Physics

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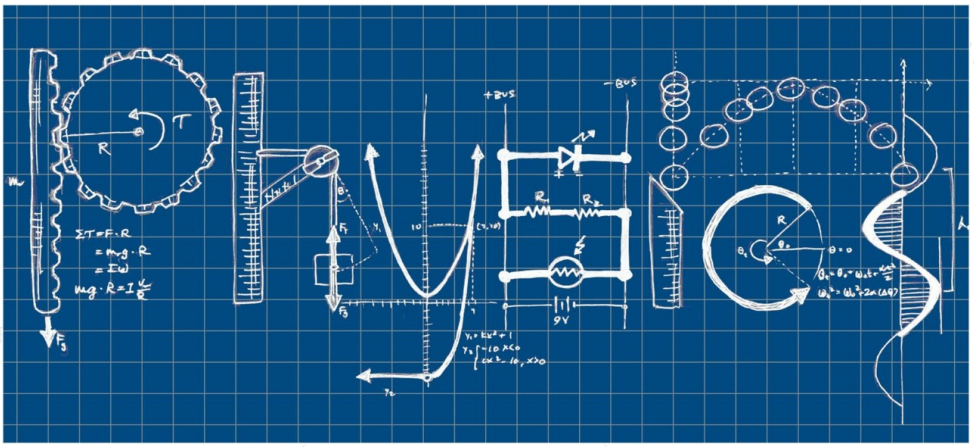

Do not ask what it is. Ask what you can say about it.

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Chapter 1
Linear Algebra

1.1 Linear Vector Space

1.1.1 Definition

Definition 1.1 Linear vector space

A linear vector space is a set of elements, called vectors, which is closed under addition and multiplication by scalars. That is to say, if ϕ and ψ are vectors then so is $a\phi + b\psi$, where a and b are arbitrary scalars. If the scalars belong to the field of complex (real) numbers, we speak of a complex (real) linear vector space. Henceforth the scalars will be complex numbers unless otherwise stated.

Example:

1. Discrete vectors, which may be represented as columns of complex numbers.

2. Spaces of functions of some type, for example the space of all differentiable functions

1.1.2 Linear independence

Definition 1.2 Linear independence

A set of vectors $\{\phi_n\}$ is said to be linearly independent if no non-trivial linear combination of them sums to zero; that is to say, if the equation $\sum_n c_n\phi_n$ can hold only when $c_n = 0$ for all n. If this condition does not hold, the set of vectors is said to be linearly dependent, in which case it is possible to express a member of the set as a linear combination of the others.

Definition 1.3 Dimension

The maximum number of linearly independent vectors in a space is called the dimension of the space.

Definition 1.4 Base

A maximal set of linearly independent vectors is called a basis for the space. Any vector in the space can be expressed as a linear combination of the basis vectors.

1.1.3 Inner product

Definition 1.5 Inner product

An inner product (or scalar product) for a linear vector space associates a scalar (ϕ, ψ) *with every ordered pair of vectors. It must satisfy the following properties:*

1. $(\phi, \psi) =$ *a complex number*
2. $(\phi, \psi) = (\psi, \phi)^*$
3. $(\phi, c_1\psi_1 + c_2\psi_2) = c_1(\phi, \psi_1) + c_2(\phi, \psi_2)$
4. $(\phi, \phi)geq0$*,with equality holding if and only if* $\phi = 0$

Example:

1. If ψ is the column vector with elements a_1, a_2, $\cdots$, and ϕ is the column vector with elements b_1, b_2, $\cdots$, then

$$(\psi, \phi) = a_1^* b_1 + a_2^* b_2 + \cdots$$

2. If ψ and ϕ are functions of x, then

$$(\phi, \psi) = \int \phi^*(x)\psi(x)w(x)dx$$

where $w(x)$ is some non-negative weight function.

Definition 1.6 Norm

$$||\phi|| = (\phi, \phi)^{\frac{1}{2}}$$

Theorem 1.1 Schwarz's inequality

$$|(\psi, \phi)|^2 \leq (\psi, \psi)(\phi, \phi)$$

Theorem 1.2 triangle inequality

$$||(\psi + \phi)|| \leq ||\phi|| + ||\psi||$$

Definition 1.7 Orthonormal

A set of vectors $\{\phi_n\}$ is said to be orthonormal if the vectors are pairwise orthogonal and of unit norm; that is to say, their inner products satisfy $(\psi_m, \phi_n) = \delta_{mn}$.

1.1.4 Dual space

Definition 1.8 Dual vector

Corresponding to any linear vector space V there exists the dual space of linear functionals on V . A linear functional F assigns a scalar $F(\phi)$ to each vector ϕ, such that

$$F(a\phi + b\psi) = aF(\phi) + bF(\psi)$$

for any vectors for ϕ and ψ, and any scalars a and b. The set of linear functionals may itself be regarded as forming a linear space V' if we define the sum of two functionals as

$$(F_1 + F_2)(\phi) = F_1(\phi) + F_2(\phi)$$

Theorem 1.3 Riesz theorem

There is a one-to-one correspondence between linear functionals F in V' and vectors f in V, such that all linear functionals have the form

$$F(\phi) = (f, \phi)$$

f being a fixed vector, and ϕ being an arbitrary vector. Thus the spaces V and V' are essentially isomorphic.

1.1.5 Dirac's bra and ket notation

In Dirac' s notation, which is very popular in quantum mechanics, the vectors in V are called ket vectors, and are denoted as $|\phi\rangle$. The linear functionals in the dual space V' are called bra vectors, and are denoted as $\langle F|$. The numerical value of the functional is denoted as

$$F(\phi) = \langle F|\phi\rangle$$

According to the Riesz theorem, there is a one-to-one correspondence between bras and kets. Therefore we can use the same alphabetic character for the functional (a member of V') and the vector (in V) to which it corresponds, relying on the bra, $\langle F|$, or ket, $|F\rangle$, notation to determine which space is referred to.So

$$\langle F|\phi\rangle = (F, \phi)$$

Note that the Riesz theorem establishes, by construction, an antilinear correspondence between bras and kets. If $\langle F| \leftrightarrow |F\rangle$, then

$$c_1^*\langle F_1| + c_2^*\langle F_2| \leftrightarrow c_1|F_1\rangle + c_2|F_2\rangle$$

1.2 Linear Operators

Definition 1.9 Linear operators

An operator on a vector space maps vectors onto vectors. A linear operator satisfies

$$A(c_1\psi_1 + c_2\psi_2) = c_1A(\psi_1) + c_2A(\psi_2)$$

Define the sum and product of operators,

$$\begin{aligned}(A+B)\psi &= A\psi + B\psi \\ AB\psi &= A(B\psi)\end{aligned}$$

Define their action to the left on bra vectors as

$$(\langle\phi|A)\psi\rangle = \langle\phi|(A|\psi\rangle)$$

So we may define the operation of A on the bra space of functionals as

$$AF_\phi(\psi) = F_\phi(A\psi)$$

According to the Riesz theorem there must exist a ket vector χ such that

$$AF_\phi(\psi) = (\chi, \psi) = F_\chi(\psi)$$

Define operator $A^\dagger$ as

$$AF_\phi = F_{A^\dagger\chi}$$

Therefore,

$$(A^\dagger\phi, \psi) = (\phi, A\psi)$$
$$\langle\psi|A^\dagger|\phi\rangle^* = \langle\phi|A|\psi\rangle$$

Definition 1.10 Outer product

$$(|\psi\rangle\langle\phi|)|\lambda\rangle \equiv |\psi\rangle(\langle\phi|\lambda\rangle)$$

Definition 1.11 Trace

$$\mathrm{Tr}A \equiv \sum \langle u_j|A|u_j\rangle$$

where $\{u_j\}$ may be any orthonormal basis. It can be shown that the value of $\mathrm{Tr}A$ is independent of the particular orthonormal basis that is chosen for its evaluation.

Proposition 1.1

$$\begin{aligned}(cA)^\dagger &= c^* A^\dagger \\ (A+B)^\dagger &= A^\dagger + B^\dagger \\ (AB)^\dagger &= B^\dagger A^\dagger\end{aligned}$$

$$(|\psi\rangle\langle\phi|)^\dagger = |\phi\rangle\langle\psi|$$

1.3 Self-Adjoint operators

Definition 1.12 Self-Adjoint operators

An operator A that is equal to its adjoint $A^\dagger$ is called self-adjoint. This means that it satisfies

$$\langle\phi|A|\psi\rangle = \langle\psi|A|\phi\rangle^*$$

and that the domain of A coincides with the domain of $A^\dagger$. An operator that only satisfies above equation is called Hermitian.

Theorem 1.4

If $\langle\psi|A|\psi\rangle = \langle\psi|A|\psi\rangle^*$ for all $|\psi\rangle$, then it follows that $\langle\phi_1|A|\phi_2\rangle = \langle\phi_2|A|\phi_1\rangle^*$ for all $|\phi_1\rangle$ and $|\phi_2\rangle$, and hence that $A = A^\dagger$.
If an operator acting on a certain vector produces a scalar multiple of that same vector,

$$A|\phi\rangle = a|\phi\rangle$$

we call the vector $|\phi\rangle$ an eigenvector and the scalar a an eigenvalue of the operator A. The antilinear correspondence between bras and kets, and the definition of the adjoint operator $A^\dagger$, imply that the left-handed eigenvalue equation

$$\langle\phi|A^\dagger = a^*\langle\phi|$$

Theorem 1.5

If A is a Hermitian operator then all of its eigenvalues are real.

Theorem 1.6

Eigenvectors corresponding to distinct eigenvalues of a Hermitian operator must be orthogonal.

If the orthonormal set of vectors $\{\phi_i\}$ is complete, then we can expand an arbitrary vector $|v\rangle$ in terms of it:

$$|v\rangle = \sum |\phi_i\rangle(\langle\phi_i|v\rangle) = \left(\sum |\phi_i\rangle\langle\phi_i|\right)|v\rangle$$

So,

$$\sum |\phi_i\rangle\langle\phi_i| = I$$

If $A|\phi_i\rangle = a_i|\phi_i\rangle$ and the eigenvectors form a complete orthonormal set, then the operator can be reconstructed in a useful diagonal form in terms of its eigenvalues and eigenvectors:

$$A = \sum a_i|\phi_i\rangle\langle\phi_i|$$

We can define a function of an operator

$$f(A) = \sum f(a_i)|\phi_i\rangle\langle\phi_i|$$

The Hermitian operators in a finite N-dimensional vector space have complete sets of eigenvectors. But This statement does not carry over to infinite-dimensional spaces. A Hermitian operator in an infinite dimensional vector space may or may not possess a complete set of eigenvectors, depending upon the precise nature of the operator and the vector space. Instead, we have spectral theorem.

Theorem 1.7

To each self-adjoint operator A there corresponds a unique family of projection operators, $E(\lambda)$, for real λ, with the properties:

1. If $\lambda_1 < \lambda_2$ then $E(\lambda_1)E(\lambda_2) = E(\lambda_2)E(\lambda_1) = E(\lambda_1)$
2. If $\epsilon > 0$, then $E(\lambda + \epsilon)|\psi\rangle \to E(\lambda)|\psi\rangle$ as $\epsilon \to 0$
3. $E(\lambda)|\psi\rangle \to 0$ as $\lambda \to -\infty$
4. $E(\lambda)|\psi\rangle \to |\psi\rangle$ as $\lambda \to \infty$
5. $\int_{-\infty}^{\infty} \lambda dE(\lambda) = A$

We can define a function of an operator

$$f(A) = \int_{-\infty}^{\infty} f(\lambda) dE(\lambda)$$

Following Dirac's pioneering formulation, it has become customary in quantum mechanics to write a formal eigenvalue equation for an operator such as Q that has a continuous spectrum,

$$Q|q\rangle = q|q\rangle$$

The orthonormality condition for the continuous case takes the form

$$\langle q'|q''\rangle = \delta(q - q')$$

Evidently the norm of these formal eigenvectors is infinite, since $\langle q|q\rangle \to \infty$. Instead of the spectral theorem for Q, Dirac would write

$$Q = \int_{-\infty}^{\infty} q|q\rangle\langle q| dq$$

Dirac's formulation does not fit into the mathematical theory of Hilbert space, which admits only vectors of finite norm. The projection operator formally given by

$$E(\lambda) = \int_{-\infty}^{\lambda} |q\rangle\langle q| dq$$

is is well defined in Hilbert space, but its derivative does not exist within the Hilbert space framework.

Theorem 1.8

If A and B are self-adjoint operators, each of which possesses a complete set of eigenvectors, and if $AB = BA$, then there exists a complete set of vectors which are eigenvectors of both A and B.

Let $(A, B, \cdots)$ be a set of mutually commutative operators that possess a complete set of common eigenvectors. Corresponding to a particular eigenvalue for each operator, there may be more than one eigenvector. If, however, there is no more than one eigenvector (apart from the arbitrary phase and normalization) for each set of eigenvalues $(a_n, b_m, \cdots)$, then the operators $(A, B, \cdots)$ are said to be a complete commuting set of operators.

Theorem 1.9

Any operator that commutes with all members of a complete commuting set must be a function of the operators in that set. ♣

1.4 Rigged Hilbert space

Definition 1.13 Rigged Hilbert spece

Formally, a rigged Hilbert space consists of a Hilbert space $\mathcal{H}$, together with a subspace Φ which carries a finer topology, that is one for which the natural inclusion $\Phi \subseteq \mathcal{H}$ is continuous. It is no loss to assume that Φ is dense in $\mathcal{H}$ for the Hilbert norm. We consider the inclusion of conjugate space $\mathcal{H}^X$ in Φ^X. Φ^X is the space of τ_Φ continuous antilinear functional on Φ.
For any $\phi \in \Phi$, $F \in \Phi^X$,we define

$$\langle \phi | F \rangle \equiv F(\phi)$$

$$\langle F | \phi \rangle \equiv [F(\phi)]^*$$

Now by applying the Riesz representation theorem we can identify $\mathcal{H}^X$ with $\mathcal{H}$. Therefore, the definition of rigged Hilbert space is in terms of a sandwich:

$$\Phi \subseteq \mathcal{H} \subseteq \Phi^X$$

♡

There may or may not exist any solutions to the eigenvalue equation $A|a_n\rangle = a_n|a_n\rangle$ for a self-adjoint operator A on an infinite-dimensional vector space. However, the generalized spectral theorem asserts that if A is self-adjoint in $\mathcal{H}$ then a complete set of eigenvectors exists in the extended space Φ^X. The precise conditions for the proof of this theorem are rather technical, so the interested reader is referred to *Gel'fand and Vilenkin (1964)* for further details.

There are many examples of rigged-Hilbert-space triplets. A Hilbert space $\mathcal{H}$ is formed by those functions that are square-integrable. That is, $\mathcal{H}$ consists of those functions $\psi(x)$ for which

$$\langle \psi | \psi \rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 dx \text{ is finite}$$

A nuclear space Φ is made up of functions $\psi(x)$ which satisfy the infinite set of conditions,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 (1 + |x|)^m dx \text{ is finite for } m = 0, 1, 2, \cdots$$

The functions $\psi(x))$ which make up Φ must vanish more rapidly than any inverse power of x in the limit $|x| \to \infty$. The extended space Φ^X, which is conjugate to Φ, consists of those functions $\chi(x)$ for which

$$\langle \chi | \psi \rangle = \int_{-\infty}^{\infty} \chi^*(x)\psi(x)dx \text{ is finite for any } \psi \text{ in } \Phi$$

In addition to the functions of finite norm, which also lie in $\mathcal{H}$, Φ^X will contain functions that are unbounded at infinity provided the divergence is no worse than a power of x. Hence Φ^X contains e^{ikx}, which is an eigenfunction of the operator $D = i\frac{d}{dx}$. It also contains the Dirac delta function, $\delta(x - \lambda)$, which is an eigenfunction of the operator X, defined by $X\psi(x) = x\psi(x)$. These two examples suffice to show that rigged Hilbert space seems to be a more natural mathematical setting for quantum mechanics than is Hilbert space.

1.5 Unitary operators

Definition 1.14 Unitary operator

A unitary operator is a bounded linear operator $U : H \to H$ on a Hilbert space H that satisfies $UU^\dagger = U^\dagger U = I$, where $U^\dagger$ is the adjoint of U, and $I : H \to H$ is the identity operator. ♡

Consider a family of unitary operators, $U(s)$, that depend on a single continuous parameter s. Let $U(0) = I$ be the identity operator, and let $U(s_1 + s_2) = U(s_1)U(s_2)$. We can demonstrate that

$$\left.\frac{dU}{ds}\right|_{s=0} = iK \text{ with } K = K^\dagger$$

The Hermitian operator K is called the generator of the family of unitary operators because it determines $U(s)$, not only for infinitesimal s, but for all s. This can be shown by differentiating

$$U(s_1 + s_2) = U(s_1)U(s_2)$$

with respect to s_2 and we can get

$$\left.\frac{dU}{ds}\right|_{s=s_1} = U(s_1)iK$$

This first order differential equation with initial condition $U(0) = I$ has the unique solution

$$U(s) = e^{iKs}$$

1.6 Antiunitary operators

Definition 1.15 Antiunitary operator

In mathematics, an antiunitary transformation, is a bijective antilinear map

$$U : H_1 \to H_2$$

between two complex Hilbert spaces such that

$$\langle Ux, Uy\rangle = \overline{\langle x, y\rangle}$$

for all x and y y in H_1, where the horizontal bar represents the complex conjugate. If additionally one has $H_1 = H_2$ then U is called an antiunitary operator.

Proposition 1.2

1. $\langle Ux, Uy\rangle = \overline{\langle x, y\rangle} = \langle y, x\rangle$ holds for all elements x, y of the Hilbert space and an antiunitary U.
2. When U is antiunitary then U^2 is unitary. This follows from
$$\langle U^2x, U^2y\rangle = \overline{\langle Ux, Uy\rangle} = \langle x, y\rangle$$
3. For unitary operator V the operator VK, where K is complex conjugate operator, is antiunitary. The reverse is also true, for antiunitary U the operator UK is unitary.
4. For antiunitary U the definition of the adjoint operator U^* is changed into
$$\langle U^*x, y\rangle = \overline{\langle x, Uy\rangle}$$
5. The adjoint of an antiunitary U is also antiunitary and $UU^* = U^*U = 1$.

Chapter 2
Formulation of quantum mechanics

2.1 Axioms of quantum mechanics

1. The properties of a quantum system are completely defined by specification of its state vector $|\psi\rangle$. The state vector is an element of a complex Hilbert space $\mathcal{H}$ called the space of states.

2. With every physical property A (energy, position, momentum, angular momentum, ...) there exists an associated linear, Hermitian operator A (usually called observable), which acts in the space of states. The eigenvalues of the operator are the possible values of the physical properties.

3. - If $|\psi\rangle$ is the vector representing the state of a system and if $|\phi\rangle$ represents another physical state, there exists a probability $P(|\psi\rangle, |\phi\rangle)$ of finding $|\psi\rangle$ in state $|\phi\rangle$, which is given by the squared modulus of the scalar product on $\mathcal{H}$: $P(|\psi\rangle, |\phi\rangle) = |\langle\psi|\phi\rangle|^2$ (Born Rule)
   - If A is an observable with eigenvalues a_k and eigenvectors $|k\rangle$, given a system in the state $|\psi\rangle$, the probability of obtaining a_k as the outcome of the measurement of A is $|\langle k|\psi\rangle|^2$. After the measurement the system is left in the state projected on the subspace of the eigenvalue a_k (Wave function collapse).

4. The evolution of a closed system is unitary. The state vector $|\psi(t)\rangle$ at time t is derived from the state vector $|\psi(t_0)\rangle$ at time t_0 by applying a unitary operator $U(t, t_0)$, called the evolution operator: $\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$.

2.2 Transformations of States

A transformation of states can be described by $|\psi\rangle \to U(\tau)|\psi\rangle \equiv |\psi'\rangle$. And we demand that

$$|\langle\phi|\psi\rangle| = |\langle\phi'|\psi'\rangle|$$

Theorem 2.1 Wigner Theorem

Any mapping of the vector space onto itself that preserves the value of $|\langle\phi|\psi\rangle|$ may be implemented by an operator U with U being either unitary (linear) or antiunitary (antilinear). ♣

Continuous transformation

Only linear operators can describe continuous transformations because every continuous transformation has a square root. Suppose, for example, that $U(l)$ describes a displacement through the distance l. This can be done by two displacements of $U(l/2)$, and hence $U(l) = U(l/2)U(l/2)$. The product of two antilinear operators is linear, since the second complex conjugation nullifies the effect of the first. Thus, regardless of the linear or antilinear character of $U(l/2)$, it must be the case that $U(l)$ is linear. A continuous operator cannot change discontinuously from linear to antilinear as a function of l, so the operator must be linear for all l.

Transformations of observables

For an observable Q,

$$\langle \phi' | Q | \phi' \rangle = \langle \phi | U^{-1} Q U | \phi \rangle$$

If $U(\tau)^{-1} Q U(\tau) = \tau Q$, we can prove that

$$U|q\rangle = |\tau q\rangle$$

Here, $|q\rangle$ is the eigenvector of Q with eigenvalue q.

2.3 Schrödinger equation

$U(t, t_0)$ is unitary and $U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0)$. We can define $H(t_0)$ as

$$\frac{d}{dt} U(t, t_0)\Big|_{t=t_0} = -iH(t_0) \text{ with } H(t_0) = H(t_0)^\dagger$$

We can demonstrate that

$$\frac{dU(t, t_0)}{dt}\Big|_{t=t_1} = -iH(t_1)U(t_1, t_0)$$

The formal solution of the differential equation is

$$U(t, t_0) = I + (-i)^n \sum_{n=1}^{\infty} \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n H(t_1)H(t_2)\cdots H(t_n)$$

Suppose that T stands for time ordering, placing all operators evaluated at later times to the left, the above equation can be written as

$$U(t, t_0) = I + \frac{(-i)^n}{n!} \sum_{n=1}^{\infty} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n T\{H(t_1)H(t_2)\cdots H(t_n)\} \equiv \exp\left[-iT\left\{\int_{t_0}^{t} H(t')dt'\right\}\right]$$

If the Hamiltonian operator H is time-dependent but the H's at different times commute. The equation above can be simplified to

$$U(t, t_0) = \exp\left[-i \int_{t_0}^{t} H(t')dt'\right]$$

If the H is time-independent, then

$$U(t,t_0) = \exp\left[-iH(t-t_0)\right]$$

Since $|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$, we can derive the Schrödinger equation

$$\frac{d|\psi(t)\rangle}{dt} = -iH(t)|\psi(t)\rangle$$

The expectation value of an observable Q is $\langle\psi|Q|\psi\rangle$, denoted by $\langle Q\rangle$. We can then derive that

$$\frac{d\langle Q\rangle}{dt} = -i\left\{\langle[Q,H]\rangle + \langle\frac{\partial Q}{\partial t}\rangle\right\}$$

This is called Ehrenfest's theorem.

2.4 Position operators

In three dimensional space, for a particle, we have three operators corresponding to the observations of its position in space, $\boldsymbol{X} = (X_1, X_2, X_3)$. If the particle has some other internal degrees of freedom, then $\boldsymbol{X}$ plus some other observables S's will form a complete commuting set of operators. The eigenstate state will be denoted by $|\boldsymbol{x}, s\rangle$, satisfying that

$$X_i|\boldsymbol{x}, s\rangle = x_i|\boldsymbol{x}, s\rangle$$

It describes a particle posited in $\boldsymbol{x}$ with internal state s. And we will normalize $|\boldsymbol{x}, s\rangle$ by

$$\langle\boldsymbol{x}, s'|\boldsymbol{x}, s\rangle = \delta_{ss'}\delta(\boldsymbol{x}-\boldsymbol{x}')$$

2.5 Momentum operators and canonical quantization

Since $\boldsymbol{X}$ plus some other observables S's form a complete commuting set of operators. So, the momentum operators can not be independent of them. Numerous experiments shows that the position and momentum of particles can not be measured simultaneously. So, we expect $[X,P] \neq 0$.

Guess For a system which has a classical correspondence, the classical equation of motion of a particle is

$$\begin{aligned}\dot{x} &= [x, H_C(x,p,t)]_C \\ \dot{p} &= [p, H_C(x,p,t)]_C\end{aligned}$$

$[\quad]_C$ is the Poisson bracket in classical mechanics. In quantum mechanics,

$$\begin{aligned}\frac{d\langle X\rangle}{dt} &= -i\langle[X,H]\rangle \\ \frac{d\langle P\rangle}{dt} &= -i\langle[P,H]\rangle\end{aligned}$$

If we assume that the classical equation of motion of a particle is an approximation of quantum mechanics, we may expect

$$[\quad] = i[\quad]_C$$

Since the Poisson bracket in classical mechanics and commutation bracket in quantum mechanics have the same algebra structure. To get the right classical equation of motion of the particle, we demand that

$$[X_i, X_j] = 0 \quad [X_i, X_j] = 0 \quad [X_i, P_j] = i\delta_{ij}$$

and

$$H = H_C(X, P, t)$$

For a general system, we formally define momentum operator $\boldsymbol{P}$ by

$$[X_i, P_j] = i\delta_{ij}$$

The form of H can not be given as a priori, which can be specified only by the hints from classical theory and experiments.

2.6 Momentum operators and translation of states

Theorem 2.2

$$\exp(iG\lambda)A\exp(-iG\lambda) = A + i\lambda[G, A] + \cdots + \frac{i^n\lambda^n}{n!}[G, [G, [G, \cdots [G, A]]]\cdots] + \cdots$$

Define $T(\boldsymbol{a}) \equiv e^{-i\boldsymbol{P}\cdot\boldsymbol{a}}$ We can get

$$T(\boldsymbol{a})^{-1}\boldsymbol{X}T(\boldsymbol{a}) = \boldsymbol{X} + \boldsymbol{a}$$

$$T(\boldsymbol{a})|\boldsymbol{x}\rangle = |\boldsymbol{x} + \boldsymbol{a}\rangle$$

So, $T(\boldsymbol{a})$ is the space translation operator. Now, we can also define the momentum operator as the generator of space translation.

2.7 Angular momentum operators and rotation of states

We define the angular momentum operators $\boldsymbol{J}$ as the generator of rotation.

$$R(\boldsymbol{\theta}) \equiv e^{-i\boldsymbol{J}\cdot\boldsymbol{n}\theta}$$

If the operator $\boldsymbol{M} = (M_1, M_2, M_3)$ is a vector in configuration space and can be rotated by R, then we can demonstrate that

$$[J_i, M_j] = i\epsilon_{ijk}M_k$$

Especially,

$$[J_i, J_j] = i\epsilon_{ijk}J_k$$

Orbital angular momentum

Orbital angular momentum of a particle is defined as $\boldsymbol{L} = \boldsymbol{X} \times \boldsymbol{P}$. It is the generator of rotation of the position of the particle, since

$$[L_i, X_j] = i\epsilon_{ijk}X_k \quad [L_i, P_j] = i\epsilon_{ijk}P_k \quad [L_i, L_j] = i\epsilon_{ijk}L_k$$

Spin angular momentum

Experiments show that some microscopic particles possess a property called spin. The state of the spin is denoted by $|s\rangle$. The corresponding operators are $\boldsymbol{S} = [S_1, S_2, S_3]$, which measure the spin along the $\mathbf{1}, \mathbf{2}, \mathbf{3}$ direction. Spin operator is the generator of rotation of the spin of the particle, so we have

$$[S_i, S_j] = i\epsilon_{ijk}S_k$$

And the rotation of position and spin is independent, so

$$[S_i, L_j] = 0$$

Total angular momentum

The total angular momentum of the particle is

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$$

It is the generator of the rotation of the entire system, which is equivalent to the rotation of the coordinates in opposite direction.

2.8 Heisenberg picture

Define

$$Q_H = U^\dagger(t, t_0)QU(t, t_0)$$

We can derive that

$$\frac{dQ_H(t)}{dt} = -i[Q_H(t), H_H(t)] + \left(\frac{\partial Q}{\partial t}\right)_H$$

Here, $H_H(t) = U^\dagger(t, t_0)H(t)U(t, t_0)$ If the state of the system at t_0 is $|\phi_0\rangle$, then

$$\langle Q\rangle_t = \langle\phi(t)|Q|\phi(t)\rangle = \langle\phi_0|Q_H(t)|\phi_0\rangle$$

If the state $|q\rangle$ is the eigenstate of the Q with the eigenvalue q, then $U^\dagger(t, t_0)|q\rangle$ is the eigenstate of the Q_H with eigenvalue q, which can be denoted by $|q_H(t)\rangle$, so we have

$$\langle q|\phi(t)\rangle = \langle q_H(t)|\phi_0\rangle$$

2.9 Symmetries and conservation laws

Let $U = e^{iKs}$ be a continuous unitary transformation with generator$K = K^\dagger$. To say that the Hamiltonian operator H is invariant under this transformation means that

$$U(s)^{-1}H(t)U(s) = H(t)$$

Then we can deduce that

$$[K, H(t)] = 0$$

Usually, K does not depend on time explicitly. If the above equation hold for all t, then in Heisenberg picture,

$$K_H(t) = K \quad |k_H(t)\rangle = |k\rangle$$

So,

$$\langle K\rangle_t = \langle K\rangle_{t_0} \quad \langle k|\phi(t)\rangle = \langle k|\phi_0\rangle$$

The probability distribution of the measurement of the observable K will not change with time for an arbitrary initial state. We can assume that the K is a constant of motion.

Note: *The concept of a constant of motion should not be confused with the concept of a stationary state. Suppose that the Hamiltonian operator H is independent of t, and that the initial state vector is an eigenvector of H, $|\phi_0\rangle = |E_n\rangle$ with $H|E_n\rangle = E_n|E_n\rangle$. This describes a state having a unique value of energy E_n. So*

$$|\phi(t)\rangle = e^{-iE_nt}|\phi_0\rangle$$

From this result it follows that the average of any dynamical variable R,

$$\langle\phi(t)|R|\phi(t)\rangle = \langle E_n|R|E_n\rangle$$

is independent of t for such a state. By considering functions of R we can further show that the probability distribution is independent of time. In a stationary state the averages and probabilities of all dynamical variables are independent of time, whereas a constant of motion has its average and probabilities independent of time for all states.

Chapter 3
Coordinate and Momentum Representation

3.1 Coordinate representation

To form a representation of an abstract linear vector space, one chooses a complete orthonormal set of basis vectors $\{|u_i\rangle\}$ and represents an arbitrary vector $|\psi\rangle$ by its expansion coefficients $\{c_i\}$, where $|\psi\rangle = \sum c_i|u_i\rangle$. The array of coefficients $\langle u_i|\psi\rangle$ can be regarded as a column vector (possibly of infinite dimension), provided the basis set is discrete.
Coordinate representation is obtained by choosing as the basis set the eigenvectors $\{|\boldsymbol{x}\rangle\}$ of the position operator . Since this is a continuous set, the expansion coefficients define a function of a continuous variable,

$$\psi(\boldsymbol{x}) \equiv \langle \boldsymbol{x}|\psi\rangle$$

We can show that the inner product of the state vector in coordinate representation is

$$\langle \phi|\psi\rangle = \int \phi^*(\boldsymbol{x})\psi(\boldsymbol{x})d^3\boldsymbol{x}$$

It is a matter of taste whether one says that the set of functions forms a representation of the vector space, or that the vector space consists of the functions $\psi(\boldsymbol{x})$.
The action of an operator A on the function space is related to its action on the abstract vector space by the rule

$$A\psi(\boldsymbol{x}) \equiv \langle \boldsymbol{x}|A|\psi\rangle$$

The action of an position operator in coordinate representation is

$$\boldsymbol{X}\psi(\boldsymbol{x}) = \boldsymbol{x}\psi(\boldsymbol{x})$$

The action of an momentum operator in coordinate representation is

$$\boldsymbol{P}\psi(\boldsymbol{x}) = -i\boldsymbol{\nabla}\psi(\boldsymbol{x})$$

For a spin-less particle in the scalar potential $W(\boldsymbol{x})$, $H = \frac{\boldsymbol{P}^2}{2M} + W(\boldsymbol{X})$. The equation of motion in the coordinate representation is

$$\left[-\frac{1}{2M}\boldsymbol{\nabla}^2 + W(\boldsymbol{x})\right]\psi(\boldsymbol{x},t) = i\frac{\partial}{\partial t}\psi(\boldsymbol{x},t)$$

3.2 Galilei transformation of Schrödinger equation

For simplicity we shall treat only one spatial dimension. Let us consider two frames of reference: F with coordinates x and t, and F' with coordinates x' and t'. F' is moving uniformly with velocity v relative to F, so that

$$x = x' + vt' \quad t = t'$$

The potential energy is given by $W(x,t)$ in F , and by $W'(x',t')$ in F', with

$$W(x,t) = W'(x',t')$$

Because the requirement of invariance under Galilei transformation, we expect in F' the Schrödinger equation has the form

$$\left[-\frac{1}{2M}\frac{\partial^2}{\partial x'^2} + W'(x')\right]\psi'(x',t') = i\frac{\partial}{\partial t'}\psi'(x',t')$$

where $\psi'(x',t')$ is the wave function in F'. The probability density at a point in space−time must be the same in the two frames of reference

$$|\psi(x,t)|^2 = |\psi'(x',t')|^2$$

and hence we must have

$$\psi(x,t) = e^{if}\psi'(x',t')$$

where f is a real function of the coordinates. Put all the conditions above together, we can derive

$$f(x,t) = Mvx - \frac{1}{2}Mv^2t$$

apart from an irrelevant constant term.

3.3 Probability flux and conditions on wave functions

Define the probability flux vector

$$\boldsymbol{J}(\boldsymbol{x},t) = \frac{1}{M}\mathrm{Im}(\psi^*\boldsymbol{\nabla}\psi)$$

We can get a continuity equation

$$\frac{d}{dt}|\psi(\boldsymbol{x},t)|^2 + \boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{x},t) = 0$$

Applying the divergence theorem, we obtain

$$\frac{\partial}{\partial t}\int_\Omega |\psi(\boldsymbol{x},t)|^2 d^3x = -\oint_\sigma \boldsymbol{J}\cdot d\boldsymbol{s}$$

The equations of continuity require that the probability flux $\boldsymbol{J}(\boldsymbol{x},t)$ be continuous across any surface, since otherwise the surface would contain sources or sinks. Although this condition applies to all surfaces, implying that $\boldsymbol{J}(\boldsymbol{x},t)$ must be everywhere continuous, its practical applications are mainly to surfaces separating regions in which the potential has different analytic forms. Usually, we have the following conditions,

1.
$$\psi(x)|_{x+0} = \psi(x)|_{x-0} \quad \frac{d\psi}{dx}|_{x+0} = \frac{d\psi}{dx}|_{x-0}$$

2.
$$\psi(x)|_{x+0} = \psi(x)|_{x-0} = 0 \quad \frac{d\psi}{dx}|_{x+0} - \frac{d\psi}{dx}|_{x-0} \text{ is finite}$$

Consider next the behavior at a singular point, assumed for convenience to be the origin of coordinates. Let S be a small sphere of radius r surrounding the singularity. The probability that the particle is inside S must be finite. Suppose that $\psi = \frac{u}{r^\alpha}$, where u is a smooth function that does not vanish at $r = 0$. Then we must have $|\psi|^2 r^3$ convergent at the origin, which implies that $\alpha < \frac{3}{2}$.
The net outward flow through the surface S is $F = \oint_S J \cdot dS$. It must vanish in the limit $r \to 0$, since otherwise the origin would be a point source or sink. One has $\frac{\partial \psi}{\partial r} = r^{-\alpha}\frac{\partial u}{\partial r} - \alpha u r^{-\alpha-1}$. The second term does not contribute to the flux, so we obtain

$$F \propto r^{2-2\alpha}$$

where the integration is over solid angle. If the integral does not vanish, then we must have $\alpha < 1$ in order for F to vanish in the limit $r \to 0$. This is a stronger condition than that derived from the probability density.
Since $|\psi|^2$ is a probability density, it must vanish sufficiently rapidly at infinity so that its integral over all configuration space is convergent and equal to 1.
The conditions that we have discussed apply to wave functions $\psi(x)$ which represent physically realizable states, but they need not apply to the eigenfunctions of operators that represent observables. Those eigenfunctions, $\chi(x)$, which play the role of filter functions in computing probabilities, are only required to lie in the extended space, Φ^X, of the rigged-Hilbert-space triplet. It has been suggested that $\psi(x)$ be restricted to the nuclear space Φ, rather than merely to the Hilbert space $\mathcal{H}$. In many cases this would amount to requiring that $\psi(x)$ should vanish at infinity more rapidly than any inverse power of the distance.

3.4 Path integrals

Theorem 3.1 Gaussian integration

$$\int dx e^{-\frac{1}{2}ax^2+Jx} = \left(\frac{2\pi}{a}\right)^{\frac{1}{2}} e^{\frac{J^2}{2a}}$$

The time evolution of a quantum state vector, $|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$, can be regarded as the propagation of an amplitude in configuration space,

$$\psi(x,t) = \int G(x,t;x',t_0)\psi(x',t_0)dx'$$

where

$$G(x,t;x',t_0) = \langle x,t|U(t,t_0)|x',t_0\rangle$$

is often called the propagator.
Making use of the multiplicative property of the time development operator, it follows that the propagator can be written as

$$G(x,t;x_0,t_0) = \int \cdots \int G(x,t;x_N,t_N) \cdots G(x_1,t_1;x_0,t_0) dx_N \cdots dx_1$$

The N-fold integration is equivalent to a sum over zigzag paths that connect the initial point (x_0,t_0) to the final point (x,t). If we now pass to the limit of $N \to \infty$ and $\Delta t = t_i - t_{i-1} \to 0$, we will have the propagator expressed as a sum (or, rather, as an integral) over all paths that connect the initial point to the final point. We can show that

$$\langle x|e^{-iH\Delta t}|x'\rangle = \sqrt{\frac{M}{2i\pi\Delta t}} \exp\left\{ i \left[\frac{M(x-x')^2}{2\Delta t^2} - V(x') \right] \Delta t \right\} \quad \Delta t \to 0$$

So,

$$G(x,t;x_0,t_0) = \lim_{N\to\infty} \int \cdots \int \left(\frac{M}{2i\pi\Delta t} \right)^{\frac{N+1}{2}} \exp\left\{ i \sum_{j=0}^{N} \left[\frac{M(x_{j+1}-x_j)^2}{2\Delta t^2} - V(x_{j+1}) \right] \Delta t \right\} dx_1 \cdots dx_N$$

The final result can be expressed as

$$G(x,t;x_0,t_0) = \int \mathcal{D}[x(\tau)] e^{iS[x(\tau)]}$$

Here, $S[x(\tau)]$ is the action associated with the path

$$S[x(\tau)] = \int_{x(\tau)} L(x,\dot{x}) d\tau$$

The integral is a functional integration over all paths $x(\tau)$ which connect the initial point (x_0,t_0) to the final point (x,t).
To conclude this section, let us generalize our path-integral formula to a more complicated systems. Consider a very general quantum system, described by arbitrary set of of coordinates q_i, conjugate momentum p^i, and Hamiltonian $H(q,p)$. We can show that

$$\langle q_{k+1}|e^{-i\epsilon H}|q_k\rangle = \left(\prod_i \int \frac{dp_k^i}{2\pi} \right) \exp\left[-i\epsilon H\left(\frac{q_{k+1}+q_k}{2}, p_k \right) \right] \exp\left[i \sum_i p_k^i (q_{i,k+1} - q_{i,k}) \right]$$

so,

$$\langle q_N|U(t,t_0)|q_0\rangle = \left(\prod_{i,k} \int \frac{dp_k^i dq_{i,k}}{2\pi} \right) \exp\left[i \sum_k \left(\sum_i p_k^i (q_{i,k+1} - q_{i,k}) - \epsilon H\left(\frac{q_{k+1}+q_k}{2}, p_k \right) \right) \right]$$

There is one momentum integral for each k from 0 to N, and on coordinate integral for each k from 1 to N. The final result can be expressed as

$$\langle q_N|U(t,t_0)|q_0\rangle = \left(\prod_i \int \mathcal{D}q(t)\mathcal{D}p(t) \right) \exp\left[i \int_0^T dt \left(\sum_i p^i \dot{q}_i - H(q,p) \right) \right]$$

where the functions $q(t)$ are constrained at the endpoints, but $p(t)$ are not. The details of this generalization can be found in chapter 9.1 of *An introduction to quantum field theory (M.E.Peskin & D.V.Schroeder)*

3.5 Momentum representation

Momentum representation is obtained by choosing as the basis set the eigenvectors $\{|\boldsymbol{p}\rangle\}$ of the momentum operator. The orthonormality condition takes the form

$$\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}')$$

Then we can derive that

$$\langle \boldsymbol{x}|\boldsymbol{p}\rangle = \frac{1}{(2\pi)^{3/2}} e^{i\boldsymbol{p}\cdot\boldsymbol{x}}$$

and

$$\phi(\boldsymbol{p}) \equiv \langle \boldsymbol{p}|\psi\rangle = \frac{1}{(2\pi)^{3/2}} \int e^{-i\boldsymbol{p}\cdot\boldsymbol{x}} \langle \boldsymbol{x}|\psi\rangle d^3x$$

The effect of position operator in momentum representation is

$$\boldsymbol{X}\phi(\boldsymbol{p}) = i\boldsymbol{\nabla}\phi(\boldsymbol{p})$$

Bloch's Theorem

A crystal is unchanged by translation through a vector displacement of the form

$$\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3$$

where n_1, n_2 and n_3 are integers, and $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{a}_2$ form the edges of a unit cell of the crystal. Corresponding to such a translation, there is a unitary operator, $U(\boldsymbol{R}_n) = \exp(-i\boldsymbol{P}\cdot\boldsymbol{R}_n)$, which leaves the Hamiltonian of the crystal invariant:

$$U^{-1}(\boldsymbol{R}_n)HU(\boldsymbol{R}_n) = H$$

These unitary operators for translations commute with each other, as well as with H, so there must exist a complete set of common eigenvectors for all of these operators,

$$H|\psi\rangle = E|\psi\rangle \quad U(\boldsymbol{R}_n)|\psi\rangle = c(\boldsymbol{R}_n)|\psi\rangle$$

By the composition relation of the translation operators, we can deduce that

$$c(\boldsymbol{R}_n) = \exp(-i\boldsymbol{p}\cdot\boldsymbol{R}_n)$$

So, in coordinate representation, we have

$$\psi(\boldsymbol{x}-\boldsymbol{R}_n) = U(\boldsymbol{R}_n)\psi(\boldsymbol{x}) = \exp(-i\boldsymbol{p}\cdot\boldsymbol{R}_n)\psi(\boldsymbol{x})$$

The vector $\boldsymbol{p}$ is called the Bloch wave vector of the state. If we expand a function of the Bloch form in a series of plane waves,

$$\psi(\boldsymbol{x}) = \sum_{\boldsymbol{k}'} a(\boldsymbol{k}')e^{i\boldsymbol{k}'\cdot\boldsymbol{x}}$$

we can show that for all $\boldsymbol{R}_n$

$$\exp(i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{R}_n) = 1$$

So $\boldsymbol{G}_n \equiv \boldsymbol{k}'-\boldsymbol{k}$ is a vector of the reciprocal lattice. So, the expansion can be written as

$$\psi(\boldsymbol{x}) = \sum_{\boldsymbol{G}_m} a(\boldsymbol{k}+\boldsymbol{G}_m)e^{i(\boldsymbol{k}+\boldsymbol{G}_m)\cdot\boldsymbol{x}}$$

3.6 Harmonic oscillator

A harmonic oscillator is an object that is subject to a quadratic potential energy, which produces a restoring force against any displacement from equilibrium that is proportional to the displacement. The Hamiltonian for such an object whose motion is confined to one dimension is

$$H = \frac{1}{2M}P^2 + \frac{M\omega^2}{2}Q^2$$

where P is the momentum, Q is the position, and M is the mass.

3.6.1 Algebraic solution

We have the commutation relation

$$[Q, P] = i$$

and the self-adjointness of the operators P and Q,

$$P = P^\dagger \quad Q = Q^\dagger$$

Define

$$p \equiv (M\omega)^{-1/2}P \quad q \equiv (M\omega)^{1/2}Q$$

So

$$[q, p] = i \quad H = \frac{1}{2}\omega(p^2 + q^2)$$

We further define

$$a \equiv \frac{q + ip}{\sqrt{2}}$$

We can verify that

$$[a, a^\dagger] = 1 \quad H = \frac{1}{2}\omega(aa^\dagger + a^\dagger a) = \omega(aa^\dagger - \frac{1}{2}) = \omega(a^\dagger a + \frac{1}{2})$$

Introduce $N \equiv a^\dagger a$, we have

$$[N, a] = -a \quad [N, a^\dagger = a^\dagger]$$

Let $N|\nu\rangle = \nu|\nu\rangle$, with $\langle\nu|\nu\rangle \neq 1$. We have

$$Na|\nu\rangle = a(N-1)|\nu\rangle = (\nu - 1)a|\nu\rangle$$

If $\nu \neq 0$, then $a|\nu\rangle$ cannot be 0, $a|\nu\rangle$ must be an eigenvector of N with eigenvalue $\nu - 1$. On the other hand, we have

$$(\langle\nu|a^\dagger)(a|\nu\rangle) = \langle\nu|N|\nu\rangle = \nu\langle\nu|\nu\rangle$$

Since the norm must be nonnegative, it follows that $\nu \geq 0$, and thus an eigenvalue cannot be negative. By applying the operator a repeatedly, it would appear that one could construct an indefinitely long sequence of eigenvectors having the eigenvalues $\nu - 1$, $\nu - 2$, $\nu - 3$ and so on. The contradiction can be avoided only if the sequence terminates with the value $\nu = 0$

and $a|0\rangle = 0$.
We also have that

$$Na^\dagger|\nu\rangle = a^\dagger(N+1)|\nu\rangle = (\nu+1)a^\dagger|\nu\rangle$$

The squared norm of the vector $a^\dagger|\nu\rangle$ is

$$(\langle\nu|a)(a^\dagger|\nu\rangle) = \langle\nu|N+1|\nu\rangle = (\nu+1)\langle\nu|\nu\rangle$$

which never vanishes because $\nu \geq 0$. Thus $a^\dagger|\nu\rangle$ is an eigenvector of N with eigenvalue $\nu+1$. By repeatedly applying the operator $a^\dagger$, one can construct an unlimited sequence of eigenvectors, each having an eigenvalue one unit greater than that of its predecessor. The sequence begins with the eigenvalue $\nu = 0$. Therefore the spectrum of N consists of the nonnegative integers, $\nu = n$.
The orthonormal eigenvectors of N will be denoted as $|n\rangle$, and we can verify that

$$|n\rangle = n^{-1/2}a^\dagger|n-1\rangle = (n!)^{-1/2}(a^\dagger)^n|0\rangle$$

The matrix elements of $a^\dagger$ and a are

$$\langle n'|a^\dagger|n\rangle = (n+1)^{1/2}\delta_{n',n+1} \quad \langle n'|a|n\rangle = (n)^{1/2}\delta_{n',n-1}$$

Finally we note that the eigenvalues and eigenvectors of the harmonic oscillator Hamiltonian are

$$H|n\rangle = E_n|n\rangle \quad E_n = (n+\frac{1}{2})\omega$$

3.6.2 Solution in coordinate representation

In the coordinate representation, we have

$$-\frac{1}{2M}\frac{d^2}{dx^2}\psi(x) + \frac{M\omega^2}{2}x^2\psi(x) = E\psi(x)$$

Define

$$q \equiv (M\omega)^{1/2}x \quad \lambda \equiv \frac{2E}{\omega}$$

The differential equation becomes

$$\frac{d^2u}{dq^2} + (\lambda - q^2)u = 0$$

When $q \to \pm\infty$, we have $u(q) \sim e^{q^2/2}$ or $e^{-q^2/2}$. The first of these is unacceptable, because it diverges so severely as to be outside of both Hilbert space and rigged Hilbert space. We would seek solutions of the form

$$u(q) = H(q)e^{-\frac{1}{2}q^2}$$

We then have

$$H'' - 2qH' + (\lambda - 1)H = 0$$

It is the so-called Hermite differential equation. When $\lambda - 1 = 2n$, we have regular solutions. Solutions are Hermite polynomials, and will be denoted as $H_n(q)$. After appropriate normalization, we have

$$\psi_n(x) = \left[\frac{\alpha}{\pi^{1/2}2^n n!}\right]^{1/2} H_n(\alpha x)e^{-\frac{1}{2}\alpha^2x^2} \quad E_n = (n+\frac{1}{2})\omega$$

where $\alpha \equiv (M\omega)^{1/2}$.

3.6.3 Path integral solution

The propagator of harmonic oscillator in terms of path integral are

$$\begin{aligned} G(x_b,t_b;x_a,t_a) &= \int \mathcal{D}[x(t)] e^{i\int_{t_a}^{t_b}(\frac{1}{2}M\dot{x}^2-\frac{1}{2}M\omega^2x^2)dt} \\ &= \lim_{N\to\infty}\int \left(\frac{M}{2i\pi\Delta t}\right)^{\frac{N+1}{2}} \exp\left\{i\sum_{j=0}^{N}\left[\frac{M(x_{j+1}-x_j)^2}{2\Delta t^2}-\frac{1}{2}M\omega^2x_{j+1}^2\right]\Delta t\right\} dx_1\cdots dx_N \end{aligned}$$

where

$$x_0 = x_a \quad x_{N+1} = x_b \quad \Delta t = \frac{t_b - t_a}{N+1}$$

Suppose $x_c(t)$ is the classical path of harmonic oscillator and we define

$$\delta x(t) \equiv x(t) - x_c(t)$$

Substitute it into the equation above, the terms which is linear in δx can be dropped, because

$$\frac{\delta S}{\delta x}|_{x(t)=x_c(t)}$$

And since $x_c(t_a) = x_a$, $x_c(t_b) = x_b$, we have

$$\delta x_0 = \delta x_{N+1} = 0$$

At last, we have

$$\begin{aligned} G(x_b,t_b;x_a,t_a) &= e^{iS_c}\lim_{N\to\infty}\int \left(\frac{M}{2i\pi\Delta t}\right)^{\frac{N+1}{2}} \exp\left\{i\sum_{j=1,k=1}^{N}\delta x_j S_{jk}\delta x_k\right\} d\delta x_1\cdots d\delta x_N \\ &= e^{iS_c}\lim_{N\to\infty}\left(\frac{M}{2i\pi\Delta t}\right)^{\frac{N+1}{2}}\sqrt{\frac{\pi^N}{\det(-iS)}} \end{aligned} \tag{3.1}$$

where

$$-iS = \frac{M}{2i\Delta t}\begin{pmatrix} 2-\omega^2\Delta t^2 & -1 & 0 & \cdots \\ -1 & 2-\omega^2\Delta t^2 & -1 & \cdots \\ 0 & -1 & 2-\omega^2\Delta t^2 & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}$$

The details of the following calculation will be eliminated here, and some discussion can be found in section 2.1.4 of *Quantum Field Theory of Many-body Systems (Xiao-Gang Wen)*. The final result is

$$G(x_b,t;x_a,0) = \left(\frac{M\omega}{2\pi i\sin\omega t}\right)^{1/2}\exp\left[\frac{iM\omega}{2\sin\omega t}\left((x_a^2+x_b^2)\cos\omega t - 2x_ax_b\right)\right]$$

In the limit $\omega\to 0$, we have

$$G(x_b,t;x_a,0) = \left(\frac{M}{2\pi it}\right)^{1/2}\exp\left[\frac{iM}{2t}(x_b-x_a)^2\right]$$

This is just the propagator of free particle.

Chapter 4
Angular Momentum

4.1 Eigenvalues of angular momentum operator

The commutation relations among the angular momentum operators are

$$[J_i, J_j] = \epsilon_{ijk} J_k$$

And these three operators are self-adjoint. We first introduce the operator $J^2 = J_x^2 + J_y^2 + J_z^2$. We can verify that $[J^2, \boldsymbol{J}] = 0$. Thus there exists a complete set of common eigenvectors of J^2 and any one component of $\boldsymbol{J}$. Particularly, we have the pair of eigenvalue equations

$$J^2|\beta, m\rangle = \beta|\beta, m\rangle \quad J_z|\beta, m\rangle = m|\beta, m\rangle$$

Since

$$\langle\beta, m|J^2|\beta, m\rangle = \langle\beta, m|J_x^2|\beta, m\rangle + \langle\beta, m|J_y^2|\beta, m\rangle + \langle\beta, m|J_z^2|\beta, m\rangle$$

we have $m^2 \leq \beta$. Thus for a fixed value of β there must be maximum and minimum values for m.
Define

$$J_+ \equiv J_x + iJ_y \quad J_- \equiv J_x - iJ_y$$

we have the commutation relations

$$[J_z, J_+] = J_+ \quad [J_z, J_-] = -J_- \quad [J_+, J_-] = 2J_z$$

So

$$J_z J_+|\beta, m\rangle = J_+(J_z + 1)|\beta, m\rangle = (m + 1)J_+|\beta, m\rangle$$

Therefore, either $J_+|\beta, m\rangle$ is an eigenvector of J_z with the raised eigenvalue $m+1$, or $J_+|\beta, m\rangle = 0$. Now for fixed β there is a maximum value of m, which we shall denote as j. It must be the case that

$$J_+|\beta, j\rangle = 0$$

Since

$$J_+ J_- = J^2 - J_z^2 - J_z$$

it is obvious that $\beta = j(j + 1)$. By similar method, we can show the minimum eigenvalue of J_z for fixed β satisfy that $\beta = k(k - 1)$. So, we have $k = -j$.
We have thus shown the existence of a set of eigenvectors corresponding to integer spaced m values in the range $-j \leq m \leq j$. Since the difference between the maximum value j and the minimum value $-j$ must be an integer, it follows that $j =$ integer$/2$. Henceforth we shall adopt the common and more convenient notation of labeling the eigenvectors by j instead of by β. Thus the vector that was previously denoted as $|\beta, m\rangle$ will now be denoted as $|j, m\rangle$.

4.2 Orbital Angular Momentum and Spin

Let $\psi(\boldsymbol{x})$ be a one-component state function in coordinate representation. When it is subjected to a rotation it is transformed into

$$\boldsymbol{R}\psi(\boldsymbol{x}) = \psi(R^{-1}\boldsymbol{x})$$

where $\boldsymbol{R}$ is the rotation operator generated by $\boldsymbol{R} = \exp(-i\boldsymbol{J}\cdot\boldsymbol{n}\theta)$. For a rotation through infinitesimal angle ϵ about the z axis, we have

$$\boldsymbol{R}_z(\epsilon)\psi(x,y,z) = \psi(x+\epsilon y, y-\epsilon x, z) = \psi(x,y,x) + \epsilon(y\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial y})$$

On the other hand,

$$\boldsymbol{R}_z(\epsilon) = I - i\epsilon J_z$$

so, we have $J_z = -i(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$. This is just the z component of the orbital angular momentum operator $L = \boldsymbol{X}\times\boldsymbol{P}$.
For a multicomponent state function, we have

$$\boldsymbol{R}\begin{pmatrix}\psi_1(\boldsymbol{x})\\ \psi_2(\boldsymbol{x})\\ \vdots\end{pmatrix} = D\begin{pmatrix}\psi_1(R^{-1}\boldsymbol{x})\\ \psi_2(R^{-1}\boldsymbol{x})\\ \vdots\end{pmatrix}$$

Thus the general form of the rotation operator will be

$$\boldsymbol{R}_n(\theta) = e^{-i\boldsymbol{L}\cdot\boldsymbol{n}\theta}D_n(\theta)$$

The two factors commute because the first acts only on the coordinate and the second acts only on the components of the column vector. The matrix D must be unitary, and so it can be written as

$$D_n(\theta) = e^{-i\boldsymbol{S}\cdot\boldsymbol{n}\theta}$$

The angular momentum operator $\boldsymbol{J}$ has the form

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$$

with $\boldsymbol{L} = \boldsymbol{X}\times\boldsymbol{P}$ and $[L_\alpha, S_\beta] = 0$. In the particular representation used in this section, we have $\boldsymbol{L} = -i\boldsymbol{x}\times\boldsymbol{\nabla}$, and the components of S are discrete matrices. The operators $\boldsymbol{L}$ and $\boldsymbol{S}$ are called the orbital and spin parts of the angular momentum.

Orbital angular momentum

The form of the gradient operator in spherical coordinates is

$$\boldsymbol{\nabla} = \boldsymbol{e}_r\frac{\partial}{\partial r} + \boldsymbol{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta} + \boldsymbol{e}_\phi\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}$$

The orbital angular momentum operator then has the form

$$\boldsymbol{L} = r\boldsymbol{e}_r\times(-i\boldsymbol{\nabla}) = (-i)\left[\boldsymbol{e}_\phi\frac{\partial}{\partial\theta} - \boldsymbol{e}_\theta\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right]$$

So,we have

$$L_z = \boldsymbol{L} \cdot \boldsymbol{e}_z = -i\frac{\partial}{\partial \phi}$$

$$L^2 = \boldsymbol{L} \cdot \boldsymbol{L} = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

We must now solve the two coupled differential equations,

$$L_z Y(\theta,\phi) = mY(\theta,\phi) \quad L^2 Y(\theta,\phi) = l(l+1)Y(\theta,\phi)$$

Apart from normalization, we have $Y(\theta,\phi) = e^{im\phi}P_l^m(\cos\theta)$. Here, P_l^m is the associated Legendre polynomials. If we assume that the solution must be single-valued under rotation, then it will follow that m must be an integer. If we further assume that it must be nonsingular at $\theta = 0$ and $\theta = \pi$, then from the standard theory of the Legendre equation it will follow that l must be a nonnegative integer in the range $l \geq |m|$. The normalized solutions that result from these assumptions are the well-known spherical harmonics

$$Y_l^m(\theta,\phi) = (-1)^{(m+|m|)/2}\left[\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}\right]^{1/2} e^{im\phi}P_l^{|m|}(\cos\theta)$$

Spin

A particular species of particle is characterized by a set of quantum numbers that includes the value of its spin s, it is often sufficient to treat the spin operators $\boldsymbol{S}$ as acting on the space of dimension $2s+1$ that is spanned by the eigenvectors of for a fixed value of s.
If $s = \frac{1}{2}$, we have

$$S_x = \frac{1}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} \quad S_y = \frac{1}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix} \quad S_z = \frac{1}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$

The spin operator in direction $\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is

$$\boldsymbol{S}_n = \frac{1}{2}\begin{bmatrix}\cos\theta & e^{-i\phi}\sin\theta\\ e^{i\phi}\sin\theta & -\cos\theta\end{bmatrix}$$

The eigenvectors are

$$\begin{bmatrix}e^{-i\phi/2}\cos\frac{\theta}{2}\\ e^{i\phi/2}\sin\frac{\theta}{2}\end{bmatrix} \quad \begin{bmatrix}-e^{-i\phi/2}\sin\frac{\theta}{2}\\ e^{i\phi/2}\cos\frac{\theta}{2}\end{bmatrix}$$

corresponding to eigenvalues $\frac{1}{2}$ and $-\frac{1}{2}$.
If $s = 1$, we have

$$S_x = \sqrt{\frac{1}{2}}\begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{bmatrix} \quad S_y = \sqrt{\frac{1}{2}}\begin{bmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{bmatrix} \quad S_z = \sqrt{\frac{1}{2}}\begin{bmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{bmatrix}$$

The spin operator in direction $\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is

$$\boldsymbol{S}_n = \begin{bmatrix}\cos\theta & \sin\theta e^{-i\phi}\sqrt{\frac{1}{2}} & 0\\ \sin\theta e^{i\phi}\sqrt{\frac{1}{2}} & 0 & \sin\theta e^{-i\phi}\sqrt{\frac{1}{2}}\\ 0 & \sin\theta e^{i\phi}\sqrt{\frac{1}{2}} & -\cos\theta\end{bmatrix}$$

The eigenvectors are

$$\begin{bmatrix} \frac{1}{2}(1+\cos\theta)e^{-i\phi} \\ \sqrt{\frac{1}{2}}\sin\theta \\ \frac{1}{2}(1-\cos\theta)e^{i\phi} \end{bmatrix} \quad \begin{bmatrix} -\sqrt{\frac{1}{2}}\sin\theta e^{-i\phi} \\ \cos\theta \\ \sqrt{\frac{1}{2}}\sin\theta e^{i\phi} \end{bmatrix} \quad \begin{bmatrix} \frac{1}{2}(1-\cos\theta)e^{-i\phi} \\ -\sqrt{\frac{1}{2}}\sin\theta \\ \frac{1}{2}(1+\cos\theta)e^{i\phi} \end{bmatrix}$$

corresponding to eigenvalues 1, 0 and -1.

4.3 Rotation operator

Three parameters are required to describe an arbitrary rotation. A common parameterization is by the Euler angles. From the fixed system of axes $Oxyz$, a new rotated set of axes $Ox'y'z'$ is produced in three steps:

- Rotate through angle α about Oz, carrying Oy into Ou
- Rotate through angle β about Ou, carrying Oz into Oz'
- Rotate through angle γ about Oz' , carrying Ou into Oy'

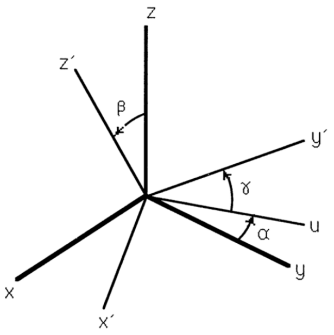

Figure 4.1: Euler angles

The net rotation is

$$\boldsymbol{R}(\alpha,\beta,\gamma) = \boldsymbol{R}_{z'}(\gamma)\boldsymbol{R}_u(\beta)\boldsymbol{R}_z(\alpha) = e^{-i\gamma J_{z'}}e^{-i\beta J_u}e^{-i\alpha J_z}$$

Since $J_u = \boldsymbol{R}_z(\alpha)J_y\boldsymbol{R}_z(-\alpha)$, we have $\boldsymbol{R}_u(\beta) = \boldsymbol{R}_z(\alpha)\boldsymbol{R}_y(\beta)\boldsymbol{R}_z(-\alpha)$. Similarly, we can obtain $\boldsymbol{R}_{z'}(\gamma) = \boldsymbol{R}_u(\beta)\boldsymbol{R}_z(\gamma)\boldsymbol{R}_u(-\beta)$. So, the rotation operator is

$$\boldsymbol{R}(\alpha,\beta,\gamma) = \boldsymbol{R}_z(\alpha)\boldsymbol{R}_y(\beta)\boldsymbol{R}_z(\gamma) = e^{-i\alpha J_z}e^{-i\beta J_y}e^{-i\gamma J_z}$$

The matrix representation of the rotation operator in the basis $|j,m\rangle$

$$\langle j',m'|\boldsymbol{R}(\alpha,\beta,\gamma)|j,m\rangle = \delta_{jj'}D^{(j)}_{m'm}(\alpha,\beta,\gamma)$$

gives rise to the rotation matrices,

$$D^{(j)}_{m'm}(\alpha,\beta,\gamma) = \langle j',m'|e^{-i\alpha J_z}e^{-i\beta J_y}e^{-i\gamma J_z}|j,m\rangle = e^{-i(\alpha m'+\gamma m)}d^{(j)}_{mm'}(\beta)$$

where

$$d^{(j)}_{mm'}(\beta) = \langle j', m'|e^{-i\beta J_y}|j, m\rangle$$

For the case of $j = \frac{1}{2}$, we have $J_y = \frac{1}{2}\sigma_y$ and $\sigma_y^2 = I$. We can obtain

$$d^{(1/2)}(\beta) = \begin{bmatrix} \cos\frac{\beta}{2} & -\sin\frac{\beta}{2} \\ \cos\frac{\beta}{2} & \sin\frac{\beta}{2} \end{bmatrix}$$

Notice that this matrix is periodic in β with period 4π, but it changes sign when 2π is added to β. This double-valuedness under rotation by 2π is a characteristic of the full rotation matrix whenever j is a half odd-integer. The matrix is single-valued under rotation by 2π whenever j is an integer.

The operator for a rotation through 2π about an axis along the unit vector $\boldsymbol{n}$ is $\boldsymbol{R}_n(2\pi) = e^{-2\pi i \boldsymbol{n}\cdot\boldsymbol{J}}$. Its effect on the standard angular momentum eigenvectors is

$$\boldsymbol{R}_n(2\pi) = (-1)^{2j}|j, m\rangle$$

We assume a rotation through 2π as a trivial operation that leaves everything unchanged, i.e. all dynamical variables are invariant under 2π rotation:

$$\boldsymbol{R}(2\pi)A\boldsymbol{R}^{-1}(2\pi) = A$$

where A may represent any physical observable.
the operator $\boldsymbol{R}_{2\pi}$ divides the vector space into two subspaces. A typical vector in the first subspace, denoted as $|+\rangle$, has the property $\boldsymbol{R}(2\pi)|+\rangle = |+\rangle$, whereas a typical vector in the second subspace, denoted as $|-\rangle$, has the property $\boldsymbol{R}(2\pi)|-\rangle = -|-\rangle$. Now, if A represents any physical observable, we have $\langle+|\boldsymbol{R}(2\pi)A|-\rangle = \langle+|A\boldsymbol{R}(2\pi)|-\rangle$, leading to

$$\langle+|A|-\rangle = 0$$

No physical observable can have nonvanishing matrix elements between states with integer angular momentum and states with half odd-integer angular momentum. This fact forms the basis of a superselection rule: There is no observable distinction among the state vectors of the form

$$|\Psi_\omega\rangle = |+\rangle + e^{i\omega}|-\rangle$$

for different values of the phase ω.

4.4 Addition of angular momentum

Let us consider a two-component system, each component of which has angular momentum degrees of freedom. Basis vectors for the composite system can be formed from the basis vectors of the components by taking all binary products of a vector from each set

$$|j_1, j_2, m_1, m_2\rangle = |j_1, m_1\rangle^{(1)}|j_2, m_2\rangle^{(2)}$$

These vectors are common eigenvectors of the four commutative operators $\boldsymbol{J}^{(1)} \cdot \boldsymbol{J}^{(1)}$, $\boldsymbol{J}^{(2)} \cdot \boldsymbol{J}^{(2)}$, $\boldsymbol{J}_z^{(1)}$, and $\boldsymbol{J}_z^{(2)}$. It is often desirable to form eigenvectors of the total angular momentum operators, $\boldsymbol{J} \cdot \boldsymbol{J}$ and $\boldsymbol{J}_z$, where the total angular momentum vector operator is

$$\boldsymbol{J} = \boldsymbol{J}^{(1)} \otimes \mathbf{1} + \mathbf{1} \otimes \boldsymbol{J}^{(2)}$$

This is useful when the system is invariant under rotation as a whole, but not under rotation of the two components separately. The eigenvectors of $\boldsymbol{J} \cdot \boldsymbol{J}$ and $\boldsymbol{J}_z$ may be denoted as $|\alpha, J, M\rangle$. It is easy to verify that the four operators $\boldsymbol{J}^{(1)} \cdot \boldsymbol{J}^{(1)}$, $\boldsymbol{J}^{(2)} \cdot \boldsymbol{J}^{(2)}$, $\boldsymbol{J} \cdot \boldsymbol{J}$ and $\boldsymbol{J}_z$ are mutually commutative, and hence they possess a complete set of common eigenvectors. Since the set of product vectors and the new set of total angular momentum eigenvectors are both eigenvectors of $\boldsymbol{J}^{(1)} \cdot \boldsymbol{J}^{(1)}$ and $\boldsymbol{J}^{(2)} \cdot \boldsymbol{J}^{(2)}$, the eigenvalues j_1 and j_2 will be constant in both sets. Therefore we may confine our attention to the vector space of dimension $(2j_1 + 1)(2j_2 + 1)$ that is spanned by product vectors with fixed values of j_1 and j_2.

Now the $2J + 1$ vectors $|\alpha, J, M\rangle$, with M in the range $-J \leq M \leq J$, span an irreducible subspace. Therefore if the vector $|\alpha, J, M\rangle$, for a particular value of M, can be constructed in the space under consideration, then so can the entire set of $2J + 1$ such vectors with M in the range $-J \leq M \leq J$. For a particular value of J, it might be possible to construct one such set of vectors, two or more linearly independent sets, or none at all.

Let $N(J)$ denote the number of independent sets that can be constructed. Let $n(M)$ be the degree of degeneracy, in this space, of the eigenvalue M . The relation between these two quantities is

$$n(M) = \sum_{J \geq |M|} N(J)$$

and hence

$$N(J) = n(J) - n(J + 1)$$

The product vectors $|j_1, m_1\rangle|j_2, m_2\rangle$ are eigenvectors of the operator $\boldsymbol{J}_z$, with eigenvalue $m_1 + m_2$, and the degree of degeneracy $n(M)$ is equal to the number of pairs (m_1, m_2) such that $M = m_1 + m_2$. Therefore,

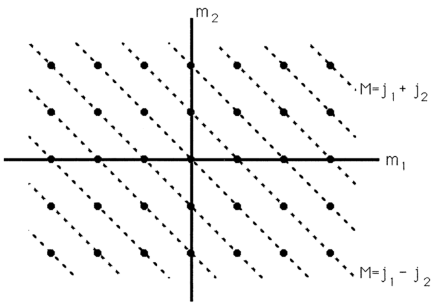

Figure 4.2: Possible values of $M = m_1 + m_2$, illustrated for $j_1 = 3$, $j_2 = 2$

$$n(M) = \begin{cases} 0 & |M| > j_1 + j_2 \\ j_1 + j_2 + 1 - |M| & |j_1 - j_2| \leq M \leq |j_1 + j_2| \\ 2j_{min} + 1 & 0 \leq |M| \leq |j_1 - j_2| \end{cases}$$

It then follows that

$$N(J) = \begin{cases} 1 & |j_1 - j_2| \leq J \leq |j_1 + j_2| \\ 0 & \text{otherwise} \end{cases}$$

It has turned out that $N(J)$ is never greater that 1, and so the vectors $|\alpha, J, M\rangle$ can be uniquely labeled by the eigenvalues of the four operators $\boldsymbol{J}^{(1)} \cdot \boldsymbol{J}^{(1)}$, $\boldsymbol{J}^{(2)} \cdot \boldsymbol{J}^{(2)}$, $\boldsymbol{J} \cdot \boldsymbol{J}$ and $\boldsymbol{J}_z$. Henceforth these total angular momentum eigenvectors will be denoted as $|j_1, j_2, J, M\rangle$. And we have the unitarity transformation

$$|j_1, j_2, J, M\rangle = \sum_{m_1, m_2} |j_1, j_2, m_1, m_2\rangle\langle j_1, j_2, m_1, m_2|j_1, j_2, J, M\rangle$$

The coefficients of this transformation are called the Clebsch–Gordan coefficients, denoted as $(j_1, j_2, m_1, m_2|J, M)$. We fix the phase of $|j_1, j_2, J, M\rangle$ by requiring that $(j_1, j_2, m_1, m_2|J, M)$ be real and positive. The CG coefficient vanishes unless the following conditions are satisfied:

- $m_1 + m_2 = M$
- $|j_1 - j_2| \leq J \leq |j_1 + j_2|$
- $j_1 + j_2 + J =$ an integer

It is possible to calculate the values of the CG coefficients by successive application of the raising or lowering operator to

$$|j_1, j_2, J, M\rangle = \sum_{m_1, m_2} |j_1, j_2, m_1, m_2\rangle\langle j_1, j_2, m_1, m_2|j_1, j_2, J, M\rangle$$

The details of the calculation can be found in section 7.7 of *Quantum mechanics - a modern development(Leslie E. Ballentine)*.And we have Table of CG coefficients and Calculator of CG coefficients on the internet. A special case of angular momentum addition is spin–orbit coupling of spin $\frac{1}{2}$ particles, and we list the corresponding CG coefficients $(l, \frac{1}{2}, M - m_s, m_s|J, M)$ here:

	$J = l + \frac{1}{2}$	$J = l - \frac{1}{2}$
$m_s = \frac{1}{2}$	$\left[\frac{l+M+\frac{1}{2}}{2l+1}\right]^{\frac{1}{2}}$	$-\left[\frac{l-M+\frac{1}{2}}{2l+1}\right]^{\frac{1}{2}}$
$m_s = -\frac{1}{2}$	$\left[\frac{l-M+\frac{1}{2}}{2l+1}\right]^{\frac{1}{2}}$	$\left[\frac{l+M+\frac{1}{2}}{2l+1}\right]^{\frac{1}{2}}$

Table 4.1: Spin-Orbit coupling

Magnetic moment

The magnetic moment operator for an atom has the form

$$\boldsymbol{\mu} = \frac{-e}{2m_e c}(g_L \boldsymbol{L} + g_s \boldsymbol{S})$$

The parameters g_L and g_S have approximately the values $g_L = 1$ and $g_S = 2$. The former is an generalization of the magnetic moment we calculated in classical electrodynamics for a

system of charged particles. The latter will be discussed in quantum field theory. We define the effective Lande factor as

$$\langle \tau, J, M' | \boldsymbol{\mu} | \tau, J, M \rangle = \frac{-e}{2m_e c} g_{eff} \langle J, M' | \boldsymbol{J} | J, M \rangle$$

So, we have

$$g_{eff} = \frac{\langle \tau, J, M | g_L \boldsymbol{L} \cdot \boldsymbol{J} + g_s \boldsymbol{S} \cdot \boldsymbol{J} | \tau, J, M \rangle}{J(J+1)} = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

A formal discussion can be found in section 7.8 of *Quantum mechanics - a modern development(Leslie E. Ballentine)*.

4.5 Spherical potential well

The stationary states of a particle in the spherical potential well are determined by

$$-\frac{1}{2M}\nabla^2 \Psi + W(r)\Psi = E\Psi$$

In spherical coordinates,

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial}{\partial r}\right] + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left[\sin\theta \frac{\partial}{\partial \theta}\right] + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}$$

So, the eigenvalue equation becomes

$$-\frac{1}{2M}\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial \Psi}{\partial r}\right] + \frac{L^2}{2Mr^2}\Psi + W(r)\Psi = E\Psi$$

Suppose the eigenfunctions have the factored form

$$\Psi(r, \theta, \phi) = Y_l^m(\theta, \phi)\frac{u(r)}{r}$$

The radial function then satisfies the equation

$$-\frac{1}{2M}\frac{d^2 u(r)}{dr^2} + \left[\frac{l(l+1)}{2Mr^2} + W(r)\right] u(r) = E u(r)$$

The radial function must satisfy the boundary condition $u(0) = 0$ since $\Psi(r, \theta, \phi)$ would otherwise have an r^{-1} singularity at the origin. The normalization $\langle \Psi | \Psi \rangle = 1$ implies that

$$\int_0^\infty = |u(r)|^2 dr = 1$$

The hydrogen atom

The hydrogen atom is a two-particle system consisting of an electron and a proton. The Hamiltonian is

$$H = \frac{P_e^2}{2M_e} + \frac{P_p^2}{2M_p} - \frac{e^2}{4\pi |\boldsymbol{Q}_e - \boldsymbol{Q}_p|}$$

We take as independent variables the center of mass and relative coordinates of the particles

$$\boldsymbol{Q}_c = \frac{M_e\boldsymbol{Q}_e + M_p\boldsymbol{Q}_p}{M_e + M_p} \quad \boldsymbol{Q}_r = \boldsymbol{Q}_e - \boldsymbol{Q}_p$$

The corresponding momentum operators are

$$\boldsymbol{P}_c = \boldsymbol{P}_e + \boldsymbol{P}_p \quad \boldsymbol{P}_r = \frac{M_p\boldsymbol{P}_e - M_e\boldsymbol{P}_p}{M_e + M_p}$$

We can verify that

$$[Q_{c\alpha}, P_{c\beta}] = [Q_{r\alpha}, P_{r\beta}] = i\delta_{\alpha\beta} \quad [Q_{c\alpha}, P_{r\beta}] = [Q_{r\alpha}, P_{c\beta}] = 0$$

The Hamiltonian becomes

$$H = \frac{P_c^2}{2(M_e + M_p)} + \frac{p_r^2}{2\mu} - \frac{e^2}{4\pi|\boldsymbol{Q}_r|}$$

where μ is called the reduced mass, and is defined by $\mu \equiv \frac{M_eM_p}{M_e+M_p}$. The center of mass behaves as a free particle, and its motion is not coupled to the relative coordinate. We shall confine our attention to the internal degrees of freedom described by the relative coordinate $\boldsymbol{Q}_r$. The energy eigenvalue equation in coordinate representation is

$$-\frac{1}{2\mu}\nabla^2\Psi(\boldsymbol{r}) - \frac{e^2}{4\pi r}\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r})$$

Suppose $\Psi(r,\theta,\phi) = Y_l^m(\theta,\phi)\frac{u(r)}{r}$, we have

$$-\frac{1}{2\mu}\frac{d^2u(r)}{dr^2} + \left[\frac{l(l+1)}{2\mu r^2} - \frac{e^2}{4\pi r}\right]u(r) = Eu(r)$$

Define

$$\rho \equiv \alpha r \quad \alpha \equiv \sqrt{8\mu|E|} \quad \lambda \equiv \frac{e^2}{4\pi}\sqrt{\frac{\mu}{2|E|}}$$

we have

$$\frac{d^2u}{d\rho^2} + \left[-\frac{1}{4} + \frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2}\right]u = 0$$

As $\rho \to \infty$, we have $u \sim e^{-\rho/2}$. And as $\rho \to 0$, we have $u \sim \rho^{l+1}$. So, we can suppose

$$u(\rho) = \rho^{l+1}e^{-\rho/2}v(\rho)$$

And we can get

$$\rho\frac{d^2v}{d\rho^2} + (2l + 2 - \rho)\frac{dv}{d\rho} + (\lambda - l - 1)v = 0$$

It is the so-called Confluent Hypergeometric Differential Equation. When $\lambda - 1 - l = n_r$, we have regular solutions. Solutions are Associated Laguerre Polynomial, and will be denoted as $L_{n-l-1}^{2l+1}(\rho)(n = n_r + l + 1)$. The energy levels are

$$E_n = -\frac{\mu e^4}{32\pi^2 n^2}$$

The degeneracy of an eigenvalue E_n is

$$\sum_{l=0}^{n-1}(2l+1) = n^2$$

Note: *The degeneracy of an energy level of a hydrogen atom is greater than this by a factor of* 4*, which arises from the two-fold orientational degeneracies of the electron and proton spin states. This four-fold degeneracy is modified by the hyperfine interaction between the magnetic moments of the electron and the proton.*

The orthonormal energy eigenfunctions for the hydrogen atom are

$$\Psi_{nlm}(r,\theta,\phi) = \left[\frac{4(n-l-1)!}{(na_0)^3 n[(n+l)!]^3}\right]^{\frac{1}{2}} \rho^l L_{n-l-1}^{2l+1}(\rho) e^{-\rho/2} Y_l^m(\theta,\phi)$$

where $\rho = \alpha r = \frac{2r}{na_0}$, and $a_0 \equiv \frac{4\pi}{\mu e^2}$ is a characteristic length for the atom, known as the Bohr radius.The ground state wave function is

$$\Psi_{000} = (\pi a_0^3)^{-\frac{1}{2}} e^{-\frac{r}{a_0}}$$

A measure of the spatial extent of the bound states of hydrogen is given by the averages of various powers of the distance r.

$$\begin{aligned}
\langle r \rangle &= n^2 a_0 \left\{1 + \frac{1}{2}\left[1 - \frac{l(l+1)}{n^2}\right]\right\} \\
\langle r^2 \rangle &= n^4 a_0^2 \left\{1 + \frac{3}{2}\left[1 - \frac{l(l+1) - 1/3}{n^2}\right]\right\} \\
\langle \frac{1}{r} \rangle &= \frac{1}{n^2 a_0}
\end{aligned}$$

Chapter 5
Quantum-mechanical Particles and Classical Electromagnetic Field

5.1 Charged Particle in EM field

In classical electrodynamics, if the velocity of the charged particle is much smaller than that of light, then the Hamiltonian of charged particles in a given EM field is

$$H = \frac{(\boldsymbol{\pi} - e\boldsymbol{A})^2}{2m} + e\phi$$

In corresponding quantum theory, we will suppose the Hamiltonian operator to be

$$H = \frac{[\boldsymbol{P} - e\boldsymbol{A}(\boldsymbol{X})]^2}{2M} + e\phi(\boldsymbol{X})$$

The corresponding field operators are

$$\boldsymbol{E} = -\nabla\phi - \frac{\partial \boldsymbol{A}}{\partial t} \quad \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$$

In Heisenberg picture, we have

$$\frac{d\boldsymbol{X}}{dt} = -i[\boldsymbol{X}, H] = \frac{1}{M}(\boldsymbol{P} - e\boldsymbol{A})$$

Define kinetic momentum $\boldsymbol{K}$ by

$$\boldsymbol{K} = \boldsymbol{P} - e\boldsymbol{A}$$

We have

$$[K_i, K_j] = ie(\partial_i A_j - \partial_j A_i) = ie\epsilon_{ijk}B_k$$

So

$$M\frac{d^2\boldsymbol{X}}{dt^2} = -i[\boldsymbol{K}, H] + \frac{\partial \boldsymbol{K}}{\partial t} = e\left[\boldsymbol{E} + \frac{1}{2}\left(\frac{d\boldsymbol{X}}{dt} \times \boldsymbol{B} - \boldsymbol{B} \times \frac{d\boldsymbol{X}}{dt}\right)\right]$$

In coordinate representation of Schrödinger picture, we have

$$\frac{1}{2M}\left[-i\boldsymbol{\nabla} - e\boldsymbol{A}\right] \cdot \left[-i\boldsymbol{\nabla} - e\boldsymbol{A}\right]\psi(\boldsymbol{x}, t) + e\phi(\boldsymbol{x})\psi(\boldsymbol{x}, t) = i\frac{\partial\psi(\boldsymbol{x}, t)}{\partial t}$$

Define probability current $\boldsymbol{j}$ as

$$\boldsymbol{j} \equiv \frac{1}{M}\mathrm{Im}(\psi^*\boldsymbol{\nabla}\psi) - \frac{e}{M}\boldsymbol{A}|\psi|^2$$

we can verify that

$$\boldsymbol{\nabla}\cdot\boldsymbol{j}+\frac{\partial\rho}{\partial t}=0$$

Transformation

$$\phi\to\phi-\frac{\partial\Lambda}{\partial t}\quad \boldsymbol{A}\to\boldsymbol{A}+\boldsymbol{\nabla}\Lambda$$

will leave $\boldsymbol{E}$ and $\boldsymbol{B}$ unchanged. The transformation is called gauged transformation. In classical electrodynamics, gauge transformation will not change the trajectory of particles, (which is the only thing we can observed in experiment). In quantum theory, suppose the state vector $|\psi\rangle$ will transform as

$$|\psi(t)\rangle\to O(t)|\psi(t)\rangle$$

where $O(t)$ is an unitary operator. If the Schrödinger equation is always satisfied, we can derive that

$$H'O-OH=i\frac{\partial O}{\partial t}$$

where H' is the Hamiltonian operator after gauge transformation. Generally, we have

$$O(t)=\exp\left[ie\Lambda(\boldsymbol{X},t)\right]$$

And so

$$O^{-1}\boldsymbol{X}O=\boldsymbol{X}\quad O^{-1}\boldsymbol{P}O=\boldsymbol{P}+e\boldsymbol{\nabla}\Lambda\quad O^{-1}(\boldsymbol{P}-e\boldsymbol{A}')O=\boldsymbol{P}-e\boldsymbol{A}$$

So, the expectation value of $\boldsymbol{X}$ and $\boldsymbol{K}$ is invariant under gauge transformation. We can also verify that $\boldsymbol{j}$ is also invariant under gauge transformation. A special case is that

$$\phi\to\phi+\phi_0(t)\quad \boldsymbol{A}\to\boldsymbol{A}$$

In this case, we have

$$O(t)=\exp\left[-i\int_{t_0}^{t}dt'e\phi_0(t')\right]$$

If ϕ_0 is a constant, then

$$O(t)=\exp\left[-ie\phi_0(t-t_0)\right]$$

5.2 Charged particle in a magnetic field

5.2.1 Motion in a uniform static magnetic field

Suppose that the magnetic field be of magnitude B in the z direction. The Hamiltonian $H=H_{xy}+H_z$ with $H_{xy}=\frac{K_x^2+K_y^2}{2M}$ and $H_z=\frac{P_z^2}{2M}$. Since $B_x=B_y=0$, then P_z commutes with P_x and P_y. Hence the operators H_{xy} and H_z are commutative, and every eigenvalue of H is just the sum of an eigenvalue of H_{xy} and an eigenvalue of H_z.
Define

$$Q'\equiv\frac{K_x}{\gamma}\quad P'\equiv\frac{K_y}{\gamma}\quad \gamma\equiv\sqrt{|eB|}$$

Then we have

$$H_{xy} = \frac{1}{2}\frac{|eB|}{M}(Q'^2 + P'^2) \text{ with } [Q', P'] = i \text{ or } -i$$

therefore the eigenvalues of H_{xy} must be equal to $(n + \frac{1}{2})\frac{|eB|}{M}$, where n is any non-negative integer.

The spectrum of K_z can be shown to be gauge-invariant. Because the magnetic field is uniform and in the z direction, it is possible to choose the vector potential such that $A_z = 0$. Therefore the spectrum of K_z is continuous from $-\infty$ to ∞, like that of P_z.

Thus the energy eigenvalues for a charged particle in a uniform static magnetic field B are

$$E_n(p_z) = \frac{(n + \frac{1}{2})|eB|}{M} + \frac{p_z^2}{2M}$$

The motion parallel to the magnetic field is not coupled to the transverse motion, and is unaffected by the field. The classical motion in the plane perpendicular to the field is in a circular orbit with angular frequency $\omega_c = \frac{eB}{M}$, and it is well known that periodic motions correspond to discrete energy levels whose separation is ω_c.

Now let us choose the vector potential to be $A_x = -yB$,$A_y = A_z = 0$. The Hamiltonian now becomes

$$H = \frac{(P_x + yeB)^2 + P_y^2 + P_z^2}{2M}$$

P_x and P_z commute with H, so it is possible to construct a complete set of common eigenvectors of H, P_x and P_z. In coordinate representation, the eigenvalue equation now takes the form

$$-\frac{1}{2M}\nabla^2\psi - \frac{ieB}{M}y\frac{\partial}{\partial x}\psi + \frac{e^2B^2}{2M}y^2\psi = E\psi$$

Substitute

$$\psi(x, y, z) = \exp(ik_x x + ik_z z)\phi(y)$$

The equation then takes the form

$$-\frac{1}{2M}\frac{d^2\phi(y)}{dy^2} + \left[\frac{M\omega_c^2}{2}(y - y_0)^2 - E'\right]\phi(y) = 0$$

where $\omega_c = \frac{eB}{M}$ is the classical cyclotron frequency, and $E' = E - \frac{k_z^2}{2M}$ is the energy associated with motion in the xy plane. This is just the energy eigenvalue equation for a simple harmonic oscillator with angular frequency $\omega = |\omega_c|$, whose eigenvalues are $E' = (n + 1/2)\omega$. Thus the energies for the charged particle in the magnetic field must be $E = (n + 1/2)|\omega_c| + \frac{k_z^2}{2M}$. Apart from a normalization constant, the eigenfunction will be

$$\psi = \exp(ik_x x + ik_z z)H_n[\alpha(y - y_0)]\exp[-\frac{1}{2}\alpha^2(y - y_0)^2]$$

with $\alpha = \sqrt{M\omega} = \sqrt{|eB|}$, and $y_0 = -\frac{k_x}{eB}$.

For fixed n and k_z, the energy eigenvalue is highly degenerate. For convenience, we assume that the system is confined to a rectangle of dimension $D_x \times D_y$ and subject to periodic boundary conditions. The allowed values of k_x are $k_x = \frac{2\pi n_x}{D_x}$, with $n_x = 0, \pm 1, \cdots$.The orbit center

coordinate $y_0 = -\frac{2\pi n_x}{D_x eB}$ must lie in the range $[0, D_y]$. In the limit as D_x and D_y become large, we may ignore problems associated with orbits lying near the boundary, since they will be a negligible fraction of the total. In this limit the number of degenerate states corresponding to fixed n and k_z will be $\frac{D_x D_y |eB|}{2\pi}$.

5.2.2 The Aharonov-Bohm effect

A long solenoid is placed perpendicular to the plane of the figure, so that a magnetic field can be created inside the solenoid while the region external to the solenoid remains field-free. The solenoid is located in the unilluminated shadow region so that no particles will reach it, and moreover it may be surrounded by a cylindrical shield that is impenetrable to the charged particles. Nevertheless it can be shown that the interference pattern depends upon the magnetic flux through the cylinder.

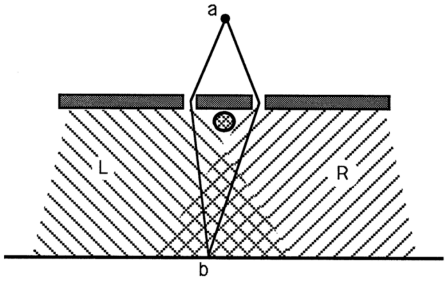

Figure 5.1: The Aharonov–Bohm experiment

Let $\Psi^{(0)}(\boldsymbol{x}, t)$ be the solution of the Schrödinger equation and boundary conditions of this problem for the case in which the vector potential is everywhere zero. Now let us consider the case in which the magnetic field is non-zero inside the cylinder but zero outside of it. The vector potential $\boldsymbol{A}$ will not vanish everywhere in the exterior region, even though $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A} = 0$ outside of the cylinder. This follows by applying Stokes's theorem to any path surrounding the cylinder

$$\oint \boldsymbol{A} \cdot d\boldsymbol{x} = \int\int (\boldsymbol{\nabla} \times \boldsymbol{A}) \cdot d\boldsymbol{S} = \int\int \boldsymbol{B} \cdot d\boldsymbol{S} = \Phi$$

If the flux through the cylinder is not zero, then the vector potential must be nonzero on every path that encloses the cylinder. However in any simply connected region outside of the cylinder, it is possible to express the vector potential as the gradient of a scalar, from the zero potential solution by means of a gauge transformation, $\Psi = \Psi^{(0)} \exp(ie\Lambda)$.
In region L, which contains the slit on the left, the wave function can be written as $\Psi_L = \Psi_L \exp(ie\Lambda_1)$, where Ψ_L is the zero potential solution in region L, and $\Lambda_1(\boldsymbol{x}, t) = \int \boldsymbol{A} \cdot d\boldsymbol{x}$, with the integral taken along a path within region L. A similar form can be written for the wave function in the region R, which contains the slit on the right.
At the point b, in the overlap of regions L and R, the wave function is a superposition of contributions from both slits. Hence we have

$$\Psi(\boldsymbol{b}) = \Psi_L \exp(ie\Lambda_1) + \Psi_R \exp(ie\Lambda_2)$$

The interference pattern depends $\exp(ie(\Lambda 1 - \Lambda_2)) = \exp(ie\Phi)$. Therefore the interference pattern is sensitive to the magnetic flux inside of the cylinder, even though the particles never pass through the region in which the magnetic field is nonzero. The AB effect is a topological effect, in that the effect depends on the flux encircled by the paths available to the particle, even though the paths may never approach the region of the flux.
At last, we conclude that in quantum theory, the potentials themselves are physically significant; however, they are subject to the requirement that all observable effects be invariant under gauge transformations.

5.2.3 The Zeeman effect

The Zeeman effect refers to the effect of a uniform magnetic field on atomic states and energy levels. The Hamiltonian for an electron in the atom is

$$H = \frac{(\boldsymbol{P} + e\boldsymbol{A})^2}{2M} + W(r) = \frac{P^2}{2M} + \frac{e}{M}\boldsymbol{A}\cdot\boldsymbol{P} + \frac{e^2A^2}{2M} + W(r)$$

where the mass of the electron is M, and its charge is $-e$. We have used the simplification $\boldsymbol{P}\cdot\boldsymbol{A} = \boldsymbol{A}\cdot\boldsymbol{P}$, which is valid if $\boldsymbol{\nabla}\cdot\boldsymbol{A} = 0$. We shall take vector potential to be $\boldsymbol{A}(\boldsymbol{X}) = \frac{1}{2}\boldsymbol{B}\times\boldsymbol{X}$. It then follows that

$$\boldsymbol{A}\cdot\boldsymbol{P} = \frac{1}{2}(\boldsymbol{B}\times\boldsymbol{X})\cdot\boldsymbol{P} = \frac{1}{2}(\boldsymbol{X}\times\boldsymbol{P})\cdot\boldsymbol{B} = \frac{1}{2}\boldsymbol{B}\cdot\boldsymbol{L}$$

For weak magnetic fields it is convenient to write this Hamiltonian in the form

$$H = H_a + \frac{e}{2M}\boldsymbol{B}\cdot\boldsymbol{L} + \frac{e^2}{8M}(\boldsymbol{B}\times\boldsymbol{X})^2$$

where $H_a = \frac{P^2}{2M} + W(r)$ is the Hamiltonian of the free atom. If we neglect the last term of H, which is of the second order in the magnetic field, and choose the magnetic field to lie along the z axis, then eigenfunctions Ψ_{nlm} of H_a will also be an eigenfunction of H. To the first order in the magnetic field, the atomic energy levels will be displaced by an amount

$$E^{(1)} = \frac{eB}{2M}m$$

The degeneracy of the $2l+1$ fold multiplet of fixed n and l, due to the spherical symmetry of the atom, is broken by the magnetic field.

Note: *There is also a magnetic dipole moment associated with the spin, $\boldsymbol{\mu}_S = -\frac{e}{M}\boldsymbol{S}$, and so in practice one must also add the spin term $-\boldsymbol{\mu}_S\cdot\boldsymbol{B}$ to the Hamiltonian.*

For strong magnetic fields the term in the Hamiltonian that is proportional to B^2 becomes important. The details of the discussion can be found in section 11.5 of *Quantum mechanics - a modern development(Leslie E. Ballentine)*.

Chapter 6
Discrete Symmetries

6.1 Space inversion

The space inversion transformation is $\boldsymbol{x} \to -\boldsymbol{x}$. The corresponding operator on state vector space is usually called the parity operator. It will be denoted by P. By definition, the parity operator reverses the signs of the position operator and the momentum operator

$$P^{-1}\boldsymbol{X}P = -\boldsymbol{X} \quad P^{-1}\boldsymbol{P}P = -\boldsymbol{P}$$

It follows that the orbital angular momentum, $\boldsymbol{L} = \boldsymbol{X} \times \boldsymbol{P}$, is unchanged by the parity transformation. This property is extended, by definition, to any angular momentum operator,

$$P^{-1}\boldsymbol{J}P = \boldsymbol{J}$$

We can verify that P must be linear by applying space inversion to the commutation relation $[X_i, P_i] = i$. Therefore the parity operator is a unitary operator rather than an anti-unitary operator. Since two consecutive space inversions produce no change at all, it follows that the states described by $|\psi\rangle$ and by $P^2|\psi\rangle$ must be the same. Thus the operator P^2 can differ from the identity operator by at most a phase factor. This phase factor is left arbitrary. It is most convenient to choose that phase factor to be unity, and hence we have

$$P = P^{-1} = P^\dagger$$

Further more, we can derive that

$$P|\boldsymbol{x}\rangle = |-\boldsymbol{x}\rangle$$

So the effect of P on a wave function is

$$P\psi(\boldsymbol{x}) \equiv \langle \boldsymbol{x}|P|\psi\rangle = \langle -\boldsymbol{x}|\psi\rangle = \psi(-\boldsymbol{x})$$

From the fact the $P^2 = 1$, it follows that P has eigenvalues ± 1. Any even function, $\psi_e(\boldsymbol{x}) = \psi_e(-\boldsymbol{x})$, is an eigenfunction on P with eigenvalue 1, and any odd function, $\psi_o(\boldsymbol{x}) = -\psi_o(-\boldsymbol{x})$, is an eigenfunction of P with eigenvalue -1. A function corresponding to parity $+1$ is also said to be of even parity, and a function corresponding to parity -1 is said to be of odd parity.

Example
Under space inversion, $\boldsymbol{x} \to -\boldsymbol{x}$, the spherical harmonic undergoes the transformation

$$Y_l^m(\theta, \phi) \to Y_l^m(\pi - \theta, \phi + \pi) = (-1)^l Y_l^m(\theta, \phi)$$

Hence the single particle orbital angular momentum eigenvector $|l, m\rangle$ is also an eigenvector of parity, with parity $(-1)^l$.
A total orbital angular momentum eigenvector for a two- electron atom is of the form

$$|l_1, l_2, L, M\rangle = \sum_{m_1,m_2} \langle l_1, l_2, m_1, m_2|l_1, l_2, L, M\rangle |l_1, m_1\rangle \otimes |l_2, m_2\rangle$$

It is apparent that

$$P|l_1, l_2, L, M\rangle = (-1)^{l_1+l_2}|l_1, l_2, L, M\rangle$$

and that $(-1)^{l_1+l_2} \neq (-1)^L$. Thus we see that, in general, the parity of an angular momentum state is not determined by its total angular momentum.

If the parity operator P commutes with the Hamiltonian H, then parity eigenvalue ± 1 is a conserved quantity. In that case an even parity state can never acquire an odd parity component, and an odd parity state can never acquire an even parity component.
If $|\psi(t)\rangle$ is a physical process of the system with Hamiltonian H, then we have Schrödinger equation

$$H|\psi\rangle = i\frac{\partial|\psi\rangle}{\partial t}$$

If $PH = HP$, we can verify that

$$HP|\psi\rangle = i\frac{\partial P|\psi\rangle}{\partial t}$$

So, the space inversion of $|\psi(t)\rangle$, $P|\psi(t)\rangle$, can also be a possible physical process of the system. Experiments have shown that parity in β decay is not conserved.

6.2 Time reversal

The effect of the time reversal operator T is to reverse the linear and angular momentum while leaving the position unchanged. Thus we require, by definition,

$$T^{-1}\boldsymbol{X}T = \boldsymbol{X} \quad T^{-1}\boldsymbol{P}T = -\boldsymbol{P} \quad T^{-1}\boldsymbol{J}T = -\boldsymbol{J}$$

We can verify that T must be anti-linear by applying space inversion to the commutation relation $[X_i, P_i] = i$. Therefore the parity operator is a anti-unitary operator.
The time evolution of a system satisfied Schrödinger equation

$$H|\psi(t)\rangle = i\frac{\partial|\psi(t)\rangle}{\partial t}$$

Suppose that $TH = HT$, we can derive that

$$HT|\psi(t)\rangle = -i\frac{\partial T|\psi(t)\rangle}{\partial t}$$

i.e.

$$HT|\psi(-t)\rangle = i\frac{\partial T|\psi(-t)\rangle}{\partial t}$$

$T|\psi(-t)\rangle$ is also a possible physical process of the system.

In coordinate representation the Schrödinger equation takes the form

$$\left[-\frac{1}{2M}\nabla^2 + W(\boldsymbol{x})\right]\psi(\boldsymbol{x},t) = i\frac{\partial\psi(\boldsymbol{x},t)}{\partial t}$$

Its complex conjugate is

$$\left[-\frac{1}{2M}\nabla^2 + W^*(\boldsymbol{x})\right]\psi^*(\boldsymbol{x},t) = -i\frac{\partial\psi^*(\boldsymbol{x},t)}{\partial t}$$

The condition for the Hamiltonian to be invariant under complex conjugation is that the potential be real: $W = W^*$. In that case it is apparent that if $\psi(\boldsymbol{x},t)$ is a solution then so is $\psi^*(\boldsymbol{x},t)$. This suggests that we may identify the time reversal operator with the complex conjugation operator in this representation,

$$T = K_0$$

where, by definition, $K_0\psi(\boldsymbol{x},t) = \psi^*(\boldsymbol{x},t)$. In this case T is its own inverse. The formal expression for an arbitrary vector in coordinate representation is $|\psi\rangle = \int \psi(\boldsymbol{x})|\boldsymbol{x}\rangle d^3\boldsymbol{x}$, where the basis vector $|\boldsymbol{x}\rangle$ is an eigenvector of the position operator. Since T is equal to the complex conjugation operator, its effect is simply $T|\psi\rangle = \int \psi^*(\boldsymbol{x})|\boldsymbol{x}\rangle d^3\boldsymbol{x}$, with $T|\boldsymbol{x}\rangle = |\boldsymbol{x}\rangle$.

In momentum representation, an arbitrary vector can be written as

$$|\psi\rangle = \int \psi(\boldsymbol{p})|\boldsymbol{p}\rangle d^3\boldsymbol{p}$$

Since

$$T|\boldsymbol{p}\rangle = \int \langle\boldsymbol{x}|\boldsymbol{p}\rangle^*|\boldsymbol{x}\rangle d^3\boldsymbol{x} = |-\boldsymbol{p}\rangle$$

so we have

$$T|\psi\rangle = \int \psi^*(\boldsymbol{p})|-\boldsymbol{p}\rangle d^3\boldsymbol{p} = \int \psi^*(-\boldsymbol{p})|\boldsymbol{p}\rangle d^3\boldsymbol{p}$$

The time reversal operator must reverse the angular momentum. For spin operator, we have

$$T^{-1}\boldsymbol{S}T = -\boldsymbol{S}$$

In the standard representation of the spin operators, S_x and S_z are real, while S_y is imaginary. The time reversal operator T cannot be equal to the complex conjugation operator K_0 in this representation, since the effect of the latter is

$$K_0 S_x K_0 = S_x \quad K_0 S_y K_0 = -S_y \quad K_0 S_z K_0 = S_z$$

Let us write the time reversal operator as $T = YK_0$, where Y is a linear operator. Y must have the following properties:

$$Y^{-1}S_xY = -S_x \quad Y^{-1}S_yY = S_y \quad Y^{-1}S_zY = -S_z$$

And Y must operate only on the spin degrees of freedom. A reasonable choice is that $Y = e^{-i\pi S_y}$, whose effect is to rotate spin (and only spin) through the angle π about the y axis. Therefore the explicit form of the time reversal in this representation is

$$T = e^{-i\pi S_y} K_0$$

Two successive applications of the time reversal transformation, must leave the physical situation unchanged. Therefore

$$T^2|\Psi\rangle = c|\Psi\rangle$$

where $|c| = 1$. And we have

$$T^2(T|\Psi\rangle) = T(T^2|\Psi\rangle) = T(c|\Psi\rangle) = c^* T|\Psi\rangle$$

so

$$T^2(|\Psi\rangle + T|\Psi\rangle) = c|\Psi\rangle + c^* T|\Psi\rangle = c'(|\Psi\rangle + T|\Psi\rangle)$$

And we can determine that $c' = c^* = c$. Thus we must have $c = \pm 1$, i.e.

$$T^2|\Psi\rangle = \pm|\Psi\rangle$$

In the particularly representation, we have

$$T^2 = e^{-i\pi S_y} K_0 e^{-i\pi S_y} K_0 = e^{-i2\pi S_y}$$

This may equivalently be written as

$$T^2 = e^{-i2\pi J_y}$$

since $e^{-i2\pi L_y} = I$. So we have an identity

$$T^2 = R(2\pi)$$

Kramer's theorem

Let us consider the energy eigenvalue equation, $H|\Psi\rangle = E|\Psi\rangle$, for a time-reversal-invariant Hamiltonian, $TH = HT$. Then $HT|\Psi\rangle = TH|\Psi\rangle = ET|\Psi\rangle$, and so both $|\Psi\rangle$ and $T|\Psi\rangle$ are eigenvectors with energy eigenvalue E. There are two possibilities: (a) $|\Psi\rangle$and $T|\Psi\rangle$ are linearly dependent, and so describe the same state. (b) $|\Psi\rangle$and $T|\Psi\rangle$ are linearly independent, and so describe two degenerate states.
Suppose that (a) is true, in which case we must have $T|\Psi\rangle = a|\Psi\rangle$ with $|a| = 1$. A second application of T yields $T^2|\Psi\rangle = |\Psi\rangle$. So for those states that satisfy $T^2|\Psi\rangle = -|\Psi\rangle$ it is necessarily true that $|\Psi\rangle$and $T|\Psi\rangle$ are linearly independent, degenerate states. This result is known as Kramer's theorem: any system for which $T^2|\Psi\rangle = -|\Psi\rangle$ has only degenerate energy levels.

Chapter 7
Approximation method

Chapter 8
Many body problem

8.1 Identical particles

8.2 Non-relativistic quantum field theory

Chapter 9
Scattering theory

9.1 Lippmann–Schwinger equation

Imagine a particle coming in and getting scattered by a short-ranged potential $V(x)$ located around the origin $x \sim 0$. The time-independent Schrödinger equation is simply

$$(H_0 + V)|\psi\rangle = E|\psi\rangle$$

Here, $H_0 = \frac{p^2}{2m}$ is the free-particle Hamiltonian operator. We can write the solution as

$$|\psi^{(\pm)}\rangle = \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{(\pm)}\rangle + |\phi\rangle$$

Here, $H_0|\phi\rangle = E|\phi\rangle$. In coordinate representation,

$$\psi^{(\pm)}(\mathbf{x}) = \phi(\mathbf{x}) + \int d^3x' \langle \mathbf{x}| \frac{1}{E - H_0 \pm i\epsilon} |\mathbf{x}'\rangle V(\mathbf{x}')\psi^{(\pm)}(\mathbf{x}')$$

Here, $\phi(\mathbf{x}) = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{\frac{3}{2}}}$. Define the Green function as

$$G_\pm(\mathbf{x}, \mathbf{x}') \equiv \frac{1}{2m} \langle \mathbf{x}| \frac{1}{E - H_0 \pm i\epsilon} |\mathbf{x}'\rangle$$

We can derive that

$$G_\pm(\mathbf{x}, \mathbf{x}') = -\frac{1}{4\pi} \frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|}$$

where $k = \sqrt{2mE}$. And it is easy to show that

$$(\nabla^2 + k^2) G_\pm(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')$$

So, we have

$$\psi^{(\pm)}(\mathbf{x}) = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{\frac{3}{2}}} - 2m \int d^3x' \frac{1}{4\pi} \frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|} V(\mathbf{x}')\psi^{(\pm)}(\mathbf{x}')$$

We now can interpret $\psi^+(\mathbf{x})$ as a superposition of incident plane wave and scattered wave which propagate from scatterer to outside region. From now on, we will denote it as $\psi(\mathbf{x})$.

The experiment is done typically by placing the detector far away from the scatterer $|\mathbf{x}| \ll a$ where a is the "size" of the scatterer. The integration over $\mathbf{x}'$, on the other hand, is limited within the "size" of the scatterer because of the $V(\mathbf{x}')$ factor. Therefore, we are in the situation $|\mathbf{x}| \ll |\mathbf{x}'|$, and hence can use the approximation

$$|\mathbf{x} - \mathbf{x}'| \approx |\mathbf{x}| - \frac{\mathbf{x}' \cdot \mathbf{x}}{|\mathbf{x}|}$$

Under this limit,

$$\psi(\mathbf{x}) = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{\frac{3}{2}}} - 2m\frac{e^{ikr}}{4\pi r}\int d^3x' e^{-\mathbf{k}'\cdot\mathbf{x}'}V(\mathbf{x}')\psi(\mathbf{x}')$$

Here, $r = |\mathbf{x}|$ and $\mathbf{k}' = k\frac{\mathbf{x}}{r}$. It is customary to write this equation in the form

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\left(e^{i\mathbf{k}\cdot\mathbf{x}} + f(\mathbf{k},\mathbf{k}')\frac{e^{ikr}}{r}\right)$$

Here,

$$f(\mathbf{k},\mathbf{k}') \equiv -\frac{m}{2\pi}(2\pi)^3\langle\mathbf{k}'|V|\psi\rangle$$

Recall the definition of cross section

$$\sigma \equiv \frac{\text{Number of Events}}{\text{Time} \times \text{Incident Flux}}$$

So, the differential cross section for particles being scattered into the solid angle is

$$d\sigma = \frac{|\mathbf{j}_{\text{scatt}}|r^2 d\Omega}{|\mathbf{j}_{\text{inc}}|} = |f(\mathbf{k},\mathbf{k}')|^2 d\Omega$$

In a more realistic situation, we should use wave packets to describe the scattering process. The basic picture is a free wave packet approaches the scattering center. After a long time, we have both the original wave packet moving in the original direction plus a spherical wave front that moves outward. The details can be found in the section 3 of the lecture notes *Scattering Theory I (Hitoshi Murayama)*.

Furthermore, if we require that the normalization of the wave function should always satisfy $\int dx^3|\psi(\mathbf{x})|^2$ for any t, as guaranteed by the unitarity of time evolution operator. This requirement leads to a special requirement on the scattered wave, and hence $f(\mathbf{k},\mathbf{k}')$, from witch we can derive the optical theorem.

Theorem 9.1 Optical theorem

$$\text{Im}f(\theta = 0) = \frac{k\sigma_{\text{tot}}}{4\pi}$$

where

$$f(\theta = 0) \equiv f(\mathbf{k},\mathbf{k}),$$

the setting of $\mathbf{k} \equiv \mathbf{k}'$ imposes scattering in the forward direction, and

$$\sigma_{\text{tot}} = \int \frac{d\sigma}{d\Omega}d\Omega$$

The meaning of this theorem is clear. Because the scattered wave takes the probability away to different directions, the total probability for the particle to go to the forward direction (unscattered) should decrease. This decrease is caused by the interference between the unscattered and scattered waves and hence is proportional to $f(0)$. On the other hand, the amount of decrease in the forward direction should equal the total probability at other directions, which is proportional to the total cross section. The proof can be found in the section 4 of the lecture notes *Scattering Theory I (Hitoshi Murayama)*.

9.2 Born approximation

If $|\psi\rangle = |\phi\rangle + O(V)$ is close to $|\phi\rangle$, we can solve the Lippmanmn-Schwinger equation by perturbation theory. The lowest order approximation in V is

$$|\psi\rangle = \frac{1}{E - H_0 + i\epsilon} V|\phi\rangle + |\phi\rangle$$

This is called Born approximation. In coordinate representation,

$$f^{(1)}(\mathbf{k}, \mathbf{k}') = -\frac{m}{2\pi} \int d^3x V(\mathbf{x}) e^{i\mathbf{q}\cdot\mathbf{x}}$$

Here, $\mathbf{q} = |\mathbf{k} - \mathbf{k}'|$. If the potential is central, we can derive that

$$f^{(1)}(\mathbf{k}, \mathbf{k}') = -\frac{2m}{q} \int_0^\infty dr\, rV(r) \sin(qr)$$

Yukawa potential

$$V = \frac{\alpha}{r} e^{-\mu r}$$

So, we can derive

$$f(\theta) = -\frac{2m\alpha}{q^2 + \mu^2}$$

Different cross section is therefore given by

$$\frac{d\sigma}{d\Omega} = (2m\alpha)^2 \frac{1}{[2k^2(1 - \cos\theta) + \mu^2]^2}$$

The total cross section is obtained by integrating over $d\Omega$,

$$\sigma = (2m\alpha)^2 \frac{4\pi}{4k^2\mu^2 + \mu^4}$$

Coulomb potential

$$V = \frac{\alpha}{r}$$

Take the limit $\mu \to 0$, we can get

$$f(\theta) = -\frac{2m\alpha}{q^2}$$

Different cross section is given by

$$\frac{d\sigma}{d\Omega} = (\frac{\alpha}{4E})^2 \frac{1}{\sin^4 \frac{\theta}{2}}$$

The total cross section diverges. The divergence is in the $\cos\theta$ integral when $\theta \to 0$. In other words, the divergence occurs for the small momentum transfer $q \to 0$, which corresponds to large distances. The reason why the total cross section diverges is because the Coulomb potential is actually a long-range force. No matter how far the incident particles are from the charge, there is always an effect on the motion of the particles and they get scattered.

Form factor

If the source of Coulomb potential has an distribution $\rho_N(\mathbf{x})$, then

$$V(\mathbf{x}) = \int d^3x \frac{\alpha}{|\mathbf{x}-\mathbf{x}'|}\rho(\mathbf{x}')$$

Note that the potential is mathematically a convolution of the Coulomb potential and the probability density. Since the first Born amplitude is nothing but the Fourier transform of the potential, the convolution becomes a product of Fourier transforms, one for the Coulomb potential and the other for the probability density. So

$$f(\theta) = f(\theta)_{\text{pointlike}} F(q)$$

Here,

$$F(q) \equiv \int d^3x \rho_N(\mathbf{x}) e^{i\mathbf{q}\cdot\mathbf{x}},$$

being called form factor.

Born expansion

Define T-matrix by

$$V|\psi\rangle = T|\phi\rangle$$

Using the definition of the T-matrix, we find

$$f(\mathbf{k},\mathbf{k}') = -\frac{m}{2\pi}(2\pi)^3\langle\mathbf{k}'|T|\mathbf{k}\rangle$$

Using the Lippmann–Schwinger equation and multiplying the both sides by V from left, we find

$$T|\phi\rangle = V\frac{1}{E-H_0+i\epsilon}T|\phi\rangle + V|\phi\rangle$$

A formal solution to the T-matrix is

$$T = \frac{1}{1-V\frac{1}{E-H_0+i\epsilon}}V$$

By Taylor expanding this operator in geometric series, we find

$$T = V + V\frac{1}{E-H_0+i\epsilon}V + V\frac{1}{E-H_0+i\epsilon}V\frac{1}{E-H_0+i\epsilon}V + \cdots$$

So,

$$|\psi\rangle = \left(1 + \frac{1}{E-H_0+i\epsilon}V + \frac{1}{E-H_0+i\epsilon}V\frac{1}{E-H_0+i\epsilon}V + \cdots\right)|\phi\rangle$$

The first term is the wave which did not get scattered. The second term is the wave that gets scattered at a point in the potential and then propagates outwards by the propagator. In the third term, the wave gets scattered at a point in the potential, propagates for a while, and gets scattered again at another point in the potential, and propagates outwards. In the $n+1$-th term, there are n times scattering of the wave before it propagates outwards.

9.3 Partial wave analysis

Partial wave expansion

When the potential is **central**, angular momentum is conserved due to Noether's theorem. Therefore, we can expand the wave function in the eigenstates of the angular momentum. Obtained waves with definite angular momenta are called partial waves. We can solve the scattering problem for each partial wave separately, and then in the end put them together to obtain the full scattering amplitude. The plane wave can be expanded as follows.

$$e^{ikz} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\theta)$$

Here, $j_l(kr)$ is spherical Bessel functions of first kind. The asymptotic behaviour of $j_l(kr)$ at large r can be written as

$$j_l(kr) \sim \frac{\sin(kr - \frac{l\pi}{2})}{kr}$$

so,

$$e^{ikz} \sim \frac{1}{2ikr}\sum_{l=0}^{\infty}(2l+1)(e^{ikr} - (-1)^l e^{-ikr})P_l(\cos\theta)$$

Meanwhile, the f factor can be expanded as

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

Optical theorem constraint

The cross section can be represented by expansion coefficient of f factor as

$$\sigma = 4\pi\sum_l (2l+1)|f_l|^2$$

On the other hand,

$$\mathrm{Im}f(0) = \sum_l (2l+1)\mathrm{Im}f_l$$

From optical theorem we can derive that

$$|f_l|^2 = \frac{1}{k}\mathrm{Im}f_l$$

This constraint can be rewritten as

$$|1 + 2ikf_l|^2 = 1$$

So we can define a phase δ_l as

$$1 + 2ikf_l = e^{i\delta_l}$$

or equivalently,

$$f_l = \frac{1}{k}e^{i\delta_l}\sin(\delta_l)$$

Phase shifts

We can derive the asymptotic behaviour of the wave function as

$$\psi(\mathbf{x}) \sim \frac{1}{2ikr}\sum_l (2l+1)P_l(\cos\theta)[e^{ikr}e^{2i\delta_l} - (-1)^l e^{-ikr}]$$

Compare it to the case of the plane wave without scattering. What this equation says is that the wave converging on the scatterer has the well-defined phase factor $-(-1)^l$, the same as in the case without scattering. On the other hand, the wave that emerges from the scatterer has an additional phase factor $e^{2i\delta_l}$. All what scattering did is to shift the phase of the emerging wave by $2\delta_l$. The reason why this is merely a phase factor is the conservation of probability. What converged to the origin must come out with the same strength. But this shift in the phase causes the interference among all partial waves different from the case without the phase shifts, and the result is not a plane wave but contains the scattered wave.
In terms of the phase shifts, the cross section is given by

$$\sigma = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l$$

Actual calculation of phase shifts is basically to solve the Schrödinger equation for each partial waves,

$$\left[-\frac{1}{r}\frac{d^2}{dr^2}r + \frac{l(l+1)}{r^2} + 2mV(r)\right]R_l(r) = k^2 R_l(r)$$

After solving the equation, we take the asymptotic limit $r \to \infty$, and write $R_l(r)$ as a linear combination of $j_l(kr)\cos\delta_l + n_l(kr)\sin\delta_l$. The relative coefficients of j_l and n_l determines the phase shift δ_l, and hence the cross section.