|\Theta A^{+}\Theta^{-1}|\beta' > . \end{aligned} \tag{4.134}$$

For hermitian operators we get

$$< \beta|A|\alpha >=< \alpha'|\Theta A\Theta^{-1}|\beta' > . \tag{4.135}$$

We say that observables are even or odd under time reversal according to whether

$$\begin{aligned} &\Theta A\Theta^{-1} = A \ \ (\text{even}) \qquad , \text{or} \\ &\Theta A\Theta^{-1} = -A \ \ (\text{odd}). \end{aligned} \tag{4.136}$$

For such definite-T-parity operators and for $|\beta >= |\alpha >$ Eq. (4.135) becomes

$$< \alpha|A|\alpha >=< \alpha'|\Theta A\Theta^{-1}|\alpha' >= \pm < \alpha'|A|\alpha' > . \tag{4.137}$$

As an example let us look at the expectation value of the momentum operator. Intuitively we expect $\mathbf{P}$ to be odd under time reversal, i.e.

$$\Theta\mathbf{P}\Theta^{-1} = -\mathbf{P}. \tag{4.138}$$

This implies that

$$\mathbf{P}\Theta|\mathbf{k}>=-\Theta\mathbf{P}\Theta^{-1}\Theta|\mathbf{k}>=-\Theta\mathbf{P}|\mathbf{k}>=-\hbar\mathbf{k}\Theta|\mathbf{k}>. \tag{4.139}$$

The above agrees with the notion that $\Theta|\mathbf{k}>$ is the momentum eigenstate with eigenvalue $-\hbar\mathbf{k}$. Thus we define

$$\Theta|\mathbf{k}>=|-\mathbf{k}>. \tag{4.140}$$

Eq. (4.140) fixes the representation of the time reversal operator under the momentum eigenbasis.

Similarly for position operator we expect

$$\Theta\mathbf{X}\Theta^{-1}=\mathbf{X}, \tag{4.141}$$

which suggest that

$$\Theta|\mathbf{x}>=|\mathbf{x}>. \tag{4.142}$$

This defines the representation of the time reversal under the position eigenbasis.

It is interesting to see the consistency of Eq. (4.138) and Eq. (4.141) with the commutation relation

$$[X_j,P_k]=i\hbar\delta_{jk}. \tag{4.143}$$

The time reversed operators obey the following commutation relation

$$[\Theta X_j\Theta^{-1},\Theta P_k\Theta^{-1}]=\Theta[X_j,P_k]\Theta^{-1}=\Theta(i\hbar)\Theta^{-1}. \tag{4.144}$$

According to Eq. (4.138) and Eq. (4.141) the first commutator is $-[X_j,P_k]=-i\hbar\delta_{jk}$. Looking at the last term of Eq. (4.144) and realize that $\Theta=UK$ hence changes i to $-i$, we get a consistent result. Since the position operator is even while the momentum operator is odd under time reversal, the orbital angular momentum operator $\mathbf{L}=\mathbf{X}\times\mathbf{P}$ obeys

$$\Theta L\Theta^{-1}=-\mathbf{L}. \tag{4.145}$$

Since the orbital angular momentum is part of the total angular momentum operator in Eq. (4.64) we require

$$\begin{aligned}\Theta\mathbf{L}\Theta^{-1}&=-\mathbf{L}\\ \Theta\mathbf{S}\Theta^{-1}&=-\mathbf{S}\\ \Theta\mathbf{J}\Theta^{-1}&=-\mathbf{J}.\end{aligned} \tag{4.146}$$

Under Eq. (4.142) the wavefunction of an state transform as follows. Let $|\psi>=\int d^3x\psi(\mathbf{x})|\mathbf{x}>$. Under time reversal

$$\begin{aligned}|\psi>\rightarrow\Theta|\psi> \quad &= \int d^3x\Theta\psi(\mathbf{x})|\mathbf{x}>=\int d^3x\psi^*(\mathbf{x})\Theta|\mathbf{x}> \\ &= \int d^3x\psi^*(\mathbf{x})|\mathbf{x}>\,. \end{aligned} \tag{4.147}$$

As the result the wavefunction corresponds to $\Theta|\psi>$ is $\psi^*(\mathbf{x})$.

Since time reversal send the wavefunction to its complex conjugate we have

$$Y_{lm}(\theta,\phi) \;\; \text{time reversal} \rightarrow Y^*_{lm}(\theta,\phi)=(-1)^m Y_{l-m}(\theta,\phi). \tag{4.148}$$

$$\Theta|l,m>=(-1)^m|l,-m>\,. \tag{4.149}$$

Finally we state an important theorem on time reversal.

Theorem. Suppose the Hamiltonian is invariant under time reversal and the energy eigenstate $|n>$ is non-degenerate; then the corresponding eigenfunction is real up to a phase factor.[6]

Proof. First we note that

$$H\Theta|n>=\Theta H|n>=E_n\Theta|n>\,. \tag{4.150}$$

Since this energy eigenstate is non-degenerate $|n>$ and $\Theta|n>$ must be the same state. Since the wavefunction of $|n>$ is the complex conjugate of the wavefunction for $\Theta|n>$ this means that

$$\psi_n(\mathbf{x})=e^{i\theta}\psi^*_n(\mathbf{x}). \tag{4.151}$$

Up to this point we have only speak of the representation of the time reversal operator in the Hilbert space of spinless particles. The representation of Θ in the spin space is of interest. This is specially true for the case of spin 1/2.

Let us find such representation using as the basis the eigenbasis of S_z. Let $|\chi>$ be a spin state

$$|\chi>=\alpha|1/2>+\beta|-1/2>\,. \tag{4.152}$$

[6]By this we mean that the complex conjugate of the wavefunction is a phase factor times the original one.

The effect of the time reversal operator on $|\chi>$ is

$$\Theta|\chi>= UK|\chi>= \alpha^* U|1/2> +\beta^* U|-1/2> . \tag{4.153}$$

The question is what is the appropriate unitary transformation on the basis.

The unitary transformation must be chosen so that if $|\eta>= \Theta|\chi>$

$$<\eta|\mathbf{S}|\eta>= -<\chi|\mathbf{S}|\chi> . \tag{4.154}$$

Equivalently we require

$$(\,\alpha \quad \beta\,)\, U^+ \vec{\sigma} U \begin{pmatrix} \alpha^* \\ \beta^* \end{pmatrix} = -(\,\alpha^* \quad \beta^*\,)\,\vec{\sigma}\begin{pmatrix} \alpha \\ \beta. \end{pmatrix}. \tag{4.155}$$

Since the right hand side of the above equation is real we can rewrite it as

$$-\left[(\,\alpha^* \quad \beta^*\,)\,\vec{\sigma}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}\right]^* = -\left[(\,\alpha \quad \beta\,)\,(\hat{x}\sigma_x - \hat{y}\sigma_y + \hat{z}\sigma_z)\begin{pmatrix} \alpha^* \\ \beta^* \end{pmatrix}\right]. \tag{4.156}$$

we conclude that

$$U^+ \vec{\sigma} U = -(\hat{x}\sigma_x - \hat{y}\sigma_y + \hat{z}\sigma_z), \tag{4.157}$$

or equivalently

$$\begin{aligned} U^+\sigma_x U &= -\sigma_x \\ U^+\sigma_y U &= \sigma_y \\ U^+\sigma_z U &= -\sigma_z. \end{aligned} \tag{4.158}$$

The operator that obviously work is

$$U = \xi\sigma_y, \tag{4.159}$$

where ξ is an arbitrary phase factor. Thus the representation of the time reversal operator under the S_z eigenbasis is

$$\Theta = \xi\sigma_y K. \tag{4.160}$$

There is an important difference between the effect on Θ on the states of a spinless particle and that of a spin 1/2 particle. For the spinless case

$$\Theta^2|\psi>=\Theta[\int d^3x\psi^*(\mathbf{x})|\mathbf{x}>]=\int d^3x\psi(\mathbf{x})|\mathbf{x}>=|\psi>. \quad (4.161)$$

Thus

$$\Theta^2=I. \quad (4.162)$$

However for the spin state $|\chi>=\alpha|1/2>+\beta|-1/2>$ of a spin 1/2 particle we have

$$\begin{aligned}\Theta^2|\chi> &= \Theta[\alpha^*\xi\sigma_y|1/2>+\beta^*\xi\sigma_y|-1/2>] \\ &= \Theta[\alpha^*\xi i|-1/2>+\beta^*\xi(-i)|1/2>] \\ &= \xi(\alpha^*\xi i)^*\sigma_y|-1/2>+\xi(\beta^*\xi(-i))^*\sigma_y|1/2> \\ &= -i\alpha(-i)|1/2>+i\beta i|-1/2>=-|\chi>. \end{aligned} \quad (4.163)$$

Thus

$$\Theta^2=-I. \quad (4.164)$$

More generally we have

$$\begin{aligned}&\Theta^2|\text{integer j}>=|\text{integer j}> \\ &\Theta^2|\text{half integer j}>=-|\text{half integer j}>. \end{aligned} \quad (4.165)$$

Therefore the eigenvalue of Θ^2 is given by $(-1)^{2j}$. Eq. (4.160) can be rewritten as

$$\Theta=\xi' e^{-\frac{i}{\hbar}\pi S_y}K \quad (4.166)$$

where $-i\xi'=\xi$. Generalized to arbitrary j we have

$$\Theta=\xi' e^{-\frac{i}{\hbar}\pi J_y}K. \quad (4.167)$$

4.8 The Kramers degeneracy

Let the Hamiltonian be time reversal invariant, i.e., $\Theta H\Theta^{-1}=H$. If $|n>$ is an energy eigenstate with eigenvalue E_n so does $\Theta|n>$. The

question is, are $|n>$ and $\Theta|n>$ the same state? If the answer is yes then

$$\Theta|n>= e^{i\phi}|n> . \tag{4.168}$$

Apply the time reversal operator again we obtain

$$\Theta^2|n>= e^{-i\phi}e^{i\phi}|n>= |n> . \tag{4.169}$$

But this relation is impossible for half-integer j systems, for which Θ^2 is -1. So we are led to conclude that $|n>$ and $\Theta|n>$ must represent distinct states – that is, there must be a degeneracy. This implies, for example, that for a system composed of an odd number of electrons in external potential $V(\mathbf{x})$, each energy level must be at least two fold degenerate no matter how complicated $V(\mathbf{x})$ may be.

Chapter 5

Approximation methods for discrete levels

5.1 A useful matrix theorem

Consider a matrix

$$\mathcal{H} = \begin{pmatrix} h & V \\ V^+ & H \end{pmatrix}. \tag{5.1}$$

In the above h is a $n \times n$ matrix, and H is $N \times N$ and V is a $n \times N$ matrix. Our goal is to solve the eigenvalue problem

$$\begin{pmatrix} h & V \\ V^+ & H \end{pmatrix} \begin{pmatrix} \phi \\ \chi \end{pmatrix} = E \begin{pmatrix} \phi \\ \chi \end{pmatrix}. \tag{5.2}$$

In Eq. (5.2) ϕ is a $n \times 1$ column vector and χ is $N \times 1$. Perform the matrix multiplication explicitly Eq. (5.2) reduces to

$$\begin{aligned} (E - h)\phi &= V\chi \\ (E - H)\chi &= V^+\phi. \end{aligned} \tag{5.3}$$

Eliminate the second of the above equation we get

$$\chi = (E - H)^{-1}V^+\phi. \tag{5.4}$$

Here we have assumed the existence of the inverse $(E-H)^{-1}$. Substitute Eq. (5.2) back into the first of Eq. (5.3) we obtain

$$(E - h)\phi = V(E - H)^{-1}V^+\phi. \tag{5.5}$$

Thus solving the original eigenvalue problem with $\mathcal{H}$ a $(n+N)\times(n+N)$ matrix is equivalent to find the eigenvalues of a $n \times n$ matrix given by

$$h_{eff}(E) = h + V(E - H)^{-1}V^{+}. \tag{5.6}$$

The eigen value E satisfies the equation

$$\det\left[h_{eff}(E)\right] = 0. \tag{5.7}$$

After obtaining the solution for E we can solve for the eigenvectors by first find ϕ via

$$(E - h_{eff})\phi = 0. \tag{5.8}$$

After obtaining ϕ we can solve for χ via Eq. (5.4).

5.2 The non-degenerate Rayleigh-Schrödinger perturbation theory

The non-degenerate Rayleigh-Schrödinger perturbation theory is based on a special case of the above matrix theorem where $n = 1$.

The problem we are concerning with are the discrete energy levels of a physical system whose Hamiltonian can be broken into two parts:

$$H = H_0 + gV. \tag{5.9}$$

In the above H_0 is regarded as the unperturbed part, and gV the perturbation. g is a real parameter. It is introduced for bookkeeping purposes. For $g = 0$ we have the unperturbed Hamiltonian and for $g = 1$ the perturbation acquires full strength. The eigenvalues and eigenfunctions of H are functions of g. Simple perturbation theory applies when these functions can be expanded in powers of g. A perturbative method is useful when only the first few terms of the expansion need be considered.

The eigenvalue problem we wish to solve is

$$(H_0 + gV)|\psi_n >= E_n|\psi_n > . \tag{5.10}$$

We suppose that the problem

$$H_0|\phi_n >= \epsilon_n|\phi_n > \tag{5.11}$$

has already been solved. Assuming first that no degeneracy has occurred here, let us inquire what happens to the eigenvalues and eigenvectors as we allow g to grow continuously from zero to some finite value. In this process the energy will change to

$$E_n = \epsilon_n + \Delta E_n. \tag{5.12}$$

and the eigenstate changes to

$$|\psi_n >= |\phi_n > + |\chi_n > . \tag{5.13}$$

In Eq. (5.13) we require that

$$< \phi_n|\chi_n >= 0, \tag{5.14}$$

or equivalently

$$< \phi_n|\psi_n >= 1. \tag{5.15}$$

A symbolic representation of the Hamiltonian matrix in the space spanned by $|\phi_n >$ and all other eigenstates of H_0 is

$$H = \begin{pmatrix} \epsilon_n + V_{nn} & gPVQ \\ gQVP & QHQ \end{pmatrix}. \tag{5.16}$$

In the above $V_{nn} =< \phi_n|V|\phi_n >$, $P = |\phi_n >< \phi_n|$, and $Q \equiv I - |\phi_n >< \phi_n|$. It is trivial to show that the eigenenergy satisfies the equation

$$E_n - \epsilon_n - V_{nn} - < \phi_n|gPVQ\frac{1}{E_n - QHQ}gQVP|\phi_n >= 0 \tag{5.17}$$

The above equation can be simplified to

$$E_n - \epsilon_n - V_{nn} - < \phi_n|gVQ\frac{1}{E_n - H}gQV|\phi_n >= 0 \tag{5.18}$$

Thus

$$\Delta E_n \quad = V_{nn} + < \phi_n|gVQ\frac{1}{E_n - QHQ}gQV|\phi_n > . \tag{5.19}$$

As to $(E_n - H)^{-1}$ in Eq. (5.19) we use the fact that

$$\begin{aligned}\frac{1}{E_n - QHQ} &= \frac{1}{E_n - QH_0Q - gQVQ} = \frac{1}{E_n - QH_0Q} \\ &+ \frac{1}{E_n - QH_0Q} gQVQ \frac{1}{E_n - QH_0Q} + ... \\ &= \frac{Q}{E_n - H_0} + \frac{Q}{E_n - H_0} gV \frac{Q}{E_n - H_0} + ... \quad (5.20)\end{aligned}$$

Substitute Eq. (5.20) into Eq. (5.19) we obtain

$$\Delta E_n = gV_{nn} + < \phi_n | gV \left[\frac{Q}{E_n - H_0} + \frac{Q}{E_n - H_0} gV \frac{Q}{E_n - H_0} + ... \right] gV | \phi_n > . \quad (5.21)$$

Insert complete set of states into Eq. (5.21) we obtain

$$\Delta E_n = gV_{nn} + g^2 \sum_{m \neq n} \frac{V_{nm} V_{mn}}{\epsilon_n - \epsilon_m + \Delta E_n} + ... \quad (5.22)$$

Thus to the lowest order in g

$$\Delta E_n = gV_{nn}. \quad (5.23)$$

To $O(g^2)$ we have

$$\Delta E_n = gV_{nn} + g^2 \sum_{m \neq n} \frac{V_{nm} V_{mn}}{\epsilon_n - \epsilon_m}. \quad (5.24)$$

To $O(g^3)$ we have

$$\begin{aligned}\Delta E_n &= gV_{nn} + g^2 \sum_{m \neq n} \frac{V_{nm} V_{mn}}{\epsilon_n - \epsilon_m} \\ &+ g^3 \sum_{k,m \neq n} \frac{V_{nm} V_{mk} V_{kn}}{(\epsilon_n - \epsilon_m)(\epsilon_n - \epsilon_k)} - g^3 \sum_{m \neq n} \frac{V_{nm} V_{mn} V_{nn}}{(\epsilon_n - \epsilon_m)^2}. \quad (5.25)\end{aligned}$$

In this way we achieve an expansion of ΔE_n in powers of g. After we obtain the eigenvalues, the eigen state are given by

$$|\chi_n > = \frac{1}{E_n - QHQ} gQVP|\phi_n > . \quad (5.26)$$

Substitute Eq. (5.20) into the above we obtain

$$|\chi_n >= \left[\frac{Q}{E_n - H_0} + \frac{Q}{E_n - H_0} gV \frac{Q}{E_n - H_0} + ...\right] gV|\phi_n > . \quad (5.27)$$

Thus to $O(g)$

$$|\psi_n >= |\phi_n > + g \sum_{m \neq n} \frac{V_{mn}}{\epsilon_n - \epsilon_m} |\phi_m > . \quad (5.28)$$

To $O(g^2)$ we have

$$\begin{aligned} |\psi_n > \quad &= |\phi_n > + g \sum_{m \neq n} \frac{V_{mn}}{\epsilon_n - \epsilon_m} |\phi_m > + g^2 \sum_{m,k \neq n} \frac{V_{km} V_{mn}}{(\epsilon_n - \epsilon_k)(\epsilon_n - \epsilon_m)} |\phi_k > \\ &- g^2 \sum_{m \neq n} \frac{V_{nn} V_{mn}}{(\epsilon_n - \epsilon_m)^2} |\phi_m > . \end{aligned} \quad (5.29)$$

In this way we achieved at an expansion of eigenstates in powers of g.

5.3 The degenerate Rayleigh-Schrödinger perturbation theory

The degenerate perturbation theory we shall discuss here is a special case of the matrix theorem at the beginning of this chapter where $n > 1$.

A symbolic representation of the Hamiltonian matrix in the space spanned by n degenerate levels $|\phi_i > \quad i = 1, ..., n$ and all other eigenstates (not degenerate with $|\phi_i >$'s) of H_0 is

$$H = \begin{pmatrix} \epsilon + PVP & gPVQ \\ gQVP & QHQ \end{pmatrix} . \quad (5.30)$$

In the above ϵ is the degenerated eigenvalue, $P = \sum_{i=1}^{n} |\phi_i >< \phi_i|$, and $Q \equiv I - P$. As discussed in the matrix theorem the effective Hamiltonian we need to diagonalize it $n \times n$ dimensional and is given by

$$H_{eff} = \epsilon + gPVP + gPVQ \frac{1}{E - QHQ} gQVP, \quad (5.31)$$

where E is the undetermined eigenenergy. Using Eq. (5.20) we obtain

$$H_{eff} = \epsilon + gPVP + gPV\left[\frac{Q}{E-H_0} + \frac{Q}{E-H_0}gV\frac{Q}{E-H_0} + ...\right]gVP \tag{5.32}$$

Thus to $O(g)$ we have

$$H_{eff} = \epsilon + gPVP, \tag{5.33}$$

which we need to diagonalize to obtain the new eigenvalues $\epsilon_j^{(1)}$. Note that at this order H_{eff} is independent of E. To $O(g^2)$ we have

$$H_{eff} = \epsilon + gPVP + g^2PV\frac{Q}{\epsilon - H_0}VP, \tag{5.34}$$

which we need to diagonalize to get $\epsilon_j^{(2)}$. To $O(g^3)$ we have

$$\begin{aligned} H_{eff} \quad &= \epsilon + gPVP + g^2PV\frac{Q}{\epsilon^{(1)} - H_0}VP \\ &+g^2PV\frac{Q}{\epsilon - H_0}V\frac{Q}{\epsilon - H_0}VP + ..., \end{aligned} \tag{5.35}$$

which we diagonalize to get $\epsilon_j^{(3)}$..etc.

As to the eigenstates we have to $O(g)$ the eigensolutions of

$$(\epsilon + gPVP)|\phi_j^{(1)}>= 0, \tag{5.36}$$

and

$$|\chi_j^{(1)}>= g\frac{Q}{\epsilon - H_0}VP|\phi_j^{(1)}> . \tag{5.37}$$

(We note that $|\phi_j^{(1)}>$ is also the eigenstate of H_0. As the result $|\phi_j^{(1)}>= |\phi_j^{(0)}>$. To $O(g^2)$ we get $|\phi_j^{(2)}>$ by solving

$$\left[\epsilon + gPVP + g^2PV\frac{Q}{\epsilon - H_0}VP\right]|\phi_j^{(2)}>= 0, \tag{5.38}$$

and we get $|\chi_j^{(2)}>$ by

$$|\chi_j^{(2)}>= g\frac{Q}{\epsilon_j^{(1)} - H_0}VP|\phi_j^{(1)}> +g^2\frac{Q}{\epsilon - H_0}V\frac{Q}{\epsilon - H_0}VP|\phi_j^{(0)}> . \tag{5.39}$$

5.4 Berry's theorem - an application of the First-order peturbation theory.

Consider the Hamiltonian

$$H = R_x\sigma_x + R_y\sigma_y + R_z\sigma_z. \tag{5.40}$$

As discussed before such Hamiltonian has two non-degenerate eigenstates as long as $|\mathbf{R}| \neq 0$. The Berry's phase is given by

$$\gamma_\pm = \oint_C d\mathbf{R}\cdot < \psi_\pm|\frac{\nabla_R}{i}|\psi_\pm > . \tag{5.41}$$

Here $|\psi_\pm >$ is the instantaneous eigen state that are single valued and differentiable over the contour C. Since $< \psi_\pm|\psi_\pm >= 1$ we have $< \nabla_R\psi_\pm|\psi_\pm > + < \psi_\pm|\nabla_R\psi_\pm >= 0$. Since $< \nabla_R\psi_\pm|\psi_\pm >=< \psi_\pm|\nabla_R\psi_\pm >^*$ we conclude that $< \psi_\pm|\nabla_R\psi_\pm >$ is pure imaginary. As the result

$$\gamma_\pm = Im\left[\oint_C d\mathbf{R}\cdot < \psi_\pm|\nabla_R|\psi_\pm >\right]. \tag{5.42}$$

Since the quantity $< \psi_\pm|\frac{\nabla_R}{i}|\psi_\pm >$ is sensitive to the phase convention of $|\psi_\pm >$ and $\nabla_R\times < \psi_\pm|\nabla_R|\psi_\pm >$ is not, we apply the Stokes theorem and convert Eq. (5.42) to a surface integral

$$\begin{aligned}\gamma_\pm \quad &= Im\left[\int\int_S d\mathbf{a}\cdot\nabla\times < \psi_\pm|\nabla_R|\psi_\pm >\right] \\ &= \epsilon_{ijk}Im\left[\int\int_S da_i\partial_j < \psi_\pm|\partial_k\psi_\pm >\right] \\ &= \epsilon_{ijk}Im\left[\int\int_S da_i < \partial_j\psi_\pm|\partial_k\psi_\pm >\right].\end{aligned} \tag{5.43}$$

Note that in order for the Stokes theorem to be applicable $< \psi_\pm|\nabla_R|\psi_\pm >$ has to be well defined and differentiable on the surface S that is bounded by C. Now let us compute $< \partial_j\psi_+|\partial_k\psi_+ > - < \partial_k\psi_+|\partial_j\psi_+ >$. By inserting complete set of states we have

$$\begin{aligned}&< \partial_j\psi_+|\partial_k\psi_+ > - < \partial_k\psi_+|\partial_j\psi_+ > \\ &=< \partial_j\psi_+|\psi_- >< \psi_-|\partial_k\psi_+ > - < \partial_k\psi_+|\psi_- >< \psi_-|\partial_j\psi_+ >\end{aligned} \tag{5.44}$$

Now let compute $< \psi_-|\partial_j\psi_+ >$ expresses the eigen states for $\mathbf{R} = \mathbf{R}_0 + \delta\mathbf{R}$ in terms of those of $\mathbf{R}_0$. This is achieved by the perturbation theory since

$$H(\mathbf{R}_0 + \delta\mathbf{R}) = H(\mathbf{R}_0) + \delta\mathbf{R} \cdot \nabla_R H. \tag{5.45}$$

According to Eq. (5.28) we have up to a phase $e^{i\delta\theta}$ and up to a normalization factor N

$$\begin{aligned} |\psi_+ >' &= \frac{e^{i\delta\theta}}{N}[|\psi_+ > + \frac{< \psi_-|\delta\mathbf{R} \cdot \nabla_R H|\psi_+ >}{E_- - E_+}|\psi_- >] \\ &= \frac{e^{i\delta\theta}}{N}[|\psi_+ > - \frac{< \psi_-|\delta\mathbf{R} \cdot \nabla_R H|\psi_+ >}{2|\mathbf{R}|}|\psi_- >]. \end{aligned} \tag{5.46}$$

Here both $\delta\theta$ and $N - 1$ are of order $|\delta\mathbf{R}|$. Thus we have

$$< \psi_-|\partial_j\psi_+ >= -\frac{< \psi_-|\partial_j H|\psi_+ >}{2|\mathbf{R}|} = \frac{< \psi_-|\sigma_j|\psi_+ >}{2|\mathbf{R}|}. \tag{5.47}$$

As the result we have

$$\begin{aligned} &< \partial_j\psi_+|\psi_- >< \psi_-|\partial_k\psi_+ > - < \partial_k\psi_+|\psi_- >< \psi_-|\partial_j\psi_+ > \\ &= \frac{1}{4|\mathbf{R}|^2}[< \psi_+|\sigma_j|\psi_- >< \psi_-|\sigma_k|\psi_+ > - < \psi_+|\sigma_k|\psi_- >< \psi_-|\sigma_j|\psi_+ >] \\ &= \frac{1}{4|\mathbf{R}|^2}\sum_{n=\pm} < \psi_+|\sigma_j|\psi_n >< \psi_n|\sigma_k|\psi_+ > - < \psi_+|\sigma_k|\psi_n >< \psi_n|\sigma_j|\psi_+ > \\ &== \frac{1}{4|\mathbf{R}|^2} < \psi_+|[\sigma_j, \sigma_k]|\psi_+ >= \frac{2i}{4|\mathbf{R}|^2}\epsilon_{jkl} < \psi_+|\sigma_l|\psi_+ > \\ &= \frac{i}{2|\mathbf{R}|^2}\epsilon_{jkl}\hat{R}_l. \end{aligned} \tag{5.48}$$

Therefore

$$\epsilon_{ijk} Im[< \partial_j\psi_\pm|\partial_k\psi_\pm >] = \frac{1}{4|\mathbf{R}|^2}\epsilon_{ijk}\epsilon_{jkl}\hat{R}_l = \frac{\hat{R}_i}{2|\mathbf{R}|^2}. \tag{5.49}$$

Substitute the above into Eq. (6.64) we obtain

$$\gamma_+ = \int\int_S da_i \frac{\hat{R}_i}{2|\mathbf{R}|^2} = \int\int_S d\mathbf{a} \cdot \frac{\hat{R}}{2|\mathbf{R}|^2}. \tag{5.50}$$

The above is the magnetic flux produced by a monopole of strength 1/2 at the origin.

5.5 The variational principle

The above perturbation approach based on an important assumption - the existence of a small parameter that can be used to expand things. In practice such small parameter rarely exists. The variational approach is a non-perturbative method which does not rely on the presence of small parameters.

The variational method is based on the following theorem. Let H be the Hamiltonian whose ground state we try to find. Let $|\psi>$ be any normalized state, then

$$<\psi|H|\psi>\geq E_0, \tag{5.51}$$

where E_0 is the ground state energy. Moreover the equality of Eq. (5.51) holds if and only if $|\psi>$ is the ground state.

Proof. Let $\{|e_n>\}$ be the complete set of eigen states of H. Then it follows that $\{|e_n>\}$ forms a orthonormal set. Let us expand $|\psi>$ in this basis

$$|\psi>=\sum_n c_n|e_n> . \tag{5.52}$$

The fact that $|\psi>$ is normalized means that $\sum_n |c_n|^2 = 1$. The expectation of H in $|\psi>$ is given by

$$<\psi|H|\psi>=\sum_n |c_n|^2 E_n \geq E_0 \sum_n |c_n|^2 = E_0. \tag{5.53}$$

Moreover we can write

$$<\psi|H|\psi>= E_0 \sum_{m;E_m=E_0} |c_m|^2 + \sum_{n;E_n>E_0} E_n|c_n|^2, \tag{5.54}$$

Thus

$$<\psi|H|\psi> - E_0 = \sum_{n;E_n>E_0} (E_n - E_0)|c_n|^2. \tag{5.55}$$

Since $E_n - E_0 > 0$, the right hand side of the above equation is equal to zero if and only if

$$c_n = 0 \quad \forall \quad E_n > E_0. \tag{5.56}$$

As the result

$$|\psi>=\sum_{m;E_m=E_0} c_m|e_m>, \tag{5.57}$$

which means that $|\psi>$ is an ground state of H.[1]

The variational approach is entirely based on the above theorem. In this approach we construct candidate ground state (ground state wavefunction) by appealing to intuition. To make the guess less restricted we usually allow the state to depend on some parameters. For example let $|\psi(\lambda_1,...,\lambda_k)>$. Usually the more variational parameters we allow the more general is the guess. Due to the above theorem we find the best set of variational parameters by minimizing the expectation value of the Hamiltonian, i.e.

$$\frac{\partial}{\partial\lambda_j}\left[\frac{<\psi(\{\lambda_i\})|H|\psi(\{\lambda_i\})>}{<\psi(\{\lambda_i\})|\psi(\{\lambda_i\})>}\right]=0. \tag{5.58}$$

In some cases we can construct states that are orthogonal to the ground state. This is mostly achieved via symmetry consideration. For example, if we know the ground state have zero angular momentum we can construct the lowest-energy non-zero angular momentum state by applying the variational principle.

There is no recipe I can offer for constructing variational wavefunctions. This is entirely done based on one's physical intuition. Some of the most important progresses in physics are achieved in this way. Examples include the Bardeen-Cooper-Schrieffer theory of superconductivity, and the Laughlin theory of the fractional quantized Hall effect.

5.6 The WKB approximation

In this subsection we will primarily be interested in the problem of a particle moving in external potential $V(\mathbf{x})$. The Hamiltonian is given by

$$H=\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x}). \tag{5.59}$$

[1]In the case where the ground state is degenerate, $|\psi>$ is just one of many possible ground state.

We shall develop an approximation scheme called the WKB approximation. This approximation is valid when the potential varies slowly with position.

We recall that the probability amplitude for a particle at position $\mathbf{x}$ at $t = 0$ to propagate to position $\mathbf{x}'$ at time t is given by

$$G(\mathbf{x}', t; \mathbf{x}, 0) = \int_{\mathbf{y}(t)=\mathbf{x}', \mathbf{y}(0)=\mathbf{x}} D[\mathbf{y}(\tau)] e^{\frac{i}{\hbar} S}, \tag{5.60}$$

where

$$S[\mathbf{y}(\tau)] = \int_0^t d\tau [\frac{m}{2} \dot{\mathbf{y}}(\tau)^2 - V(\mathbf{y}(\tau))]. \tag{5.61}$$

In fact if the particle has wavefunction $\psi(\mathbf{x})$ at $t = 0$, then at time t its wavefunction becomes

$$\psi(\mathbf{x}, t) \propto \int d^3x' G(\mathbf{x}, t; \mathbf{x}', 0) \psi(\mathbf{x}'). \tag{5.62}$$

Let us consider the case where $V(\mathbf{x}) = 0$ and $\psi(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}$. The Feynman propagator for this case is given by

$$G_0(\mathbf{x}', t; \mathbf{x}, 0) = \int_{\mathbf{y}(t)=\mathbf{x}'; \mathbf{y}(0)=\mathbf{x}} D[\mathbf{y}(\tau)] e^{\frac{i}{\hbar} \int_0^t d\tau \frac{m}{2} \dot{\mathbf{y}}^2}. \tag{5.63}$$

For simplicity let us evaluate it for the one dimensional case.

$$G_0(x', t; x, 0) \quad = \int_{y(t)=x'; y(0)=x} D[y(\tau)] e^{\frac{i}{\hbar} \int_0^t d\tau \frac{m}{2} \dot{y}^2}. \tag{5.64}$$

Let us redefine the variable so that

$$y(\tau) \equiv x + \frac{x' - x}{t} \tau + z(\tau), \tag{5.65}$$

so that

$$\begin{aligned} G_0(x', t; x, 0) \quad &= \int_{z(t)=0; y(0)=0} D[z(\tau)] e^{\frac{i}{\hbar} \int_0^t d\tau \frac{m}{2} (\dot{z} + \frac{x'-x}{t})^2} \\ &\sim e^{\frac{i}{\hbar} t \frac{m}{2} (\frac{x'-x}{t})^2} \\ &= e^{i \frac{m}{2\hbar} \frac{(x'-x)^2}{t}}. \end{aligned} \tag{5.66}$$

We note that the quantity $\frac{m}{2\hbar}$ has the dimension $time/length^2$ which is the dimension of inverse diffusion constant. As the result we define

$$D \equiv \frac{\hbar}{m}, \tag{5.67}$$

under which

$$G_0(x', t; x, 0) \sim e^{i\frac{(x-x')^2}{2Dt}}. \tag{5.68}$$

In general three dimensional case the above result becomes

$$G_0(\mathbf{x}', t; \mathbf{x}, 0) \sim e^{i\frac{|\mathbf{x}-\mathbf{x}'|^2}{2Dt}}. \tag{5.69}$$

Using Eq. (5.69) we can prove that the plane wave is an stationary state of the free-particle Hamiltonian.

Proof. Let us assume that at $t = 0$ the wavefunction is $e^{i\mathbf{k}\cdot\mathbf{x}}$. According to Eq. (5.62) the wavefunction at time t is

$$\begin{aligned}
\psi(\mathbf{x}, t) \quad &\sim \int d^3x' G_0(\mathbf{x}, t; \mathbf{x}', 0) e^{i\mathbf{k}\cdot\mathbf{x}} \\
&\sim \int d^3x' e^{i\frac{|\mathbf{x}-\mathbf{x}'|^2}{2Dt}} e^{i\mathbf{k}\cdot\mathbf{x}} \\
&\sim e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\frac{Dtk^2}{2}} \\
&= e^{i\mathbf{k}\cdot\mathbf{x}} e^{-\frac{i}{\hbar}\frac{\hbar^2k^2}{2m}t}.
\end{aligned} \tag{5.70}$$

We can project out the wavefunction with constant energy by performing the Fourier transform:

$$\begin{aligned}
&\int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar}Et} \int d^3x' G_0(\mathbf{x}, t; \mathbf{x}', 0) e^{i\mathbf{k}\cdot\mathbf{x}'} \\
&= \int d^3x' [\int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar}Et} G_0(\mathbf{x}, t; \mathbf{x}', 0)] e^{i\mathbf{k}\cdot\mathbf{x}'} \\
&\equiv \int d^3x' G_0(E; \mathbf{x}, \mathbf{x}') e^{i\mathbf{k}\cdot\mathbf{x}'}.
\end{aligned} \tag{5.71}$$

In the above

$$\begin{aligned}
G_0(E; \mathbf{x}, \mathbf{x}') \quad &= \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar}Et} G_0(\mathbf{x}, t; \mathbf{x}', 0) \\
&\sim \int_{-\infty}^{\infty} dt e^{\frac{i}{\hbar}Et} e^{i\frac{(x-x')^2}{2Dt}}
\end{aligned}$$

$$\sim \int_{-\infty}^{\infty} dt \int d^3p e^{\frac{i}{\hbar}Et} e^{-i\frac{Dtp^2}{2}} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}$$
$$= (2\pi) \int d^3p \delta(\frac{E}{\hbar} - \frac{Dp^2}{2}) e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}$$
$$= 2\pi\hbar \int d^3p \delta(E - \frac{\hbar^2 p^2}{2m}) e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}. \qquad (5.72)$$

(The above integral can be done to yield $8\pi^2 \frac{m}{\hbar} \frac{\sin(\sqrt{2mE}|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|}$.) As the result

$$\int d^3x' G_0(E;\mathbf{x},\mathbf{x}') e^{i\mathbf{k}\cdot\mathbf{x}'} \sim \int d^3p \delta(E - \frac{\hbar^2 p^2}{2m}) e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} e^{i\mathbf{k}\cdot\mathbf{x}'}$$
$$= (2\pi)^3 \int d^3p \delta(E - \frac{\hbar^2 p^2}{2m}) e^{i\mathbf{p}\cdot\mathbf{x}} \delta(\mathbf{p}-\mathbf{k})$$
$$\sim e^{i\mathbf{k}\cdot\mathbf{x}} \delta(E - \frac{\hbar^2 k^2}{2m}). \qquad (5.73)$$

Now let us compute $G(\mathbf{x}', t; \mathbf{x}, 0)$ in the presence of a smooth potential. We recall that in general

$$G(\mathbf{x}', t; \mathbf{x}, 0) = \int_{\mathbf{y}(t)=\mathbf{x}', \mathbf{y}(0)=\mathbf{x}} D[\mathbf{y}(\tau)] e^{\frac{i}{\hbar}\int_0^t d\tau [\frac{m}{2}\dot{\mathbf{y}}(\tau)^2 - V(\mathbf{y}(\tau))]}. \qquad (5.74)$$

In the case where $V(\mathbf{x})$ is constant V the above reduces to

$$G(\mathbf{x}', t; \mathbf{x}, 0) = e^{-\frac{i}{\hbar}Vt} \int_{\mathbf{y}(t)=\mathbf{x}', \mathbf{y}(0)=\mathbf{x}} D[\mathbf{y}(\tau)] e^{\frac{i}{\hbar}\int_0^t d\tau [\frac{m}{2}\dot{\mathbf{y}}(\tau)^2]}$$
$$= e^{-\frac{i}{\hbar}Vt} G_0(\mathbf{x}', t; \mathbf{x}, 0). \qquad (5.75)$$

Thus

$$G(E;\mathbf{x}',\mathbf{x}) \sim \int d^3p \delta(E - V - \frac{\hbar^2 p^2}{2m}) e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}. \qquad (5.76)$$

To proceed further let us first consider the case of one dimension. Let ϵ be a length scale over which V hardly changes, we split the distance $x' - x$ into N pieces of length ϵ.

$$G(E; x', x) \approx \prod_{i=1}^{N} \int dp_i \delta(E - V(x_i) - \frac{\hbar^2 p_i^2}{2m}) e^{ip_i(x_{i+1}-x_i)}$$
$$\sim e^{\frac{i}{\hbar}\int_x^{x'} dy \sqrt{2m(E-V(y))}}. \qquad (5.77)$$

Thus

$$\psi(x) \sim e^{\frac{i}{\hbar}\int_x^{x'} dy\sqrt{2m(E-V(y))}}\psi(0). \tag{5.78}$$

In three dimension we have to choose sum over all possible paths leading from $\mathbf{x}$ to $\mathbf{x}'$. Along a particular path parametrized by s the one-dimensional result above applies. In that case along each path we have a contribution

$$e^{\frac{i}{\hbar}\int_{s_0}^{s_t} ds\sqrt{2m(E-V(s))}}. \tag{5.79}$$

In this case further simplification of the result require the semiclassical approximation where we replace the whole path integral by the contribution from the classical path.

The above discussion suggests we write the eigenwavefunction as

$$\psi(\mathbf{x}) = Ae^{\frac{i}{\hbar}S(\mathbf{x})}, \tag{5.80}$$

and expand S in powers of $\hbar$. Substitute Eq. (5.80) into the Schródinger equation we get

$$\frac{i}{\hbar}\nabla^2 S - \frac{1}{\hbar^2}\nabla S\cdot\nabla S + \frac{2m}{\hbar^2}(E-V) = 0. \tag{5.81}$$

If we write

$$S = S_0 + \frac{\hbar}{i}S_1 + (\frac{\hbar}{i})^2 S_2 + ... \tag{5.82}$$

and substitute the above into Eq. (5.81) and equating terms with equal power of $\hbar$ we obtain

$$\begin{aligned}
&\nabla S_0\cdot\nabla S_0 = 2m(E-V)\\
&2\nabla S_0\cdot\nabla S_1 = -\nabla^2 S_0\\
&\nabla^2 S_1 - \nabla S_1\cdot\nabla S_1 = 2\nabla S_2\cdot\nabla S_0.
\end{aligned} \tag{5.83}$$

5.7 The time dependent perturbation theory

5.8 Fermi's golden rule

Suppose the Hamiltonian of a system is given by

$$H = H_0 + V(t), \tag{5.84}$$

where H_0 is a Hamiltonian whose eigenstates are familiar, and $V(t)$ is a weak perturbation. Due to the presence of V the eigenstates of H_0 ceases to be a steady state, i.e., as time evolve the perturbation causes the system to make transition from one eigen state $|i>$ of H_0 to another. In this subsection we calculate the rate at which this transition occur.

To be more specific let us assume that the system is in $|i>$ at $t = 0$. The question is what is the probability per unit time that it will end up in state $|f>$. According to

$$|\psi(t)>= T_t\{e^{-\frac{i}{\hbar}\int_0^t d\tau(H_0+V(\tau))}\}|i> . \tag{5.85}$$

In the case where the external perturbation is weak we expand the time evolution operator to the first order in V. The result is

$$\begin{aligned} T_t\{e^{-\frac{i}{\hbar}\int_0^t d\tau(H_0+V(\tau))}\} \quad &\approx e^{-\frac{i}{\hbar}H_0 t}[I - \frac{i}{\hbar}\int_0^t d\tau V_H(\tau)] \\ &= e^{-\frac{i}{\hbar}H_0 t} - \frac{i}{\hbar}\int_0^t d\tau e^{-\frac{i}{\hbar}(t-\tau)H_0}V(\tau)e^{-\frac{i}{\hbar}\tau H_0}. \end{aligned} \tag{5.86}$$

where

$$V_H(\tau) = e^{\frac{i}{\hbar}H_0\tau}V(\tau)e^{-\frac{i}{\hbar}H_0\tau}. \tag{5.87}$$

As the result

$$|\psi(t)>\approx e^{-\frac{i}{\hbar}E_i t}|i> -\frac{i}{\hbar}\sum_n \int_0^t d\tau e^{-\frac{i}{\hbar}E_n(t-\tau)} < n|V(\tau)|i > e^{-\frac{i}{\hbar}E_i\tau}|n > \quad (5.88)$$

Thus the probability amplitude that after time t the system ends up in $e^{-\frac{i}{\hbar}E_f t}|f>$ is

$$A_{fi}(t) \approx -\frac{i}{\hbar}\int_0^t d\tau e^{\frac{i}{\hbar}(E_f-E_i)\tau} < f|V(\tau)|i > . \quad (5.89)$$

Thus the transition probability is

$$P_{fi}(t) = \frac{1}{\hbar^2}|\int_0^t d\tau e^{\frac{i}{\hbar}(E_f-E_i)\tau} < f|V(\tau)|i > |^2. \quad (5.90)$$

The transition rate is defined as

$$W_{fi}(t) \quad = \frac{dP_{fi}}{dt} = \frac{dA^*_{fi}}{dt}A_{fi} + A^*_{fi}\frac{dA_{fi}}{dt}. \quad (5.91)$$

Explicit differentiation gives

$$\frac{dA_{fi}}{dt} \approx -\frac{i}{\hbar}e^{\frac{i}{\hbar}(E_f-E_i)t} < f|V(t)|i > . \quad (5.92)$$

As the result

$$W_{fi}(t) = \frac{1}{\hbar^2}\int_0^t d\tau \left[e^{\frac{i}{\hbar}(E_f-E_i)(t-\tau)} < f|V(\tau)|i >^* < f|V(t)|i > + c.c.\right] \quad (5.93)$$

In the following we shall workout two special cases where i) V is independent of t and ii) $V(t) = \cos(\omega t)V$.

5.8.1 V independent of t

In this case Eq. (5.93) becomes

$$\begin{aligned} W_{fi}(t) \quad &\approx \frac{1}{\hbar}\left[\frac{e^{\frac{i}{\hbar}(E_f-E_i)t}-1}{i(E_f-E_i)}| < f|V|i > |^2 + c.c.\right] \\ &= \frac{4}{\hbar}\cos\left(\frac{(E_f-E_i)t}{2\hbar}\right)\frac{\sin\left(\frac{(E_f-E_i)t}{2\hbar}\right)}{(E_f-E_i)}| < f|V|i > |^2 \end{aligned} \quad (5.94)$$

However since

$$\lim_{\omega t\to\infty}\frac{\sin(\omega t)}{\omega}=\pi\delta(\omega), \tag{5.95}$$

Eq. (5.94) reduces to

$$W_{fi}(t)=\frac{2\pi}{\hbar}|<f|V|i>|^2\delta(E_f-E_i). \tag{5.96}$$

Eq. (5.96) is often referred to as "Fermi's golden rule".

5.8.2 $V(t)$ is harmonic in t

If $V(t)=V\cos(\omega t)$ Eq. (5.93) reduces to

$$\begin{aligned}
W_{fi}(t) &\approx \frac{1}{\hbar^2}\int_0^t d\tau\left[e^{\frac{i}{\hbar}(E_f-E_i)(t-\tau)}\cos(\omega t)\cos(\omega\tau)|<f|V|i>|^2+c.c\right]\\
&= \frac{2}{\hbar}\cos(\omega t)|<f|V|i>|^2\frac{\sin\left(\frac{(\hbar\omega-E_f+E_i)t}{2\hbar}\right)}{\hbar\omega-E_f+E_i}\cos\left(\frac{(\hbar\omega+E_f-E_i)t}{2\hbar}\right)\\
&+ \frac{2}{\hbar}\cos(\omega t)|<f|V|i>|^2\frac{\sin\left(\frac{(\hbar\omega+E_f-E_i)t}{2\hbar}\right)}{\hbar\omega+E_f-E_i}\cos\left(\frac{(\hbar\omega-E_f+E_i)t}{2\hbar}\right)\\
&\to \frac{\pi}{\hbar}\cos^2(\omega t)|<f|V|i>|^2\left[\delta(\hbar\omega-E_f+E_i)+\delta(\hbar\omega+E_f-E_i)\right].
\end{aligned} \tag{5.97}$$

5.9 Beyond Fermi's golden rule

We reiterate that given the time-dependent Hamiltonian

$$H=H_0+V(t), \tag{5.98}$$

the states evolves according to

$$|\psi(t)>=T_t\{e^{-\frac{i}{\hbar}\int_0^t d\tau(H_0+V(\tau))}\}|i>. \tag{5.99}$$

In the case where the external perturbation is weak we expand the time evolution operator the result is

$$T_t\{e^{-\frac{i}{\hbar}\int_0^t d\tau(H_0+V(\tau))}\} = e^{-\frac{i}{\hbar}H_0t}T_te^{-\frac{i}{\hbar}\int_0^t d\tau V_H(\tau)}. \tag{5.100}$$

where

$$V_H(\tau) = e^{\frac{i}{\hbar}H_0\tau}V(\tau)e^{-\frac{i}{\hbar}H_0\tau}. \tag{5.101}$$

In Eq. (5.100)

$$T_t e^{-\frac{i}{\hbar}\int_0^t d\tau V_H(\tau)} = \sum_n \left(-\frac{i}{\hbar}\right)^n \int_0^t d\tau_n ... d\tau_1 T_t[V_H(\tau_n)...V_H(\tau_1)]. \tag{5.102}$$

In previous section we kept none but the lowest order term of Eq. (5.102). In this section we will include higher order terms. The probability amplitude that a system starts off in $|i>$ (an eigenstate of H_0) will end up in $e^{-\frac{i}{\hbar}H_0 t}|f>$ is

$$\begin{aligned} A_{fi} \quad &=< f|T_t e^{-\frac{i}{\hbar}\int_0^t d\tau V_H(\tau)}|i> \\ &= \sum_n \left(-\frac{i}{\hbar}\right)^n \int_0^t d\tau_n ... d\tau_1 < f|T_t[V_H(\tau_n)...V_H(\tau_1)]|i> . \end{aligned} \tag{5.103}$$

The way we evaluate $< f|V_H(\tau_n)...V_H(\tau_1)|i>$ is by inserting complete set of states between each pair of V_H. The most convenient such states are the eigenstates of H_0. In the following we concentrate on the case $t > 0$ and assume that $\tau_n \geq \tau_{n-1} \geq ... \geq \tau_1$. Thus

$$\begin{aligned} < f|T_t[V_H(\tau_n)...V_H(\tau_1)]|i> \quad &= \sum_{\alpha_1,...,\alpha_{n-1}} \prod_{j=1}^{n} < \alpha_j|V_H(\tau_j)|\alpha_{j-1}> \\ &= \sum_{\alpha_1,...,\alpha_{n-1}} \prod_{j=1}^{n} e^{\frac{i}{\hbar}(E_{\alpha_j}-E_{\alpha_{j-1}})\tau_j} < \alpha_j|V|\alpha_{j-1}> . \end{aligned} \tag{5.104}$$

In the above we have defined $|\alpha_0>=|i>$ and $|\alpha_n>=|f>$. Next we need to perform the integral

$$\begin{aligned} &\int_{\tau_n>...>\tau_1} d\tau_n ... d\tau_1 \prod_{j=1}^{n} e^{\frac{i}{\hbar}(E_{\alpha_j}-E_{\alpha_{j-1}})\tau_j} \\ &= \int d\tau_n ... d\tau_1 \prod_{k=0}^{n} \theta(\tau_{k+1}-\tau_k) \prod_{j=1}^{n} e^{\frac{i}{\hbar}(E_{\alpha_j}-E_{\alpha_{j-1}})\tau_j}. \end{aligned} \tag{5.105}$$

Here we have defined $\tau_{n+1} = t$ and $\tau_0 = 0$. Next we use the fact that

$$\theta(t-t') = \int \frac{d\omega}{2\pi i} \frac{1}{w - i\eta} e^{i\omega(t-t')}. \tag{5.106}$$

Thus

$$\begin{aligned}
&\int d\tau_n ... d\tau_1 \prod_{k=0}^{n} \theta(\tau_{k+1} - \tau_k) \prod_{j=1}^{n} e^{\frac{i}{\hbar}(E_{\alpha_j} - E_{\alpha_{j-1}})\tau_j} \\
&= \int d\tau_n ... d\tau_1 \prod_{k=0}^{n} \int \frac{d\omega_k}{2\pi i} \frac{1}{\omega_k - i\eta} e^{i\omega_k(\tau_{k+1} - \tau_k)} \prod_{j=1}^{n} e^{\frac{i}{\hbar}(E_{\alpha_j} - E_{\alpha_{j-1}})\tau_j} \\
&= \int \frac{d\omega_n}{2\pi i} e^{i\omega_n t} \frac{1}{\omega_n - i\eta} \prod_{k=0}^{n-1} \int d\omega_k \frac{1}{\omega_k - i\eta} \\
&\times \prod_{j=1}^{n} \delta\left(\omega_j - \omega_{j-1} - \frac{E_{\alpha_j} - E_{\alpha_{j-1}}}{\hbar}\right) \\
&= \int \frac{d\omega}{2\pi i} e^{i\omega t} \left(\frac{1}{\omega - i\eta}\right) \prod_{k=0}^{n-1} \left(\frac{1}{\omega - \frac{1}{\hbar}(E_{\alpha_{k+1}} - E_{\alpha_k}) - i\eta}\right).
\end{aligned} \tag{5.107}$$

The above ω integral can be done as a complex integral. Since $t > 0$ we close the ω contour in the upper half plane, hence enclosing all the poles. The result is

$$\begin{aligned}
&(-\hbar)^n \prod_{k=0}^{n-1} \left(\frac{1}{E_{\alpha_{k+1}} - E_{\alpha_k}}\right) - (-\hbar)^n \sum_{l=0}^{n-1} e^{\frac{i}{\hbar}(E_{\alpha_{l+1}} - E_{\alpha_l})t} \frac{1}{E_{\alpha_{l+1}} - E_{\alpha_l}} \\
&\times \prod_{k \neq l} \left(\frac{1}{E_{\alpha_{k+1}} - E_{\alpha_k} - E_{\alpha_{l+1}} + E_{\alpha_l}}\right)
\end{aligned} \tag{5.108}$$

Thus

$$\begin{aligned}
A_{fi}(t) \quad &= \sum_n (i)^n \sum_{\alpha_1, ..., \alpha_{n-1}} \{ \prod_{k=0}^{n-1} \left(\frac{< \alpha_{k+1}|V|\alpha_k >}{E_{\alpha_{k+1}} - E_{\alpha_k}}\right) - \sum_{l=0}^{n-1} e^{\frac{i}{\hbar}(E_{\alpha_{l+1}} - E_{\alpha_l})t} \\
&\times \frac{< \alpha_{l+1}|V|\alpha_l >}{E_{\alpha_{l+1}} - E_{\alpha_l}} \prod_{k \neq l} \left(\frac{< \alpha_{k+1}|V|\alpha_k >}{E_{\alpha_{k+1}} - E_{\alpha_k} - E_{\alpha_{l+1}} + E_{\alpha_l}}\right) \}.
\end{aligned} \tag{5.109}$$

For $t < 0$ we have

$$A_{fi}(t) = \sum_n (-i)^n \sum_{\alpha_1,\ldots,\alpha_{n-1}} \{\prod_{k=0}^{n-1} \left(\frac{< \alpha_{k+1}|V|\alpha_k >}{E_{\alpha_k} - E_{\alpha_{k+1}}} \right) - \sum_{l=0}^{n-1} e^{\frac{i}{\hbar}(E_{\alpha_{l+1}} - E_{\alpha_l})t} \times \frac{< \alpha_{l+1}|V|\alpha_l >}{E_{\alpha_l} - E_{\alpha_{l+1}}} \prod_{k \neq l} \left(\frac{< \alpha_{k+1}|V|\alpha_k >}{E_{\alpha_k} - E_{\alpha_{k+1}} - E_{\alpha_l} + E_{\alpha_l+1}} \right) \}. \quad (5.110)$$

We note that

$$A_{if}(-|t|) = [A_{fi}(|t|)]^*, \quad (5.111)$$

i.e. when we reverse the time the transition amplitude becomes its complex conjugate.

Chapter 6

Scattering theory

6.1 The scattering of a wave packet

This section follows closely the discussion in "Quantum mechanics" by Merzbacher, page 219-249.

Let us concentrate on the scattering of a particle by a static potential. The Hamiltonian is given by

$$H = \frac{p^2}{2\mu} + U = H_0 + U. \tag{6.1}$$

Here U is appreciably different from zero only within a sphere of radius a around the origin. At $t = 0$ a particle is represented by a wave packet given by

$$\begin{aligned} \psi(\mathbf{x}, 0) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \phi(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}_0)} \\ &= \int \frac{d^3k}{(2\pi)^3} \phi(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}_0)}. \end{aligned} \tag{6.2}$$

where ϕ is non-zero within a narrow width Δk around a mean momentum $\mathbf{k}_0$. For example if $\phi(\mathbf{k}) = \frac{1}{(\sqrt{2\pi}\Delta k)^3} e^{-\frac{|\mathbf{k}-\mathbf{k}_0|^2}{2\Delta k^2}}$, $\psi(\mathbf{x}, 0) = \frac{1}{(2\pi)^3} e^{i\mathbf{k}_0\cdot(\mathbf{x}-\mathbf{x}_0)} e^{-\frac{1}{2}\Delta k^2|\mathbf{x}-\mathbf{x}_0|^2}$ which is a wave packet of width $1/\Delta k$ around $\mathbf{x}_0$. From now on we shall refer to the above as ψ_{pk}, i.e.

$$\psi_{pk}(\mathbf{k}_0, \mathbf{x} - \mathbf{x}_0) = \frac{1}{(2\pi)^3} e^{i\mathbf{k}_0\cdot(\mathbf{x}-\mathbf{x}_0)} e^{-\frac{1}{2}\Delta k^2|\mathbf{x}-\mathbf{x}_0|^2}. \tag{6.3}$$

Let us assume that

$$\mathbf{k}_0 = -k_0 \hat{x}_0 \tag{6.4}$$

so that the wave packet if unhindered in its motion would move freely toward the origin. We also assume that $|\mathbf{x}_0|$ is large enough so that $\psi(\mathbf{x}, 0)$ lies entirely outside the range of the scatterer.

The dynamic problem to be solved is this: What is the shape of the wave packet at a much later time, when the packet has hit the scatterer and been eventually dispersed by it? In principle the answer can be given easily if we expand $\psi(\mathbf{x}, 0)$ in terms if eigenfunctions, $\psi_n(\mathbf{x})$, of H. Indeed if we express

$$\psi(\mathbf{r}, 0) = \sum_n c_n \psi_n(\mathbf{x}), \tag{6.5}$$

then the wave packet at time t is

$$\psi(\mathbf{x}, t) = \sum_n c_n e^{-\frac{i}{\hbar} E_n t}. \tag{6.6}$$

Unfortunately Eq. (6.2) is an expansion in terms of plane waves, the eigenfunctions of H_0. In general the eigenfunctions of the full H is complicated, in particular near $\mathbf{x} = 0$. However Since $U(\mathbf{r}) = 0$ for $|\mathbf{r}| > a$ these eigenfunctions must reduces to linear combination of the solution of the free Schödinger equation. We shall show that for $|\mathbf{x}| >> a$ the exact eigenfunctions reduces to the following form

$$\psi^{(+)}_{\mathbf{k}}(\mathbf{x}) = \frac{1}{(2\pi)^3} \left(e^{i\mathbf{k}\cdot\mathbf{x}} + f_{\mathbf{k}}(\hat{x}) \frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|} \right), \tag{6.7}$$

and

$$\psi(\mathbf{x}, 0) = \int d^3k \phi(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}_0} \psi^{(+)}_{\mathbf{k}}(\mathbf{x}) \tag{6.8}$$

First we prove that for $|\mathbf{x}| >> a$ Eq. (6.8) reduces to the same wavepacket as that in Eq. (6.2). Again let us choose $\phi(\mathbf{k}) = \frac{1}{(\sqrt{2\pi}\Delta k)^3} e^{-\frac{|\mathbf{k}-\mathbf{k}_0|^2}{2\Delta k^2}}$. Since $\phi(\mathbf{k})$ peaks around $\mathbf{k}_0$ therefore to an excellent approximation we can replace $k|\mathbf{x}|$ in Eq. (6.8) by

$$k|\mathbf{x}| \approx \mathbf{k} \cdot \hat{k}_0 |\mathbf{x}|. \tag{6.9}$$

Using the above approximation and the assumption that $f_{\mathbf{k}}$ varies little within the range of Δk and hence can be replaced by $f_{\mathbf{k}_0}$ we obtain

$$\begin{aligned}
&\int d^3k\phi(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}_0}\psi_{\mathbf{k}}^{(+)}(\mathbf{x}) \\
&\approx \frac{1}{(2\pi)^3}e^{i\mathbf{k}_0\cdot(\mathbf{x}-\mathbf{x}_0)}e^{-\frac{1}{2}\Delta k^2|\mathbf{x}-\mathbf{x}_0|^2} + \frac{f_{\mathbf{k}_0}(\hat{x})e^{i(k_0|\mathbf{x}|-\mathbf{k}_0\cdot\mathbf{x}_0)}}{(2\pi)^3|\mathbf{x}|} \\
&\times e^{-\frac{1}{2}\Delta k^2||\mathbf{x}|\hat{k}_0-\mathbf{x}_0|^2} \\
&= \psi_{pk}(\mathbf{k}_0,\mathbf{x}-\mathbf{x}_0) + \frac{f_{\mathbf{k}_0}(\hat{x})}{|\mathbf{x}|}\psi_{pk}(\mathbf{k}_0,|\mathbf{x}|\hat{k}_0-\mathbf{x}_0). \qquad (6.10)
\end{aligned}$$

We note that for $\mathbf{x}\approx\mathbf{x}_0$ we have, by Eq. (6.4), $|\mathbf{x}|\hat{k}_0\approx-\mathbf{x}_0$, as the result

$$\psi_{pk}(\mathbf{k}_0,|\mathbf{x}|\hat{k}_0-\mathbf{x}_0)\approx\psi_{pk}(\mathbf{k}_0,-2\mathbf{x}_0)\approx 0. \qquad (6.11)$$

At a later time t,

$$\psi(\mathbf{x},t)=\int d^3k e^{-i\mathbf{k}\cdot\mathbf{x}_0-i\omega t}\psi_{\mathbf{k}}^{(+)}(\mathbf{x}), \qquad (6.12)$$

where

$$\hbar\omega=\frac{\hbar^2k^2}{2\mu}. \qquad (6.13)$$

Again since $\phi(\mathbf{k})$ sharply peaks around $\mathbf{k}_0$ we can approximate ω by

$$\omega=\frac{\hbar k^2}{2\mu}=\frac{\hbar|\mathbf{k}_0+(\mathbf{k}-\mathbf{k}_0)|^2}{2\mu}\approx\frac{\hbar(-k_0^2+2\mathbf{k}_0\cdot\mathbf{k})}{2\mu}=-\omega_0+\mathbf{v}_0\cdot\mathbf{k}, \qquad (6.14)$$

[1] where

$$\hbar\omega_0=\frac{\hbar^2k_0^2}{2\mu},\quad \mathbf{v}_0=\frac{\hbar\mathbf{k}_0}{\mu}. \qquad (6.16)$$

[1]The validity of this approximation is based on the assumption that

$$\frac{\hbar}{2\mu}\Delta k^2 t << 1. \qquad (6.15)$$

Substitute the above into Eq. (6.12) we obtain

$$\begin{aligned}
\psi(\mathbf{x},t) &= \int d^3k\phi(\mathbf{k})e^{-i\mathbf{k}\cdot(\mathbf{x}_0+\mathbf{v}_0t)+i\omega_0t}\psi^{(+)}_{\mathbf{k}}(\mathbf{x}) \\
&= \int d^3k\phi(\mathbf{k})e^{-i\mathbf{k}\cdot(\mathbf{x}_0+\mathbf{v}_0t)+i\omega_0t}[\frac{1}{(2\pi)^3}\left(e^{i\mathbf{k}\cdot\mathbf{x}}+f_{\mathbf{k}}(\hat{x})\frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|}\right)] \\
&\approx \int d^3k\phi(\mathbf{k})e^{-i\mathbf{k}\cdot(\mathbf{x}_0+\mathbf{v}_0t)+i\omega_0t}[\frac{1}{(2\pi)^3}\left(e^{i\mathbf{k}\cdot\mathbf{x}}+f_{\mathbf{k}_0}(\hat{x})\frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|}\right)] \\
&= e^{i\omega_0t}\psi_{pk}(\mathbf{k}_0,\mathbf{x}-\mathbf{v}_0t-\mathbf{x}_0) \\
&+e^{i\omega_0t}\frac{f_{\mathbf{k}_0}(\hat{x})}{|\mathbf{x}|}\psi_{pk}(\mathbf{k}_0,\hat{k}_0[|\mathbf{x}|-v_0t+|\mathbf{x}_0|])
\end{aligned} \tag{6.17}$$

The first term of Eq. (6.17) is appreciable when $|\mathbf{x}-\mathbf{v}_0t-\mathbf{x}_0|\approx 0$. The solution of this is

$$\mathbf{x}\approx\mathbf{x}_0+\mathbf{v}_0t \tag{6.18}$$

, i.e. the trajectory of the center of the wavepacket. The second term in Eq. (6.17) is appreciable when $|\mathbf{x}|-v_0t+|\mathbf{x}_0|=0$. The solution of that is

$$|\mathbf{x}|=v_0t-|\mathbf{x}_0|. \tag{6.19}$$

Consequently for $t<T_0=\frac{|\mathbf{x}_0|}{v_0}$ the second component is negligible. For $t>T_0$ Eq. (6.19) describes a outgoing spherical wave front

$$|\mathbf{x}|=v_0(t-T_0). \tag{6.20}$$

Except for the phase factor $e^{i\omega_0t}$, the first term on the right hand side represents the initial wave packet displaced without the change of shape, as if no scattering has occurred. The second term is a scattered spherical wave packet representing a radially expanding replica of the initial wave packet, and $f_{\mathbf{k}_0}(\hat{x})$ is called the scattering amplitude.

The probability flux ($\frac{\hbar}{m}Im[\psi^*\nabla\psi]$ is the probability current density) of the particle incident at a detector placed out at a distance $r>>a$ from the scatterer and expand a solid angle $d\Omega$ is

$$I_{det} = r^2d\Omega|f_{\mathbf{k}_0}(\hat{r})|^2\int_{-\infty}^{\infty}dt\frac{\hbar}{m}Im[\frac{\psi^*_{pk}(\mathbf{k}_0,\hat{k}_0[r-v_0t+|\mathbf{x}_0|])}{r}$$

$$\begin{aligned} & \times \quad \frac{\partial}{\partial r}\frac{\psi_{pk}(\mathbf{k}_0, \hat{k}_0[r - v_0 t + |\mathbf{x}_0|])}{r}] \\ & = \quad d\Omega |f_{\mathbf{k}_0}(\hat{r})|^2 v_0 \int_{-\infty}^{\infty} |\psi_{pk}(\mathbf{k}_0, \hat{k}_0[r - v_0 t + |\mathbf{x}_0|])|^2 \end{aligned} \tag{6.21}$$

The incident probability flux per unit area in the beam ($\mathbf{r} = -r\hat{k}_0$) is

$$\begin{aligned} I_{in} &= \frac{\hbar}{m}\int_{\infty}^{\infty} dt \hat{k}_0 \cdot Im[\psi^*_{pk}(\mathbf{k}_0, -r\hat{k}_0 - \mathbf{v}_0 t - \mathbf{x}_0)\nabla\psi_{pk}(\mathbf{k}_0, -r\hat{k}_0 - \mathbf{v}_0 t - \mathbf{x}_0)] \\ &= v_0 \int_{\infty}^{\infty} dt |\psi_{pk}(\mathbf{k}_0, \hat{k}_0[-r - v_0 t + |\mathbf{x}_0|])|^2. \end{aligned} \tag{6.22}$$

Since

$$\int_{\infty}^{\infty} dt |\psi_{pk}(\mathbf{k}_0, \hat{k}_0[-r - v_0 t + |\mathbf{x}_0|])|^2 = \int_{-\infty}^{\infty} |\psi_{pk}(\mathbf{k}_0, \hat{k}_0[r - v_0 t + |\mathbf{x}_0|])|^2, \tag{6.23}$$

we have

$$I_{det} = d\Omega I_{in}\frac{d\sigma}{d\Omega}, \tag{6.24}$$

where the differential cross section is

$$\frac{d\sigma}{d\Omega} = |f_{\mathbf{k}_0}(\hat{x})|^2. \tag{6.25}$$

As the result to compute the differential cross section we need to obtain the scattering amplitude in Eq. (6.7).

6.2 Calculating $\psi^{(+)}_{\mathbf{k}}(\mathbf{x})$

In this subsection we shall show that Eq. (6.7) is indeed the asymptotic form of the eigensolution of

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V\right)\psi = E\psi. \tag{6.26}$$

The above equation can be reduced to

$$(\nabla^2 + k^2)\psi = U\psi, \tag{6.27}$$

where

$$k^2 = \frac{2\mu E}{\hbar^2}, \quad U = \frac{2\mu V}{\hbar^2}. \tag{6.28}$$

It is useful to view $U\psi$ on the right hand side of Eq. (6.28) temporarily as a given inhomogeneity, even though it contains the unknown function ψ. Formally, then a particular "solution" of Eq. (6.28) is conveniently constructed in terms of the Greens function $G(\mathbf{x}-\mathbf{x}')$ which the solution of equation

$$(\nabla^2 + k^2)G(\mathbf{r}-\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{6.29}$$

As usual unique solution to Eq. (6.29) requires boundary condition. We shall require, as our boundary condition that

$$G(\mathbf{x}-\mathbf{x}') \to 0, \quad \text{as } |\mathbf{x}| \to \infty. \tag{6.30}$$

In the following we shall prove that the above boundary condition amounts to adding a infinitesimal imaginary part to k, i.e. $k \to k + i\eta$ in Eq. (6.29) so that

$$[\nabla^2 + (k+i\eta)^2]G_+(\mathbf{r}-\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{6.31}$$

We shall show that in the limit $\eta \to 0$, G_+ satisfies the appropriate boundary condition. In that case

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{x}) = \frac{1}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} + \int d^3x' G_+(\mathbf{x}-\mathbf{x}')U(\mathbf{x}')\psi_{\mathbf{k}}^{(+)}(\mathbf{x}') \tag{6.32}$$

will be a general solution of Eq. (6.28). In the above the first term is the solution of the homogeneous equation

$$(\nabla^2 + k^2)\psi = 0. \tag{6.33}$$

In order to solve Eq. (6.31) let us apply Fourier transform method. Let us write

$$G_+(\mathbf{r}) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} G_+(\mathbf{q}), \tag{6.34}$$

and

$$\delta(\mathbf{r}) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}}. \tag{6.35}$$

Substitute Eq. (6.34) and Eq. (6.35) into Eq. (6.29) we obtain

$$[(k+i\eta)^2 - q^2]G_+(\mathbf{q}) = 1, \tag{6.36}$$

or

$$G_+(\mathbf{q}) = \frac{1}{(k+i\eta)^2 - q^2}. \tag{6.37}$$

Hence

$$\begin{aligned} G_+(\mathbf{r}) &= \int \frac{d^3q}{(2\pi)^3} \frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{(k+i\eta)^2 - q^2} \\ &= 2\int_0^\infty \frac{q^2 dq}{(2\pi)^2} \frac{\sin(qr)}{qr} \frac{1}{(k+i\eta)^2 - q^2} \\ &= \int_0^\infty \frac{qdq}{(2\pi)^2} \frac{1}{r} \left(\frac{e^{iqr} - e^{-iqr}}{i} \right) \frac{1}{(k+i\eta)^2 - q^2} \\ &= \int_{-\infty}^\infty \frac{qdq}{(2\pi)^2} \frac{1}{ir} e^{iqr} \frac{1}{(k+i\eta)^2 - q^2} \\ &= \frac{1}{(2\pi)^2 r} \frac{d}{dr} \int_{-\infty}^\infty dq \frac{e^{iqr}}{q^2 - (k+i\eta)^2}. \end{aligned} \tag{6.38}$$

The integrand in Eq. (6.38) has poles at

$$q = \pm(k+i\eta), \tag{6.39}$$

in the complex q-plane. The integral can be easily evaluated by contour integral and the result is

$$G_+(\mathbf{r}) = -\frac{1}{4\pi} \frac{e^{i(k+i\eta)r}}{r}. \tag{6.40}$$

As promised before G_+ vanishes as $r \to \infty$. If we now substitute the above into Eq. (6.32) we obtain, for any finite $|\mathbf{x}|$

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{x}) = \frac{1}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{4\pi} \int d^3x' \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} U(\mathbf{x}') \psi_{\mathbf{k}}^{(+)}(\mathbf{x}'). \tag{6.41}$$

Since $U(\mathbf{x}')$ is non-zero only within a range $|\mathbf{x}'| \leq a$, we can perform multipole expansion for $|\mathbf{x}| >> a$ to obtain

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{x}) \approx \frac{1}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|} \int d^3x' e^{-ik\hat{x}\cdot\mathbf{x}'} U(\mathbf{x}') \psi_{\mathbf{k}}^{(+)}(\mathbf{x}'). \tag{6.42}$$

Eq. (6.42) is precisely of the form Eq. (6.7) with

$$\begin{aligned} f_{\mathbf{k}}(\hat{x}) &= -2\pi^2 \int d^3x' e^{-ik\hat{x}\cdot\mathbf{x}'} U(\mathbf{x}')\psi_{\mathbf{k}}^{(+)}(\mathbf{x}') \\ &= -\frac{4\pi^2\mu}{\hbar^2} \int d^3x' e^{-ik\hat{x}\cdot\mathbf{x}'} V(\mathbf{x}')\psi_{\mathbf{k}}^{(+)}(\mathbf{x}'). \end{aligned} \tag{6.43}$$

6.3 Approximate solution of $f_{\mathbf{k}}$

To calculate the scattering amplitude through Eq. (6.43) we need $\psi_{\mathbf{k}}^{(+)}$ as an input. However to get $\psi_{\mathbf{k}}^{(+)}$ we need to solve the integral equation Eq. (6.42). In following we introduce several well-known approximate solution.

6.3.1 The Born approximation

In the limit that the scattering potential is weak we can replace the $\psi_{\mathbf{k}}^{(+)}$ on the right hand side of Eq. (6.42) by $\frac{1}{(2\pi)^3}e^{i\mathbf{k}\cdot\mathbf{x}}$. In that case

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{x}) \approx \frac{1}{(2\pi)^3}e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{1}{(2\pi)^3}\frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|}\int d^3x' e^{-ik\hat{x}\cdot\mathbf{x}'}U(\mathbf{x}')e^{i\mathbf{k}\cdot\mathbf{x}'}. \tag{6.44}$$

and hence

$$\begin{aligned} f_{\mathbf{k}}(\hat{x}) &= -2\pi^2 \int d^3x' e^{-ik\hat{x}\cdot\mathbf{x}'} U(\mathbf{x}')\frac{1}{(2\pi)^3}e^{i\mathbf{k}\cdot\mathbf{x}'} \\ &= -\frac{1}{4\pi}\int d^3x' e^{-i(k\hat{x}-\mathbf{k})\cdot\mathbf{x}'}U(\mathbf{x}') \\ &= -\frac{\mu}{2\pi\hbar^2}\int d^3x' e^{-i(k\hat{x}-\mathbf{k})\cdot\mathbf{x}'}V(\mathbf{x}'). \end{aligned} \tag{6.45}$$

Since $k\hat{x}$ is the final momentum and $\mathbf{k}$ is the initial one

$$\Delta\mathbf{k} = k\hat{x} - \mathbf{k}, \tag{6.46}$$

is the momentum transfer. Thus Born approximation predicts that

$$f_{\mathbf{k}}(\hat{x}) = -\frac{\mu}{2\pi\hbar^2}V(\Delta\mathbf{k}), \tag{6.47}$$

where

$$V(\Delta\mathbf{k}) \equiv \int d^3x e^{-i\Delta\mathbf{k}\cdot\mathbf{x}} V(\mathbf{x}) \tag{6.48}$$

is the Fourier transform of the scattering potential. In the case where $V(\mathbf{r}) = V_0\theta(a-r)$, we have

$$V(\Delta\mathbf{k}) = \frac{a4\pi V_0}{\Delta k^2}\cos(\Delta k a). \tag{6.49}$$

Thus

$$f_{\mathbf{k}}(\hat{x}) = -\frac{a\mu V_0}{\hbar^2\Delta k^2}\cos(\Delta k a), \tag{6.50}$$

We note that $\frac{\mu V_0}{\hbar^2}$ has the dimension of $length^{-2}$, thus we define the scattering length

$$\lambda^2 \equiv \frac{\hbar^2}{\mu V_0}, \tag{6.51}$$

andEq. (6.50) becomes

$$f_{\mathbf{k}}(\hat{x}) = -a\frac{\cos(\Delta k a)}{(\Delta k\lambda)^2}. \tag{6.52}$$

Thus the differential cross section is

$$\frac{d\sigma}{d\Omega} = a^2\frac{\cos^2(\Delta k a)}{(\Delta k\lambda)^4}. \tag{6.53}$$

Similar calculation can be carried out for potential of the form

$$V(r) = V_0\frac{e^{-\alpha r}}{\alpha r} \tag{6.54}$$

to obtain

$$f_{\mathbf{k}}(\hat{x}) = -\frac{2\mu V_0}{\hbar^2\alpha}\frac{1}{\Delta k^2+\alpha^2}. \tag{6.55}$$

The case of Coulomb scattering is given by $\alpha \to 0$ and $V_0/\alpha = q_1q_2$. In which case the above equation becomes

$$f_{\mathbf{k}}(\hat{x}) = -\frac{2\mu}{\hbar^2}\frac{q_1q_2}{\Delta k^2}. \tag{6.56}$$

Note that

$$\Delta k = 2k \sin\left(\frac{\theta}{2}\right), \tag{6.57}$$

where θ is the scattering angle. Substitute the above into Eq. (6.56) we obtain

$$f_{\mathbf{k}}(\hat{x}) = -\frac{2\mu}{\hbar^2}\frac{q_1 q_2}{4k^2 \sin^2\left(\frac{\theta}{2}\right)} = -\frac{q_1 q_2}{4E^2 \sin^2\left(\frac{\theta}{2}\right)}, \tag{6.58}$$

where $E = \frac{\hbar^2 k^2}{2\mu}$.

Hence according to the Born-approximation the differential cross section for Coulomb scattering is given by

$$\frac{d\sigma}{d\Omega} = \frac{q_1^2 q_2^2}{16E^2 \sin^2\left(\frac{\theta}{2}\right)}, \tag{6.59}$$

which is the classical Rutherford cross section. What is even more amazing is that the above result agrees with the exact evaluation of the quantum-mechanical Coulomb scattering cross section – one of many coincidence peculiar to the Coulomb potential.

It is worth emphasize that in Born approximation the differential cross section is independent on the sign of V_0. The validity of the Born approximation is given by the requirement that at $\mathbf{x} = 0$ the first term of Eq. (6.42) is much greater than the second, or,

$$1 >> \frac{1}{4\pi}\left|\int d^3x' \frac{e^{ik|\mathbf{x}'|}}{|\mathbf{x}'|} U(\mathbf{x}') e^{i\mathbf{k}\cdot\mathbf{x}'}\right|. \tag{6.60}$$

For central potential this reduces to

$$1 >> \int dr' e^{ikr'} \sin(kr') U(r') = \frac{2\mu}{\hbar^2}\int dr' e^{ikr'} \sin(kr') V(r'). \tag{6.61}$$

Substitute for V Eq. (6.54) we obtain

$$1 >> \frac{\mu|V_0|}{k\hbar^2\alpha}\sqrt{\left(\log\sqrt{1+\frac{4k^2}{\alpha^2}}\right)^2 + \left(\tan^{-1}\frac{2k}{\alpha}\right)^2}. \tag{6.62}$$

If $k/\alpha << 1$ this simplifies to

$$\frac{2\mu|V_0|}{\hbar^2\alpha^2} << 1. \tag{6.63}$$

Using the fact that the range of force $a = 1/\alpha$ we may write Eq. (6.63) as

$$|V_0| << \frac{\hbar^2}{2\mu}\frac{1}{a^2}. \tag{6.64}$$

The right hand side of Eq. (6.64) is the mean kinetic energy of a particle that is confined within $r \leq a$. If V_0 is negative the existence of bound state requires that $|V_0| \geq \frac{\hbar^2}{2\mu}\frac{1}{a^2}$. Broadly speaking, we may therefore say that in the limit of low momentum the Born approximation is valid if the potential is too weak to produce a bound state. If $k/\alpha >> 1$ Eq. (6.63) simplifies to

$$\frac{\mu|v_0|}{k\hbar^2\alpha}\log(2k/\alpha) = \frac{|V_0|a}{\hbar v}\log 2ka << 1. \tag{6.65}$$

In the above $v = \frac{\hbar k}{\mu}$ is the velocity of the particle.

Generally, the Born approximation affords a quick estimate of scattering cross section and is accurate for reasonably high energies in comparison with the interaction energy.

6.3.2 Beyond Born approximation

To obtain $f_{\mathbf{k}}$ which is accurate to second order in V, we substitute Eq. (6.44) for $\psi^{(+)}_{\mathbf{k}}$ on the right hand side of Eq. (6.32). Go to the third order we substitute the second order result, ... etc. If we denote the plane wave state by $|\mathbf{k}>$ then Born approximation amounts to

$$|\psi^{(+)}_{\mathbf{k}}> = |\mathbf{k}> + \frac{1}{E - H_0 + i\epsilon}V|\mathbf{k}> . \tag{6.66}$$

In the above we have used the fact that

$$(k + i\eta)^2 = k^2 + i\epsilon. \tag{6.67}$$

The next order approximation is given by

$$|\psi_{\mathbf{k}}^{(+)}>=|\mathbf{k}>+\frac{1}{E-H_0+i\epsilon}V|\mathbf{k}>+\frac{1}{E-H_0+i\epsilon}V\frac{1}{E-H_0+i\epsilon}V|\mathbf{k}>. \tag{6.68}$$

In this way it is clear that the generalization to all order is given by

$$\begin{aligned}|\psi_{\mathbf{k}}^{(+)}>&=\left[I+\frac{1}{E-H_0+i\epsilon}T\right]|\mathbf{k}> \\ T&=V+V\frac{1}{E-H_0+i\epsilon}V+V\frac{1}{E-H_0+i\epsilon}V\frac{1}{E-H_0+i\epsilon}V+...\end{aligned} \tag{6.69}$$

¿From Eq. (6.69) it is clear that T satisfies

$$T=V+V\frac{1}{E-H_0+i\epsilon}T. \tag{6.70}$$

Combining Eq. (6.69) and Eq. (6.70) we have

$$\begin{aligned}V|\psi^{(+)}>\quad&=V\left[I+\frac{1}{E-H_0+i\epsilon}T\right]|\mathbf{k}>=\left[V+V\frac{1}{E-H_0+i\epsilon}T\right]|k> \\ &=T|\mathbf{k}>.\end{aligned} \tag{6.71}$$

Using Eq. (6.43) the scattering amplitude can now be written as

$$f_{\mathbf{k}}(\hat{x})=-(2\pi)^3\frac{4\pi^2\mu}{\hbar^2}<k\hat{x}|T|\mathbf{k}>. \tag{6.72}$$

In the above we have chosen the convention that $<\mathbf{x}|\mathbf{k}>=\frac{1}{(2\pi)^3}e^{i\mathbf{k}\cdot\mathbf{x}}$. We note that since $k\hat{x}$ is the momentum of the detected particle we can rewrite the above equation in a more physically transparent way

$$f(\mathbf{k}_f,\mathbf{k}_i)=-(2\pi)^3\frac{4\pi^2\mu}{\hbar^2}<\mathbf{k}_f|T|\mathbf{k}_i>, \tag{6.73}$$

where $\mathbf{k}_i$ is the momentum of the incoming particle and $\mathbf{k}_f$ is the momentum of the detected one.

6.4 Optical theorem

There is a very famous relationship due to Bohr, Peirls and Placzek, called the optical theorem. This theorem relates the imaginary part of the forward scattering (i.e. $\mathbf{k}_f = \mathbf{k}_i$) amplitude to the total cross section as follows;

Optical theorem

$$Im[f(\mathbf{k},\mathbf{k})] = \frac{k}{4\pi}\sigma_{tot}, \tag{6.74}$$

where

$$\sigma_{tot} = \int d\Omega \frac{d\sigma}{d\Omega}. \tag{6.75}$$

Proof. From Eqhty we have

$$Im[f(\mathbf{k}_f,\mathbf{k}_i)] = -(2\pi)^3 \frac{4\pi^2\mu}{\hbar^2} Im[<\mathbf{k}|T|\mathbf{k}>]. \tag{6.76}$$

We next evaluate $Im[<\mathbf{k}|T|\mathbf{k}>]$. From Eq. (6.71) we have

$$Im[<\mathbf{k}|T|\mathbf{k}>] = Im[<\mathbf{k}|V|\psi_{\mathbf{k}}^{(+)}>]. \tag{6.77}$$

Since

$$|\psi_{\mathbf{k}}^{(+)}>= \left[I + \frac{1}{E - H_0 + i\epsilon}T\right]|\mathbf{k}>= |\mathbf{k}> + \frac{1}{E - H_0 + i\epsilon}V|\psi_{\mathbf{k}}^{(+)}>, \tag{6.78}$$

we have

$$Im[<\mathbf{k}|T|\mathbf{k}>] = Im[\left(<\psi_{\mathbf{k}}^{(+)}| - <\psi_{\mathbf{k}}^{(+)}|V\frac{1}{E - H_0 - i\epsilon}\right)V|\psi_{\mathbf{k}}^{(+)}>]. \tag{6.79}$$

Since $<\psi_{\mathbf{k}}^{(+)}|V|\psi_{\mathbf{k}}^{(+)}>$ is real we have

$$Im[<\mathbf{k}|T|\mathbf{k}>] = -Im\left[<\psi_{\mathbf{k}}^{(+)}|V\frac{1}{E - H_0 - i\epsilon}V|\psi_{\mathbf{k}}^{(+)}>\right]. \tag{6.80}$$

Now we use the well-known relation

$$\frac{1}{E - H_0 - i\epsilon} = \frac{P}{E - H_0} + i\pi\delta(E - H_0). \tag{6.81}$$

(here P projects out the zeros of $E - H_0$) we have

$$Im[< \mathbf{k}|T|\mathbf{k} >] = -Im\left[< \psi_{\mathbf{k}}^{(+)}|V\frac{P}{E-H_0}V + i\pi V\delta(E-H_0)V|\psi_{\mathbf{k}}^{(+)} >\right]. \tag{6.82}$$

Since $V\frac{P}{E-H_0}V$ is hermitian we have

$$\begin{aligned} Im[< \mathbf{k}|T|\mathbf{k} >] \quad &= -\pi < \psi_{\mathbf{k}}^{(+)}|V\delta(E-H_0)V|\psi_{\mathbf{k}}^{(+)} > \\ &= -\pi < \mathbf{k}|T\delta(E-H_0)T|\mathbf{k} > . \end{aligned} \tag{6.83}$$

Let us now insert complete set of momentum states between T and $\delta(E - H_0)$ we obtain

$$\begin{aligned} Im[< \mathbf{k}|T|\mathbf{k} >] \quad &= -\pi(2\pi)^3 \int d^3q < \mathbf{k}|T|\mathbf{q} > \delta(E - \frac{\hbar^2 q^2}{2\mu}) < \mathbf{q}|T|\mathbf{k} > \\ &= -\pi(2\pi)^3 \int d\Omega_q \frac{\mu k}{\hbar^2}| < \mathbf{q}|T|\mathbf{k} > |^2. \end{aligned} \tag{6.84}$$

Using Eq. (6.73) we obtain

$$\begin{aligned} Im[f(\mathbf{k},\mathbf{k})] \quad &= \frac{k}{4\pi}\int d\Omega_q |f(\mathbf{q},\mathbf{k})|^2 \\ &= \frac{k}{4\pi}\int d\Omega_q \frac{d\sigma}{d\Omega} \\ &= \frac{k}{4\pi}\sigma_{tot}. \end{aligned} \tag{6.85}$$

6.5 Scattering by central potentials - partial wave analysis

Let us reiterate the two important equation obtained before

$f(\mathbf{k}_f, \mathbf{k}_i) = -(2\pi)^3 \frac{4\pi^2\mu}{\hbar^2} < \mathbf{k}_f|T|\mathbf{k}_i >$,

and

$T = V + V\frac{1}{E-H_0+i\epsilon}V + ...$

In the case where the scattering potential is spherically symmetric we have

$$U^+TU = T, \tag{6.86}$$

where U is the rotation operator. In that case it is advantageous to express $|\mathbf{k}_i>$ and $|\mathbf{k}_f>$ in terms of the spherical harmonics so that we can use the Wigner-Eckart theorem.

If we write

$$|\mathbf{k}>=\sum_{lm} C_{\mathbf{k},lm}|k,l,m>, \tag{6.87}$$

then

$$f(\mathbf{k}_f,\mathbf{k}_i) = -(2\pi)^3\frac{4\pi^2\mu}{\hbar^2}\sum_{lm,l'm'} C^*_{\mathbf{k}_f,l'm'}C_{\mathbf{k}_i,lm} < k,l'm'|T|k,lm> . \tag{6.88}$$

In Eq. (6.87)

$$|k,lm>\equiv \int d\Omega_k Y^*_{lm}(\Omega_k)|\mathbf{k}> . \tag{6.89}$$

As the result

$$C_{\mathbf{k},lm} = Y^*_{lm}(\hat{k}). \tag{6.90}$$

Due to the Wigner Eckart theorem we have

$$< k,l'm'|T|k,lm >= T_l(k)\delta_{l'l}\delta_{m'm}, \tag{6.91}$$

Eq. (6.88) simplifies to

$$\begin{aligned} f(\mathbf{k}_f,\mathbf{k}_i) &= -(2\pi)^3\frac{4\pi^2\mu}{\hbar^2}\sum_{lm} C^*_{\mathbf{k}_f,lm}C_{\mathbf{k}_i,lm}T_l(k) \\ &= -(2\pi)^3\frac{4\pi^2\mu}{\hbar^2}\sum_{lm} Y_{lm}(\hat{k}_f)Y^*_{lm}(\hat{k}_i)T(k). \end{aligned} \tag{6.92}$$

Use the fact that[2]

$$\sum_{lm} Y^*_{lm}(\hat{k}_i)Y_{lm}(\hat{k}_f) = \sum_l \frac{2l+1}{4\pi}P_l(\hat{k}_i\cdot\hat{k}_f), \tag{6.93}$$

[2]See, e.g., "Mathematical methods of physics", 2nd edition, Mathews and Walker, page 117.

we simplifies Eq. (6.92) to

$$f(\mathbf{k}_f, \mathbf{k}_i) = \sum_l f_l(k)(2l+1)P_l(\hat{k}_i \cdot \hat{k}_f), \tag{6.94}$$

where

$$f_l(k) \equiv -\frac{8\pi^4\mu}{\hbar^2} T_l(k). \tag{6.95}$$

We note that Eq. (6.94) completely determines the angular distribution of differential cross section, i.e.,

$$\frac{d\sigma}{d\Omega} = |\sum_l f_l(k)(2l+1)P_l(\hat{k}_i \cdot \hat{k}_f)|^2. \tag{6.96}$$

Thus by measuring $\frac{d\sigma}{d\Omega}$ distribution one can deduce $f_l(k)$. By integrating the above equation over the scattering angle we obtain

$$\sigma_{tot} = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi \sum_l |f_l(k)|^2(2l+1). \tag{6.97}$$

At this point we should not have the impression that we have solved the scattering problem. All we did was to find a good way to parametrize the scattering amplitude. The quantity $f_l(k)$ in Eq. (6.95) is still unknown.

To appreciate the physical significance of $f_l(k)$ let us study the asymptotic behavior of $\psi^{(+)}_{\mathbf{k}}(\mathbf{x})$. Let us recall Eq. (6.7) namely,

$$\psi^{(+)}_{\mathbf{k}}(\mathbf{x}) = \tfrac{1}{(2\pi)^3}\left(e^{i\mathbf{k}\cdot\mathbf{x}} + f(k\hat{x}, \mathbf{k})\tfrac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|}\right).$$

By substituting Eq. (6.94) into the above we obtain

$$\begin{aligned}\psi^{(+)}_{\mathbf{k}}(\mathbf{x}) &= \frac{1}{(2\pi)^3}\left(e^{i\mathbf{k}\cdot\mathbf{x}} + \sum_l f_l(k)(2l+1)P_l(\hat{k}\cdot\hat{x})\frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|}\right) \\ &= \frac{1}{(2\pi)^3}\left(e^{ik|\mathbf{x}|(\hat{k}\cdot\hat{x})} + \sum_l f_l(k)(2l+1)P_l(\hat{k}\cdot\hat{x})\frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|}\right).\end{aligned} \tag{6.98}$$

Using the fact that[3]

$$\frac{1}{(2\pi)^3}e^{ik|\mathbf{x}|(\hat{k}\cdot\hat{x})} = \frac{1}{(2\pi)^3}\sum_l (2l+1)j_l(k|\mathbf{x}|)P_l(\hat{k}\cdot\hat{x}), \tag{6.99}$$

and the fact that as $|\mathbf{x}| \to \infty$[4]

$$j_l(|\mathbf{x}|) \to \frac{e^{i(k|\mathbf{x}|-l\pi/2)-e^{-i(k|\mathbf{x}|-l\pi/2)}}}{2ik|\mathbf{x}|} \tag{6.100}$$

we have as $|\mathbf{x}| \to \infty$

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{x}) \to \frac{1}{2ik(2\pi)^3}\sum_l (2l+1)P_l(\hat{k}\cdot\hat{x})\left([1+2ikf_l(k)]\frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|} - \frac{e^{-i(k|\mathbf{x}|-l\pi)}}{|\mathbf{x}|}\right). \tag{6.101}$$

The physics of scattering is now clear. When the scatterer is absent, we can analyze the plane wave as sum of a spherically outgoing wave $\sim \frac{e^{ik|\mathbf{x}|}}{|\mathbf{x}|}$ and a spherically incoming wave $\sim -\frac{e^{i(k|\mathbf{x}|-l\pi)}}{|\mathbf{x}|}$ for each l. While the scatterer leaves the incoming wave completely unaffected it changes the coefficient of the outgoing wave as follows

$$1 \to 1 + i2kf_l(k) \equiv S_l(k). \tag{6.102}$$

Due to probability conservation, that is whatever coming in the lth angular momentum channel must go out, we expect the coefficient of $e^{ik|\mathbf{x}|}/|\mathbf{x}|$ to have the same magnitude as the coefficient of $e^{-ik|\mathbf{x}|}/|\mathbf{x}|$. This means

$$|S_l(k)| = 1, \tag{6.103}$$

or

$$S_l(k) = e^{2i\delta_l}. \tag{6.104}$$

We thus see that the only change in the wavefunction at a large distance as a result of scattering is to change the phase of the outgoing wave. Returning to f_l we can write

$$f_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{e^{i\delta_l}\sin\delta_l}{k}. \tag{6.105}$$

[3]See, e.g., "Modern quantum mechanics" Sakurai, page 398.

[4]See, e.g., "Modern quantum mechanics" Sakurai, page 398.

Substitute the above in Eq. (6.94) we obtain

$$f(\mathbf{k}_f, \mathbf{k}_i) = \sum_l (2l+1) e^{i\delta_l} \sin\delta_l P_l(\hat{k}_i \cdot \hat{k}_f). \tag{6.106}$$

Put the above into Eq. (6.97) we obtain

$$\sigma_{tot} = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi \sum_l (2l+1) \sin^2\delta_l. \tag{6.107}$$

Chapter 7

A few words on many-body problems

Quantum mechanical problems are seldomly solvable. Some take the point of view that with the help of modern computer this is no longer a problem at least in principle. While this viewpoint might be true for one-body problems it is fundamentally wrong for the many-body problems. As we discussed in the example of quantum spin chains the size of Hilbert space grows exponentially with the number of degrees of freedom. [1] Because of this fast increase of the dimension of the Hamiltonian, brute force diagonalization approach is in-tractable. In fact unless some special condition exist many-body problems are in general non-integrable.

7.1 Identical particles and their quantum statistics

For reason that we will not step into here, in quantum mechanics "identical particles" not only mean that the Hamiltonian operator $H(\mathbf{r}_1, \mathbf{p}_1; \mathbf{r}_2, \mathbf{p}_2; ...)$ is invariant under the permutation of particle labels i.e.,

$$H(\mathbf{r}_{P1}, \mathbf{p}_{P1}; \mathbf{r}_{P2}, \mathbf{p}_{P2}; ...) = H(\mathbf{r}_1, \mathbf{p}_1; \mathbf{r}_2, \mathbf{p}_2; ...), \tag{7.1}$$

[1] For the spin chain it grows as 2^N

but also require that the wavefunction has to be symmetric or antisymmetric

$$\psi(\mathbf{r}_{P1}, ...\mathbf{r}_{PN}; \sigma_{P1}, ..., \sigma_{PN}) = (\pm 1)^P \psi(\mathbf{r}_1, ..., \mathbf{r}_N; \sigma_1, ..., \sigma_N). \quad (7.2)$$

Particles whose wavefunction satisfies the upper sign is call bosons while those satisfying the lower sign are call fermions.

7.2 Many electron atoms

The success of hydrogen atom is largely responsible for the early acceptance of the quantum theory. From this point of view it is ironic that except for the simplest atom, hydrogen, none of the other atoms are exactly solved under the framework of quantum mechanics. The next simplest atom in the periodic table is Helium. Helium has a nucleus of charge $2e$ and two electrons. After redefining the coordinate from $\mathbf{x}_1, \mathbf{x}_2, \mathbf{X}$ to $\mathbf{R} = \frac{m\mathbf{x}_1 + m\mathbf{x}_2 + M\mathbf{R}}{2m+M}, \mathbf{r}_1 = \mathbf{x}_1 - \mathbf{X}, \mathbf{r}_2 = \mathbf{x}_2 - \mathbf{X}$, the Hamiltonian read

$$H = \left[-\frac{1}{2\mu}\nabla_1^2 - \frac{1}{2\mu}\nabla_2^2 - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \right]. \quad (7.3)$$

(Here $\mu = \frac{Mm}{m+M}$.) The reason that Eq. (7.3) is difficult to solve is due to the presence of electron-electron interaction, $\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$. In addition to the above the helium problem has a new feature that we have not encounter before, namely, it consists of two identical electrons.

Electrons are, of course, fermions. As the result we require

$$\psi(\mathbf{r}_1, \mathbf{r}_2; \sigma_1, \sigma_2) = -\psi(\mathbf{r}_1, \mathbf{r}_2; \sigma_1, \sigma_2). \quad (7.4)$$

Since the the Hamiltonian in Eq. (7.3) does not depend on the spin variables, we can separate ψ into the products of orbital and spin parts:

$$\psi(\mathbf{r}_1, \mathbf{r}_2; \sigma_1, \S_2) = \phi(\mathbf{r}_1, \mathbf{r}_2)\chi(\sigma_1, \sigma_2). \quad (7.5)$$

Since spin rotation commute with the Hamiltonian, we can choose the eigen state to be that of the total S^2 and S_z. For two electrons there are only two possibilities.

$$\begin{aligned} &i) S^2\chi(\sigma_1, \sigma_2) = 0(0+1)\chi(\sigma_1, \sigma_2) \quad or \\ &ii) S^2\chi(\sigma_1, \sigma_2) = 1(1+1)\chi(\sigma_1, \sigma_2). \end{aligned} \quad (7.6)$$

In the first case we say that the two atoms are in the singlet state, and in the second we say that they are in the triplet state. The singlet state consists of only one state

$$\chi_s(\sigma_1, \sigma_2) = \delta_{\sigma_1,1/2}\delta_{\sigma_2,-1/2} - \delta_{\sigma_1,-1/2}\delta_{\sigma_2,1/2}. \tag{7.7}$$

The triplet consists of three states

$$\begin{aligned}
&\chi_{t+1}(\sigma_1, \sigma_2) = \delta_{\sigma_1,1/2}\delta_{\sigma_2,1/2} \\
&\chi_{t0}(\sigma_1, \sigma_2) = \delta_{\sigma_1,1/2}\delta_{\sigma_2,-1/2} + \delta_{\sigma_1,-1/2}\delta_{\sigma_2,1/2} \\
&\chi_{t-1}(\sigma_1, \sigma_2) = \delta_{\sigma_1,-1/2}\delta_{\sigma_2,-1/2}.
\end{aligned} \tag{7.8}$$

While χ_s is antisymmetric under the exchange of σ_1 and σ_2, $\chi_{t,m}$ are symmetric. As the result the Helium eigenfunctions are of the form

$$\begin{aligned}
&\phi_{sym}(\mathbf{r}_1, \mathbf{r}_2)\chi_s(\sigma_1, \sigma_2), \quad \textit{or} \\
&\phi_{antsym}(\mathbf{r}_1, \mathbf{r}_2)\chi_{t,m}(\sigma_1, \sigma_2).
\end{aligned} \tag{7.9}$$

Since Eq. (7.3) is rotational invariant we expect on symmetry ground that $\phi(\mathbf{r}_1, \mathbf{r}_2)$ can be chosen to be the eigen state of L^2 and L_z. Here $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$ is the total orbital angular momentum operator. So clearly the eigenfunctions of helium can be labeled by $|L, L_z, S, S_z>$. For example one choice of coordinate gives

$$\phi_{lm}(\mathbf{r}_1, \mathbf{r}_2) = Y_{lm}(\hat{r}_1)R(r_1, r_2, \hat{r}_1 \cdot \hat{r}_2). \tag{7.10}$$

Thus after the symmetry reduction, we have an effective 3-dimensional $(r_1, r_2, \hat{r}_1 \cdot \hat{r}_2)$ problem. This is analogous to the hydrogen case where the symmetry reduction deduce the problem to one dimensional (r).

There are many other possible choices of coordinate. Although they all inevitably lead to a three dimensional problem, the complexity of the actual equation can depend greatly on the choice of coordinate. Recently Prof. Wu-Yi Hsiang of Berkeley has achieved a very elegant choice of the coordinate. Hopefully this will lead to progress in the final analytic solution of the helium atom.

So after a century of quantum mechanics, none but the simplest atom in nature can be exactly solved.

In general in the presence of spin-orbit interaction $\mathbf{L} \cdot \mathbf{S}$ the eigen states of a many-electron atom can be classified as $|L, S, J, J_z>$ In the

absence of rotational symmetry breaking, such as external magnetic field, the energy is a function of L, S and J. The atomic symbol is designed to be

$$^{2S+1}L_J, \tag{7.11}$$

where

L=	0	1	2	3	...
	S	P	D	F	...

7.3 Delta-function interacting particles in one-dimension

It turns out that in one space dimension if the interaction between particles is delta-function like, i.e.

$$H = -\frac{\hbar^2}{2m}\sum_i \partial_{x_i}^2 + V\sum_{(i,j)}\delta(x_i - x_j), \tag{7.12}$$

the problem is exactly solvable. The technique used to solve these problems is called Bethe ansatz. This technique is a bit to technical for us to get into here but we can demonstrate part of this technique by looking at its application to the two-particle case.

7.3.1 The two-particle case

In one space dimension two particles of momenta k_1 and k_2 collide with each other must end up with two particles with momenta k_1 and k_2. The momenta of the particle can switch, but that is the maximum allowed change. This is a simple consequence of the energy and momentum conservation:

$$\begin{aligned} k_1^2 + k_2^2 &= k_1'^2 + k_2'^2 \\ k_1 + k_2 &= k_1' + k_2'. \end{aligned} \tag{7.13}$$

Squaring the second equation and compare with the first, we obtain

$$k_1 k_2 = k_1' k_2'. \tag{7.14}$$

Let $k_1 k_2 = k_1' k_2' = C$ and $k_1 = \frac{C}{r}$, $k_2 = Cr$, and $k_1' = \frac{C}{r'}$, $k_2' = Cr'$. Then the second of Eq. (7.13) implies

$$\frac{1}{r} + r = \frac{1}{r'} + r'. \tag{7.15}$$

We notice that

$$x + \frac{1}{x} = K \tag{7.16}$$

has two solutions

$$x = \frac{K \pm \sqrt{K^2 - 4}}{2}. \tag{7.17}$$

It is simple to see that the two roots are reciprocal of each other. Thus

$$r' = r \quad , or, \quad r' = \frac{1}{r}. \tag{7.18}$$

Thus

$$\begin{aligned} k_1' = k_1; \quad k_2' = k_2, \quad or \\ k_1' = k_2; \quad k_2' = k_1. \end{aligned} \tag{7.19}$$

The second thing we should get familiar with is the two-particle scattering problem, Let us assume $k_1 > k_2$ and imagine originally $x_1 < x_2$. The incoming 2-particle wavefunctions is $e^{i(k_1 x_1 + k_2 x_2)}$. The reflected wavefunction is then $Re^{i(k_2 x_1 + k_1 x_2)}$ in $x_1 < x_2$. The transmitted wavefunction sits in the configuration space $x_1 > x_2$ and the wavefunction is $Te^{i(k_1 x_1 + k_2 x_2)}$. Thus this scattering state solution read

$$\begin{aligned} \Psi_{scatt,1}(x_1, x_2) \quad &= e^{i(k_1 x_1 + k_2 x_2)} + Re^{i(k_2 x_1 + k_1 x_2)} \quad ; x_1 < x_2 \\ &= Te^{i(k_1 x_1 + k_2 x_2)} \quad ; x_1 > x_2, \end{aligned} \tag{7.20}$$

where

$$\begin{aligned} R &= -\frac{1}{1 + iz} \\ T &= \frac{iz}{1 + iz} \\ z &= \frac{k_2 - k_1}{c}. \end{aligned} \tag{7.21}$$

In the above

$$c = \frac{mV}{\hbar^2}. \tag{7.22}$$

In addition to Eq. (7.20) there is another scattering state solution: i.e. in $x_1 > x_2$ the momentum of the first/second particle is k_2/k_1. The reflected wave in $x_1 > x_2$ is $R'e^{i(k_1x_1+k_2x_2)}$, and the transmitted wave in $x_1 < x_2$ is $T'e^{i(k_2x_1+k_1x_2)}$. Thus

$$\begin{aligned} \Psi_{scatt,2}(x_1, x_2) \quad &= e^{i(k_2x_1+k_1x_2)} + Re^{i(k_1x_1+k_2x_2)} \quad ; x_1 > x_2 \\ &= Te^{i(k_2x_1+k_1x_2)} \quad ; x_1 < x_2. \end{aligned} \tag{7.23}$$

We note that

$$\Psi_{scatt,2}(x_1, x_2) = \Psi_{scatt,1}(x_2, x_1). \tag{7.24}$$

Since $\Psi_{scatt,1}$ and $\Psi_{scatt,2}$ have the same energy, the eigen solution is a linear combination of them

$$\Psi(x_1, x_2) = \Psi_{scatt,1}(x_1, x_2) + A\Psi_{scatt,2}(x_1, x_2). \tag{7.25}$$

Thus

$$\begin{aligned} \Psi(x_1, x_2) \quad &= \{e^{i(k_1x_1+k_2x_2)} + Re^{i(k_2x_1+k_1x_2)}\} \\ &+A\{Te^{i(k_2x_1+k_1x_2)}\} \quad ; x_1 < x_2 \\ &= \{Te^{i(k_1x_1+k_2x_2)}\} + A\{e^{i(k_2x_1+k_1x_2)} \\ &+Re^{i(k_1x_1+k_2x_2)}\} \quad ; x_1 > x_2 \end{aligned} \tag{7.26}$$

7.3.2 Two Bosons

The symmetry on the bosonic wavefunction requires

$$\Psi(x_1, x_2) = \Psi(x_2, x_1), \tag{7.27}$$

which implies

$$A = 1. \tag{7.28}$$

As the result,

$$\begin{aligned}\Psi(x_1,x_2) &= e^{i(k_1x_1+k_2x_2)} + (R+T)e^{i(k_2x_1+k_1x_2)} \quad ; x_1 < x_2 \\ &= (R+T)e^{i(k_1x_1+k_2x_2)} + e^{i(k_2x_1+k_1x_2)} \quad ; x_1 > x_2,\end{aligned} \tag{7.29}$$

where

$$R+T = -\frac{1-iz}{1+iz} = e^{i2\phi}, \tag{7.30}$$

where

$$tan^{-1}(2\phi) = -\frac{2z}{1-z^2}. \tag{7.31}$$

or

$$\phi = -tan^{-1}z. \tag{7.32}$$

Thus we have

$$\begin{aligned}\Psi(x_1,x_2) &= e^{i(k_1x_1+k_2x_2)} + e^{i\theta}e^{i(k_2x_1+k_1x_2)} \quad ; x_1 < x_2 \\ &= e^{i\theta}e^{i(k_1x_1+k_2x_2)} + e^{i(k_2x_1+k_1x_2)} \quad ; x_1 > x_2 \\ \theta &= 2\tan^{-1}(\frac{k_1-k_2}{c}),\end{aligned} \tag{7.33}$$

where $k_1 > k_2$ and $|tan^{-1}x| \leq \frac{\pi}{2}$.

In order to quantize the allowed momenta we impose the periodic boundary condition. Let L be the dimension of the system and let $x_1 < x_2$. The periodic boundary condition requires that

$$e^{i(k_1x_1+k_2x_2)} + e^{i\theta}e^{i(k_2x_1+k_1x_2)} = e^{i\theta}e^{i(k_1(x_1+L)+k_2x_2)} + e^{i(k_2(x_1+L)+k_1x_2)} \tag{7.34}$$

Similarly

$$e^{i(k_1x_1+k_2(x_2+L))} + e^{i\theta}e^{i(k_2x_1+k_1(x_2+L))} = e^{i\theta}e^{i(k_1x_1+k_2x_2)} + e^{i(k_2x_1+k_1x_2)}. \tag{7.35}$$

These equation requires

$$\begin{aligned}e^{ik_1L} &= e^{-i\theta} = e^{-2i\tan^{-1}(\frac{k_1-k_2}{c})} \\ e^{ik_2L} &= e^{i\theta} = e^{2i\tan^{-1}(\frac{k_1-k_2}{c})},\end{aligned} \tag{7.36}$$

and the eigen energy is

$$E = \frac{\hbar^2}{2m}(k_1^2+k_2^2). \tag{7.37}$$

7.3.3 Two fermions

For two fermions if the spin wavefunction is a singlet then the orbital wavefunction is symmetric. In that case the orbital wavefunction is the same as that of two bosons. In the case where the spin wavefunction is a triplet, the orbital wavefunction has to be antisymmetric. In that case A in Eq. (7.25) is

$$A = -1. \tag{7.38}$$

, and

$$\begin{aligned} \Psi(x_1, x_2) &= e^{i(k_1 x_1 + k_2 x_2)} + (R - T) e^{i(k_2 x_1 + k_1 x_2)} \quad ; x_1 < x_2 \\ &= (T - R) e^{i(k_1 x_1 + k_2 x_2)} - e^{i(k_2 x_1 + k_1 x_2)} \quad ; x_1 > x_2, \end{aligned} \tag{7.39}$$

where

$$T - R = \frac{1 + iz}{1 + iz} = 1. \tag{7.40}$$

Thus we have

$$\begin{aligned} \Psi(x_1, x_2) &= e^{i(k_1 x_1 + k_2 x_2)} - e^{i(k_2 x_1 + k_1 x_2)} \quad ; x_1 < x_2 \\ &= e^{i(k_1 x_1 + k_2 x_2)} - e^{i(k_2 x_1 + k_1 x_2)} \quad ; x_1 > x_2. \end{aligned} \tag{7.41}$$

As the result

$$\Psi(x_1, x_2) = \det \begin{pmatrix} e^{ik_1 x_1} & e^{ik_1 x_2} \\ e^{ik_2 x_1} & e^{ik_2 x_2} \end{pmatrix}, \tag{7.42}$$

the solution of the free-fermion problem. This is expected because for antisymmetric orbital wavefunction (which vanishes when two particle coincide) delta-function interaction is invisible.