PHYS-C0252 - Quantum Mechanics - Brief summary

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This is a brief summary of the key concepts, notation and formulas presented in the course. It is not intended to replace the coursebook or lecture notes.

Contents

1 Notation

- The Planck constant is generally denoted by h and the reduced Planck constant by $\hbar = h/2\pi$. In this course, $\hbar$ occurs more often than h.
- We typically denote the mass of a particle by m.
- Angular frequency is typically denoted by ω. Note that the frequency f is different from angular frequency. They are related by $f = \omega/(2\pi)$. The SI unit of frequency is Hz, but Hz is not the unit of angular frequency!
- In the case of a one-dimensional harmonic oscillator, the classical potential energy is given by $V(x) = m\omega^2 x^2/2$ provided that x is chosen as the free coordinate of the system.
- In this course, a hat on top of a symbol indicates that it is an operator acting on quantum states. For example, the Hamiltonian operator is typically denoted by $\hat{H}$. Always use a hat on top of operators with the exception that no hat is used on top of bra or ket vectors, nor the combinations of them.
- In Dirac notation, a quantum state is denoted by the ket vector $|\psi\rangle$. The kets are independent of any particular representation basis and the same state can be represented in many different bases. For example, we can represent a state vector using the eigenstates $|x\rangle$ of the position operator $\hat{x}$ as

$$|\psi\rangle = \int \langle x|\psi\rangle |x\rangle \, \mathrm{d}x = \int \psi(x)|x\rangle \, \mathrm{d}x. \tag{1}$$

  The amplitude $\psi(x)$ is a wave function. In general, using any set of basis states $\{|\phi_n\rangle\}$, we may express $|\psi\rangle$ as

$$|\psi\rangle = \sum_n |\phi_n\rangle\langle\phi_n|\psi\rangle = \sum_n \langle\phi_n|\psi\rangle|\phi_n\rangle = \sum_n a_n|\phi_n\rangle, \tag{2}$$

  where $a_n = \langle\phi_n|\psi\rangle$ is the amplitude of state $|\phi_n\rangle$. Note that in the case of continuous bases such as that of $\hat{x}$, the summation should be interpreted as an integral.
- The inner product for two quantum states is denoted by $\langle\phi|\psi\rangle$.
- The notation $\langle\hat{A}\rangle$ means the expectation value of the operator $\hat{A}$, i.e.

$$\langle\hat{A}\rangle = \langle\psi|\hat{A}|\psi\rangle = \int \mathrm{d}x \, \psi^*(x)\hat{A}\psi(x), \tag{3}$$

  where the last equality provides merely an example, where the whole Hilbert space can be described by the eigenstates of the position operator.

2 Complex numbers

One way to define the set of complex numbers $\mathbb{C}$ is using number pairs. Let $z = (a, b)$ and $w = (c, d)$ be ordered pairs of real numbers $a, b, c, d \in \mathbb{R}$. Then, we define addition and multiplication in the following way:

$$z + w = (a, b) + (c, d) \coloneqq (a + c, b + d), \tag{4}$$

$$z \cdot w \coloneqq zw = (a, b) \cdot (c, d) \coloneqq (ac - bd, bc + ad). \tag{5}$$

Then, we may just denote $(a, b) := a + b\mathrm{i}$, and recover from the above definitions the usual relation $\mathrm{i}^2 = (0, 1) \cdot (0, 1) = (-1, 0) = -1$. With $z = a + b\mathrm{i}$, we call a the *real part* of z, $\operatorname{Re} z = a$ and b the *imaginary part* of z, $\operatorname{Im} z = b$.

Complex numbers behave as usual in arithmetic with respect to parenthesis. With z as above and $w = c + d\mathrm{i}$, we have

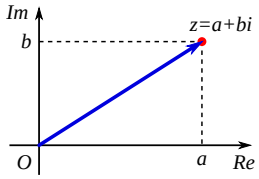
$$z + w = a + b\mathrm{i} + c + d\mathrm{i} = (a + c) + (b + d)\mathrm{i}, \tag{6}$$

and

$$zw = (a + b\mathrm{i})(c + d\mathrm{i}) = ac + ad\mathrm{i} + bc\mathrm{i} + bd\mathrm{i} \cdot \mathrm{i} \tag{7}$$

$$= ac + ad\mathrm{i} + bc\mathrm{i} - bd = (ac - bd) + (ad + bc)\mathrm{i}. \tag{8}$$

In some sense, it can be helpful to think of the imaginary unit i being "orthogonal" to the real numbers. With this in mind, a complex number $z = a + b\mathrm{i}$ can be represented as the point (a, b) on the *complex plane*, like so:



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We define the following useful operations for a complex number $z = a + b\mathrm{i}$, $a, b \in \mathbb{R}$:

- **Complex conjugate**: $z^* = a - b\mathrm{i}$ (sometimes also denoted as $\bar{z}$). This corresponds to mirroring z along the real axis in the complex plane.
- **Magnitude**: $|z| = |z^*| = \sqrt{z \cdot z^*} = \sqrt{a^2 + b^2}$. Sometimes called *absolute value* or *modulus*. This is the length of the "vector" (a, b) in the complex plane.
- **Argument**: $\arg(z) = \operatorname{atan2}(b, a)$, which is the angle between the real axis and z in the complex plane, usually denoted by φ. Sometimes called *phase* or just the *angle* of z.

Some useful relations:

- $z + z^* = a + b\mathrm{i} + a - b\mathrm{i} = 2a = 2 \operatorname{Re} z$
- $-\mathrm{i}(z - z^*) = -\mathrm{i}(a + b\mathrm{i} - a + b\mathrm{i}) = -2\mathrm{i}^2 b = 2b = 2 \operatorname{Im} z$
- $1/\mathrm{i} = (1/\mathrm{i}) \cdot (\mathrm{i}/\mathrm{i}) = \mathrm{i}/\mathrm{i}^2 = \mathrm{i}/-1 = -\mathrm{i}$

The exponential function may be generalized for complex numbers using the usual definition $e^z = \exp(z) = \sum_k^\infty z^k/k!$ with $z \in \mathbb{C}$. From this, it follows that for purely imaginary $y = b\mathrm{i}$ ($b \in \mathbb{R}$), we have

$$e^y = e^{b\mathrm{i}} = \cos b + \mathrm{i} \sin b. \tag{9}$$

(This can be obtained using the series definitions for $\sin$ and $\cos$.) This is called Euler's formula. This is a very useful relation: we can see from the complex plane picture that any complex number z can be written as

$$z = |z|\,(\cos(\arg(z)) + \mathrm{i}\sin(\arg(z))) = |z|\exp(\mathrm{i}\arg(z)) = re^{\mathrm{i}\varphi}, \tag{10}$$

where $r = |z|$ and $\varphi = \arg(z)$. With this and $w = se^{\mathrm{i}\theta}$, we observe that the product $zw = rse^{\mathrm{i}(\varphi+\theta)}$ is equal to z rotated by the angle $\theta = \arg(w)$ and scaled by $s = |w|$ in the complex plane. In particular, with $s = 1$, we see that multiplying by $e^{\mathrm{i}\theta}$ rotates points in the complex plane by θ, which is very useful in quantum mechanics.

These relations are sufficient for our course, but for example Wikipedia lists a lot of other important properties.

3 Basic Postulates of Quantum Mechanics

- **Postulate I:** For every physically measurable quantity (observable or dynamical variable) A, there is a corresponding linear Hermitian operator $\hat{A}$, such that measurements of A yields eigenvalues of $\hat{A}$.
- **Postulate II:** If we measure a certain eigenvalue, the quantum state "collapses" into the corresponding eigenstate of the measured operator.
- **Postulate III:** The state of the system at any time t is represented by a state vector $|\psi(t)\rangle$. $|\psi(t)\rangle$ contains all the information needed to describe the system.
- **Postulate IV:** The time evolution of the wave function is given by the time-dependent Schrödinger's equation:

$$\mathrm{i}\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle. \tag{11}$$

4 Time Evolution of a System

The time evolution of the state vector $|\psi(t)\rangle$ of a system is governed by the time-dependent Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle, \tag{12}$$

where $\hat{H}$ is the Hamiltonian of the system. A formal solution of $|\psi(t)\rangle$ is given by

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}t\hat{H}/\hbar}|\psi(t=0)\rangle = \hat{U}|\psi(t=0)\rangle, \tag{13}$$

where $\hat{U} = \mathrm{e}^{-\mathrm{i}t\hat{H}/\hbar}$ is called the time evolution operator, and the exponential of an operator $\hat{A}$ is defined as $\exp(\hat{A}) = \sum_{n=0}^{\infty}\hat{A}^n/n!$. Note that it is often not possible to find an analytical solution for $\hat{U}$.

One-dimensional particle states are often represented using a basis formed by the eigenstates of the position operator, i.e., a complex valued function $\psi(x,t)$.

If the particle experiences the potential $V(x)$, one can write the time-dependent Schrödinger equation as

$$\mathrm{i}\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t). \tag{14}$$

If the system is initially in an eigenstate $\phi_n(x)$ of $\hat{H}$, the time evolution is given by

$$\psi(x,t) = \phi_n(x)\mathrm{e}^{-\mathrm{i}E_n t/\hbar}, \tag{15}$$

where E_n is the energy corresponding to $\phi_n(x)$. The initial state can also be a superposition of the eigenstates of the Hamiltonian operator:

$$\psi(x,t=0) = \sum_n a_n\phi_n(x), \tag{16}$$

in which case the time evolution is

$$\psi(x,t) = \sum_n a_n\mathrm{e}^{-\mathrm{i}E_n t/\hbar}\phi_n(x). \tag{17}$$

5 Eigenstates and eigenvalues

The eigenstates $|\psi_n\rangle$ corresponding to any observable $\hat{O}$, are the solutions of the eigenvalue equation

$$\hat{O}|\psi_n\rangle = c_n|\psi_n\rangle, \tag{18}$$

where $c_n \in \mathbb{R}$ is the eigenvalue. For example, consider the momentum operator in one dimension in the position basis: $\hat{p} = -\mathrm{i}\hbar\partial/\partial x$. Then, the eigenvalue equation

$$\hat{p}|\psi_k\rangle = p_k|\psi_k\rangle \tag{19}$$

$$\Rightarrow -\mathrm{i}\hbar\frac{\partial\psi_k(x)}{\partial x} = p_k\psi_k(x) \tag{20}$$

has the solution $\psi_k(x) = \exp(\mathrm{i}kx)$, with eigenvalues $p_k = \hbar k$.

6 Measurement probabilities and superposition

The state $|\psi\rangle$ can be represented by a linear superposition of eigenstates $|\phi_n\rangle$

$$|\psi\rangle = \sum_n a_n|\phi_n\rangle, \tag{21}$$

where a_n is the amplitude corresponding to the state $|\phi_n\rangle$. When we perform a measurement on the system, the probability of finding it in one particular nondegenerate eigenstate $|\phi_n\rangle$ is given by

$$P_n = |\langle\phi_n|\psi\rangle|^2 = |a_n|^2. \tag{22}$$

The expectation value of an operator $\hat{O}$ with respect to a state $|\psi\rangle$ is defined as $\langle\psi|\hat{O}|\psi\rangle$. In the position representation

$$\langle\psi|\hat{O}|\psi\rangle = \int_{-\infty}^{\infty}\psi^*(x)\hat{O}\psi(x)\mathrm{d}x. \tag{23}$$

The standard deviation $\Delta\hat{O}$ can be calculated from the expected value for variance

$$(\Delta\hat{O})^2 = \langle\psi|\hat{O}^2|\psi\rangle - \langle\psi|\hat{O}|\psi\rangle^2. \tag{24}$$

7 Vectors and matrices

Matrix representation: Consider a state vector expanded in a given basis $|\phi_n\rangle$

$$|\psi\rangle = \sum_n a_n |\phi_n\rangle. \tag{25}$$

The information about the state is encoded in the amplitudes a_n, which may also be written as a column vector

$$\bar{\psi} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix} \tag{26}$$

and corresponding bra is a row vector

$$\bar{\psi}^\dagger = \left(a_1^*, a_2^*, \ldots, a_N^*\right). \tag{27}$$

The "dagger operation" or just "dagger" † means to transposition and complex conjugation (i.e. you change the columns to rows and you take the complex conjugate of each element). Consider the operator $\hat{O}$, that converts the state ψ to ϕ $\hat{O}|\psi\rangle = |\phi\rangle = \sum_n b_n |\phi_n\rangle$, which has some amplitudes b_n. The same can be written in vector form as

$$\hat{O}|\psi\rangle = \sum_n O_{mn} a_n |\phi_m\rangle \hat{=} \begin{bmatrix} O_{11} & O_{12} & \ldots & O_{1N} \\ O_{21} & O_{22} & \ldots & \ldots \\ \vdots & \ldots & \ldots & \ldots \\ O_{N1} & \ldots & \ldots & O_{NN} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{bmatrix}. \tag{28}$$

Here $\hat{=}$ stands for *represented by*. The operator $\hat{O}$ in the matrix form is

$$\hat{O} \hat{=} \begin{bmatrix} O_{11} & O_{12} & \ldots O_{1N} & \\ O_{21} & O_{22} & \ldots & \ldots \\ \vdots & \ldots & \ldots & \ldots \\ O_{N1} & \ldots & \ldots & O_{NN} \end{bmatrix}, \tag{29}$$

and the coefficients b_m of $|\phi\rangle$ are given by the sum $\sum_n O_{mn} a_n$, according to the rules of standard matrix-vector multiplication.

Let's choose $|\psi\rangle = |\phi_n\rangle$, which is equivalent to $a_i = \delta_{i,n}$, and $\langle\phi| = \langle\phi_m|$ and $a_j^* = \delta_{j,m}$.

$$\langle\phi_m|\hat{O}|\phi_n\rangle \hat{=} (0, 0, \ldots, 1_m \ldots 0) \begin{bmatrix} O_{11} & O_{12} & \ldots O_{1N} & \\ O_{21} & O_{22} & \ldots & \ldots \\ \vdots & \ldots & \ldots & \ldots \\ O_{N1} & \ldots & \ldots & O_{NN} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1_n \\ \vdots \end{bmatrix} = O_{mn}. \tag{30}$$

One can represent the operator by calculating the corresponding matrix $O_{mn} = \langle\phi_m|\hat{O}|\phi_n\rangle$ for all m and for n values. If operator $\hat{O}$ is Hermitian then the matrix elements $O_{n,m} = O_{m,n}^*$.

The eigenvalues and states corresponding to any Hamiltonian $\hat{H}$ can be obtained from the matrix equation

$$\hat{H}|\psi\rangle = E|\psi\rangle \hat{=} \begin{bmatrix} H_{11} & H_{12} & \dots H_{1N} & \\ H_{21} & H_{22} & \dots & \dots \\ \vdots & \dots & \dots & \dots \\ H_{N1} & \dots & \dots & H_{NN} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} Ea_1 \\ Ea_2 \\ \vdots \\ Ea_N \end{bmatrix}, \tag{31}$$

and

$$\det(H - EI) = 0, \tag{32}$$

where I is the identity matrix.

8 Commutators

In general, for two operators $\hat{A}$ and $\hat{B}$, we have $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. We often want to talk about "how much" $\hat{A}\hat{B}$ differs from $\hat{B}\hat{A}$. To this end, we define the *commutator* of the operators as $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$. If $\hat{A}$ and $\hat{B}$ commute, i.e. $\hat{A}\hat{B} = \hat{B}\hat{A}$, we have $[\hat{A}, \hat{B}] = 0$. Note also that $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$. As an example, the commutator between the position and the momentum operators is

$$[\hat{x}, \hat{p}] = \mathrm{i}\hbar. \tag{33}$$

This is an important commutator, called the *canonical commutation relation*.

When the operators $\hat{A}$ and $\hat{B}$ commute, they have a common set of eigenstates, provided only that each has a complete set of eigenstates. If $|\phi_a\rangle$ is an eigenstate of $\hat{A}$ with eigenvalue a,

$$\hat{A}|\phi_a\rangle = a|\phi_a\rangle, \tag{34}$$

then we have

$$\hat{A}\hat{B}|\phi_a\rangle = \hat{B}\hat{A}|\phi_a\rangle = a\hat{B}|\phi_a\rangle. \tag{35}$$

Thus $\hat{B}|\phi_a\rangle$ is also an eigenstate of $\hat{A}$, with the same eigenvalue a.

The generalized uncertainty principle is defined in terms of a commutator:

$$\Delta\hat{A}\Delta\hat{B} \geq \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle|, \tag{36}$$

where $\Delta\hat{A} = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2}$ is the standard deviation.

9 Time evolution of expectations values / Ehrenfest principle

In a system with Hamiltonian $\hat{H}$, the time evolution of the expectation value of an operator $\hat{O}$ is given by

$$\frac{d\langle\hat{O}\rangle}{dt} = \frac{\mathrm{i}}{\hbar}\left\langle[\hat{H}, \hat{O}]\right\rangle + \left\langle\frac{\partial\hat{O}}{\partial t}\right\rangle. \tag{37}$$

If the operator commutes with the Hamiltonian operator and does not explicitly depend on time, i.e., the right-hand side of Eq. (37) is zero, the expectation value $\langle\hat{O}\rangle$ is a constant of motion.

Ehrenfest's principle follows from the above equation. It says that the classical equations of motion can be obtained from quantum mechanics by calculating the operator expectation values. For example, consider a particle moving in the potential $V(x)$, we obtain the equations of motion

$$\frac{d\langle\hat{p}\rangle}{dt} = -\left\langle\frac{\partial V(x)}{\partial x}\right\rangle = \langle F\rangle, \tag{38}$$

and

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}\rangle}{m}. \tag{39}$$

10 Harmonic oscillator

The Hamiltonian for a harmonic oscillator is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2. \tag{40}$$

The so-called lowering (or annihilation) and raising (or creation) operators are defined as

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{\mathrm{i}\hat{p}}{m\omega}\right), \tag{41}$$

and

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{\mathrm{i}\hat{p}}{m\omega}\right). \tag{42}$$

From the canonical commutation relation, it follows that $[\hat{a}, \hat{a}^\dagger] = 1$. Using this, the Hamiltonian operator (40) can be written as

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + 1/2\right) = \hbar\omega\left(\hat{N} + 1/2\right), \tag{43}$$

where $\hat{N} = \hat{a}^\dagger\hat{a}$ is the number operator. The eigenvalues of $\hat{H}$ are

$$E_n = \hbar\omega(n + 1/2), \tag{44}$$

where $n = 0, 1, 2\ldots$. The eigenstates of the Hamiltonian operator are also the eigenstates of the number operator. Using creation operators, the eigenstate can be represented in the following form

$$|\phi_n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|\phi_0\rangle, \tag{45}$$

where $|\phi_0\rangle$ is the state with lowest energy, called the ground state. These states are orthonormal:

$$\langle\phi_n|\phi_m\rangle = \delta_{nm}. \tag{46}$$

Usually the eigenstates of a harmonic oscillator are denoted just with the ket vector $|n\rangle$. The result of operating with the annihilation operator on the eigenstate $|n\rangle$ is

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \tag{47}$$

while for the creation operator we have

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{48}$$

This is where the names come from, $\hat{a}$ lowers and $\hat{a}^\dagger$ raises the energy of the oscillator by one quantum of energy $\hbar\omega$. Note that the operators $\hat{a}$ and $\hat{a}^\dagger$ can be written as a sum of outer products of the form $|n-1\rangle\langle n|$ and $|n\rangle\langle n-1|$:

$$\hat{a} = \sum_{n=1}^{\infty} \sqrt{n}|n-1\rangle\langle n|, \tag{49}$$

$$\hat{a}^\dagger = \sum_{n=0}^{\infty} \sqrt{n+1}|n+1\rangle\langle n|. \tag{50}$$

11 Scattering from a 1D potential

A general method for solving 1D scattering problems:

1. In the regions (n) where the energy is greater than the potential value V_n, write an oscillating solution

$$\psi_n(x) = A_n e^{ik_n x} + B_n e^{-ik_n x}, \tag{51}$$

where $k_n = \sqrt{2m(E-V_n)/\hbar^2}$.

2. In the regions (n) where the energy is less than the potential value V_n the solution take form

$$\psi_n(x) = A_n e^{\kappa_n x} + B_n e^{-\kappa_n x} \tag{52}$$

where $\kappa_n = \sqrt{2m(V_n-E)/\hbar^2}$.

3. If the particle current comes from the left, the solution at the far left is

$$\psi_0(x) = e^{ikx} + Re^{-ikx} \tag{53}$$

where R is the reflection coefficient, $k = \sqrt{2mE/\hbar^2}$ and the second term describes the reflected part.

4. At the far right, the solution is

$$\psi_N(x) = Te^{ik_N x}, \tag{54}$$

which describes the part tunneled through the potential barrier.

5. At all boundaries of x_s,

   - the wave function should be continuous, $\lim_{\epsilon\to 0} \psi(x_s-\epsilon) = \psi(x_s+\epsilon)$.
   - the first derivative of the wave function should be continuous, $\lim_{\epsilon\to 0} \frac{d\psi(x_s-\epsilon)}{dx} = \frac{d\psi(x_s+\epsilon)}{dx}$. Note that the derivative need not be continuous at points where the potential is infinite (for example, in the case of the delta-function potential $\delta(x)$).

6. This gives a linear set of equations for the amplitudes $R, T, \cdots A_n, B_n$.

7. The transmission T and reflection coefficient R are the ratios of transmitted or reflected **current density** to incoming current. In the one-dimensional case, the current density can be obtained from the wave function

$$J = \frac{\hbar}{2m\mathrm{i}} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi *}{\partial x} \right]. \tag{55}$$

   For example, if particles whose wave functions are plane waves $A_1 \mathrm{e}^{\mathrm{i}k_1 x - \mathrm{i}\omega_1 t}$ strike a potential barrier, then the current density is $J = \hbar k_1 |A_1|^2 / m$.

12 Qubit

A qubit can refer either to a physical system or to a mathematical construction. We can model a qubit with a two-level quantum system. All possible quantum states of a qubit can be represented in an orthonormal basis $\{|0\rangle, |1\rangle\}$. The Hamiltonian has just two eigenvalues E_0 and E_1 corresponding to eigenstates $|0\rangle$ and $|1\rangle$. Thus we may write

$$\hat{H} = E_0 |0\rangle\langle 0| + E_1 |1\rangle\langle 1|. \tag{56}$$

Bloch sphere representation of the state: Any pure qubit state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$ can be written in the following way:

$$|\psi\rangle = \cos(\theta/2)|0\rangle + \mathrm{e}^{\mathrm{i}\phi} \sin(\theta/2)|1\rangle,$$

where $0 \leq \theta \leq \pi$ and $0 \leq \phi < 2\pi$ are parameters that equal the polar and the azimuthal angle, respectively, of the Bloch sphere representation of the state, i.e., the Bloch sphere representation of $|\psi\rangle$ is given by the Bloch vector $\vec{\psi} = (\cos\phi \sin\theta, \sin\phi \sin\theta, \cos\theta)$.

13 Density matrix

Given a quantum state $|\psi\rangle$, we can form the **density matrix**

$$\hat{\rho} = |\psi\rangle\langle\psi|, \tag{57}$$

containing the same information. The density matrix has a few general properties:

1. $\mathrm{Tr}\,\hat{\rho} = 1$.

2. $\hat{\rho}$ is Hermitian.

3. Positivity, that is, all eigenvalues of $\hat{\rho}$ are greater than or equal to zero.

If we know the state $|\psi\rangle$ of the system, the density matrix does not seem very useful. However, there are often situations with degrees of freedom which we can't keep track of. Thus, the "information" contained in the system leaks into degrees of freedom unknown to us. In such a situation, the reduced density matrix will be useful.

Consider a composite system composed of two subsystems A and B. The total density matrix of the whole system $\hat{\rho} = |\psi\rangle\langle\psi|$ and the reduced density matrix in section A (this is the part of the whole system under consideration) is

$$\hat{\rho}_A = \mathrm{Tr}_B\, \hat{\rho}, \tag{58}$$

where Tr_B means a "partial trace" operation.

14 Periodic potentials: Bloch's theorem

A potential V is periodic with period d if

$$V(x + d) = V(x). \tag{59}$$

In this case, the eigenstates of the Hamiltonian operator $\hat{H} = \hat{p}^2/2m + V(x)$ are of the form

$$\phi_k(x) = \mathrm{e}^{\mathrm{i}kx} u_k(x), \tag{60}$$

where $u_k(x + d) = u_k(x)$ is periodic for the same period as the potential. These eigenstates are called **Bloch states**. This follows from the fact that the eigenstates of the translation operator $\hat{D}$

$$\hat{D} f(x) = f(x + d) \tag{61}$$

are $\phi = \mathrm{e}^{\mathrm{i}kx} u(x)$, where $u(x+d) = u(x)$. When the potential is periodic, $[\hat{D}, \hat{H}] = 0$ and the eigenstates of $\hat{D}$ are also eigenstates of $\hat{H}$.

15 Fourier transform

The Fourier transform of $\psi(x)$ is defined as

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} \psi(x). \tag{62}$$

The inverse transform is in turn

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}kx} \phi(k). \tag{63}$$

The initial constant is the same in both the forward and inverse transforms, so that $\phi(x)$ and $\psi(x)$ remain properly normalized and thus as acceptable wavefunctions. If the transformations are between the position and momentum instead of the wave vector k, we have

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}px/\hbar} \psi(x) \tag{64}$$

and

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{d}p\, \mathrm{e}^{\mathrm{i}px/\hbar} \phi(p). \tag{65}$$

The Fourier transform of the function $f(t)$ of time t is a function of the angular frequency $F(\omega)$

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} f(t) \tag{66}$$

and

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}\omega \, \mathrm{e}^{-\mathrm{i}\omega t} F(\omega). \tag{67}$$