

Quantum Mechanics

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Contents

Chapter 1

Waves and particles

1.1 Electromagnetic waves and photons

1.1.1 Light quanta and the Planck-Einstein relations

The study of **black hole** lead to the prompt of Plank to come up with the hypothesis of **quantization energy**, and later Einstein forwarded the concept of **photon**, and made it possible to explain **photoelectric effect**. And years later **Compton effect** showed that photon exists indeed. All these result lead to the conclusion: the interaction of an electromagnetic wave with matter occurs by means of **elementary indivisible process**, in which the radiation appears to be composed of particles, the photons. Particle parameters and wave parameters are linked by the **Planck-Einstein relations**:

$$\begin{aligned} E &= h\nu = \hbar\omega \\ \mathbf{p} &= \hbar\mathbf{k} \end{aligned}$$

where $\hbar = \frac{h}{2\pi}$ and h is a new fundamental constant. And during each elementary process, energy and total momentum must be conserved.

1.1.2 Wave-particle duality

The Young's well-known double-slit experiment show that a complete interpretation of the phenomena can be obtained **only** by conserving both the wave aspect and the particle aspect of light (although they seem a **priori** irreconcilable).

What really happened when \mathcal{S} emit photons?

- (a) If we cover \mathcal{E} with a photographic plate and increase the exposure time to capture a large number of photons on each photograph, when developing, no fringes disappear.
- (b) On the other hand, if expose the photographic plate during a short time that it can only receive a few photons. We observe that each photon produces a localized impact on \mathcal{E} and not a very weak interference pattern.

If we want to detect the photons, using photomultipliers, it would absorb the photons and thus fail. And experiment told us: **it is impossible to observe the interference pattern and**

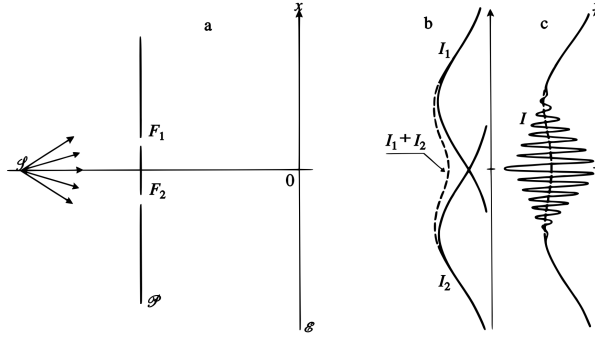


Figure 1.1: Young's experiment

to know at the same time through which slit each photon has passed. And new property occur in this new domain (microscopic): **when one performs a measurement on a microscopic system, one disturbs it in a fundamental fashion**. Also Since these photons are all emitted under the same conditions. Thus another classical idea has been destroyed: **that the initial conditions completely determine the subsequent motion of a particle**.

We summarize the concept of **wave-particle duality** as:

- (a) Light behaves simultaneously like a wave and like a flux of particles, the wave enabling us to calculate the probability of the manifestation of a particle.
- (b) Predictions about the behavior of a photon can only be probabilistic.
- (c) The information about a photon at time t is given by the wave $E(\mathbf{r}, t)$. We say that this wave characterizes the state of the photons at time t ; $E(\mathbf{r}, t)$ is interpreted as the **probability amplitude** of a photon appearing, at time t , at the point r . This means that the corresponding probability is proportional to $|E(\mathbf{r}, t)|^2$.

1.1.3 The principle of spectral decomposition

Classical explanation: **Malus' law**:

$$I' = I \cos^2 \theta$$

On quantum level: The photons pass one-by-one, and the result is only **pass** or **absorb**, and we can't predict which happens. But finally when the number of photons are large, the total result returns to the classical explanation. And in this description we get these concepts:

- (a) The measurement device only gives certain privileged results, which we shall call **eigen** (or proper) results. And in this case is

$$\mathbf{e}_p = \mathbf{e}_x \quad \text{or} \quad \mathbf{e}_p = \mathbf{e}_y$$

- (b) To each of these eigen results corresponds an **eigenstate**. And if the particle before the measurement is in one of the eigenstates, the result of this measurement is certain: it can only be the associated eigen result.

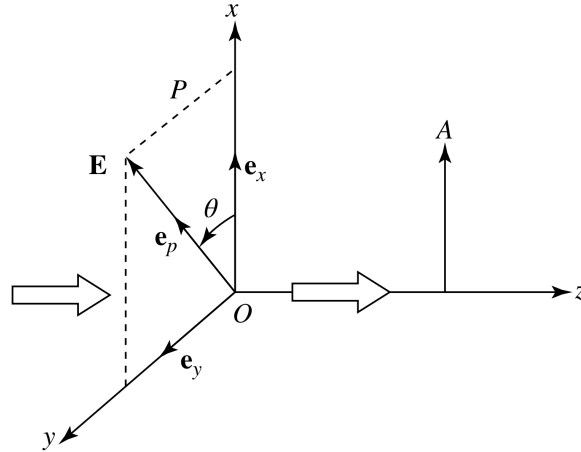


Figure 1.2: Polarization experiment

- (c) When the state before the measurement is arbitrary, only the **probabilities** of obtaining the different eigen results can be predicted. To find these probabilities, one decomposes the state of the particles into a **linear combination** of the various eigenstates. In this case is

$$\mathbf{e}_p = \mathbf{e}_x \cos^2 \theta + \mathbf{e}_y \sin^2 \theta$$

This rule is called the **principle of spectral decomposition**.

- (d) When the particle pass the polarization, the state of it changes abruptly, from \mathbf{e}_p . And this verifies the statement ??.

1.2 Material particles and matter waves

1.2.1 The de Broglie relations

The study of atomic emission and absorption spectra uncovered that spectra are composed of **narrow lines**. And this is natural if **the energy of the atom is quantized**. And de Broglie put forth the following hypothesis: **material particles, just like photons, can have a wavelike aspect**. And later **Electron diffraction experiments** (Davisson and Germer, 1927) strikingly confirmed the existence of a wavelike aspect of matter by showing that **interference patterns could be obtained with material particles such as electrons**. And thus the de Broglie relation is

$$\lambda = \frac{2\pi}{|\mathbf{k}|} = \frac{h}{|\mathbf{p}|}$$

1.2.2 Wave functions. Schrödinger equation

Use the de Broglie's hypothesis, we apply those ideas of photons to all material particles:

- (a) Use time-varying **state** instead of classical concept (position, momentum), which is characterized by **wave function** $\psi(\mathbf{r}, t)$, to describe particle.

- (b) $\psi(\mathbf{r}, t)$ is interpreted as a probability amplitude of the particle's presence. And its modular is the **probability density**:

$$d\mathcal{P} = C|\psi(\mathbf{r}, t)|^2 d^3r$$

- (c) The principle of spectral decomposition applies to the measurement of an arbitrary physical quantity:

- (i) Result must be set of eigen results $\{a\}$.
- (ii) Eigenvalue $a \longleftrightarrow$ eigenstate $\psi_a(\mathbf{r})$. And if at sometime t_0 measurement is performed and $\psi(\mathbf{r}, t_0) = \psi_a(\mathbf{r})$, then the result is always a .
- (iii) The possibility gets from decomposition:

$$\psi(\mathbf{r}, t_0) = \sum_a c_a \psi_a(\mathbf{r})$$

and

$$\mathcal{P}_a = \frac{|c_a|^2}{\sum_a |c_a|^2}$$

- (iv) If the result is a , then the wave function immediately is

$$\psi(\mathbf{r}, t_0) = \psi_a(\mathbf{r})$$

- (d) The evolution of $\psi(\mathbf{r}, t)$ is by **Schrödinger equation**: When particle with mass m is in potential field $V(\mathbf{r}, t)$, it takes on the form

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) + V(\mathbf{r}, t) \psi(\mathbf{r}, t)$$

Notice it is **linear** and **homogeneous**, also is first-order w.r.t time, and thus it is determined by $\psi(\mathbf{r}, t_0)$.

1.3 Quantum description of a particle. Wave packets

1.3.1 Free particle

When $V(\mathbf{r}, t) \equiv 0$, the Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t)$$

and solution

$$\psi(\mathbf{r}, t) = A e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)}$$

satisfies, where

$$\omega = \frac{\hbar \mathbf{k}^2}{2m}$$

Then use the de Broglie relations, we get

$$E = \hbar\omega = \frac{\hbar\mathbf{k}^2}{2m} = \frac{\mathbf{p}^2}{2m}$$

is the relation in classical mechanics.

And this state means that the possibility is

$$|\psi(\mathbf{r}, t)|^2 = A^2 = \text{Const.}$$

which means the possibility is uniform in all space. Moreover, use the superposition, we get that

$$\psi(\mathbf{r}, t) = \frac{1}{(2\pi)^{3/2}} \int g(\mathbf{k}) e^{i[\mathbf{k}\cdot\mathbf{r} - \omega(k)t]} d^3k$$

is also solution (can be complex), and actually, all square integrable function can be written in this form.

1.3.2 Form of the wave packet at a given time

Consider 1-D case, let $\alpha(k)$ be the argument of $g(k)$:

$$g(k) = |g(k)| e^{i\alpha(k)}$$

and assume $\alpha(k)$ is smoothly in $[k_0 - \frac{\Delta k}{2}, k_0 + \frac{\Delta k}{2}]$, where $g(k)$ is appreciable, then

$$\alpha(k) \approx \alpha(k_0) + (k - k_0) \left. \frac{d\alpha}{dk} \right|_{k=k_0}$$

Thus the wave function becomes:

$$\begin{aligned} \psi(x, 0) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} |g(k)| e^{i[\alpha(k_0) + (k - k_0)\alpha'(k_0)]} e^{ikx} dk \\ &= \frac{1}{\sqrt{2\pi}} e^{i[k_0x + \alpha(k_0)]} \int_{-\infty}^{\infty} |g(k)| e^{i(k - k_0)(x - x_0)} dk \end{aligned}$$

where

$$x_M(0) = x_0 = - \left. \frac{d\alpha}{dk} \right|_{k=k_0}$$

is the center of the wave packet. This can also be obtained by the **stationary phase** condition:

$$\frac{d\varphi}{dk} = \frac{d}{dk}(kx + \alpha(k)) = 0$$

Also, for $|x - x_0| > \Delta k$ and $|x - x_0| < \delta k$: So for $|x - x_0| \gg 1$, This decrease becomes appreciable if $e^{i(k - k_0)(x - x_0)}$ oscillates approximately once when k traverses the domain Δk , that is, when:

$$\Delta k \cdot (x - x_0) \approx 1$$

or

$$\Delta k \cdot \Delta x \approx 1$$

if the length of wave is Δx .

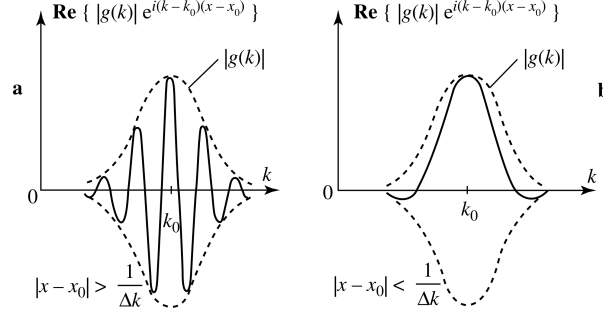


Figure 1.3: Variations w.r.t. k of the function to be integrated

1.3.3 Heisenberg relations

For the plane wave solution $e^{i(k_0 x - \omega_0 t)}$, the possibility is constant at x -axis, and thus $\Delta x \rightarrow \infty$. While the plane wave can also be obtained by set $g(k) = \delta(k - k_0)$, thus $\Delta k = 0$.

Use spectral decomposition, we can also interpret this another way. Since for $\psi(x, 0) = A e^{ikx}$, according to the de Broglie relations, the momentum of particle is determined by $p = \hbar k$, and then we say that e^{ikx} **characterizes the eigenstate corresponding to $p = \hbar k$** . And since k can be arbitrary number and any k corresponding to a wave e^{ikx} , thus any measurement on any state, the eigenvalue is also real number, as in classical mechanics.

For general cases, since $g(k)$ is the coefficient of the superposition, since k is continuous, $|g(k)|^2$ is proportional to **possibility density** $\overline{d\mathcal{P}}(k)$. More precisely, if we write as

$$\psi(x, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int \overline{\psi}(p) e^{ipx/\hbar} dp$$

then use Parseval-Plancherel relation,

$$\int_{-\infty}^{\infty} |\psi(x, 0)|^2 dx = \int_{-\infty}^{\infty} |\overline{\psi}(p)|^2 dp = C$$

we have

$$d\mathcal{P}(x) = \frac{1}{C} |\psi(x, 0)|^2$$

and

$$d\mathcal{P}(p) = \frac{1}{C} |\overline{\psi}(p)|^2$$

is the possibility to found particle at $(x, x+dx)$ and the measurement of momentum is at $(p, p+dp)$ respectively.

Back to $\Delta k \cdot \Delta x \geq 1$, we rewrite it as

$$\Delta p \cdot \Delta x \geq \hbar$$

where $\Delta p = \hbar \Delta k$ is the width of $\overline{\psi}(p)$. This inequality restrict the precision of the position of particle and the measurement of momentum, which is called as **Heisenberg relation** (or **uncertainty relation**). And for classical mechanics, it is like the limit $\hbar \rightarrow 0$.

1.3.4 Time evolution of a free wave packet

We know for plane wave $e^{i(kx-\omega t)}$, the **phase velocity** is

$$V_\varphi(k) = \frac{\omega}{k}$$

and for an electromagnetic wave propagating in a vacuum, V_φ is independent of k and is equal to c , and thus the wave packet's shape does not change. But for dispersive medium,

$$V_\varphi(k) = \frac{c}{n(k)}$$

varies.

And our case is similar to dispersive medium, because

$$V_\varphi(k) = \frac{\hbar k}{2m}$$

And also the maximum x_M of the packet is not the average velocity $\frac{\omega_0}{k_0} = \frac{\hbar k_0}{2m}$. Still use **stationary phase** condition, we get

$$x_M(t) = \left. \frac{d\omega}{dk} \right|_{k=k_0} t - \left. \frac{d\alpha}{dk} \right|_{k=k_0}$$

thus

$$V_G(k_0) := \frac{dx_M}{dt} = \left. \frac{d\omega}{dk} \right|_{k=k_0}$$

is the **group velocity** of the wave packet. Use the dispersion relation we get

$$V_G(k_0) = \frac{\hbar k_0}{m} = 2V_\varphi(k_0)$$

And this is just as particle in classical mechanics, which means for macroscopic particle the uncertainty relation have no restrict on accuracy and hence $\Delta x, \Delta p$ is negligible, and then its position and velocity are just x_M and $p_0 = \hbar k_0$ respectively.

1.4 Particle in a time-independent scalar potential

1.4.1 Separation of variables. Stationary states

For time-independent potential, the Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) + V(\mathbf{r}) \psi(\mathbf{r}, t)$$

Suppose the solution has the form

$$\psi(\mathbf{r}, t) = \varphi(\mathbf{r}) \chi(t)$$

then we get

$$\frac{i\hbar}{\chi(t)} \frac{d\chi(t)}{dt} = -\frac{\hbar^2}{2m} \frac{1}{\varphi(\mathbf{r})} \nabla^2 \varphi(\mathbf{r}) + V(\mathbf{r}) = \text{Const.} = \hbar\omega$$

Then we obtain that

$$\chi(t) = e^{-i\omega t}$$

and then

$$\psi(\mathbf{r}, t) = \varphi(\mathbf{r}) e^{-i\omega t}$$

with $\varphi(\mathbf{r})$ satisfies

$$-\frac{\hbar^2}{2m} \nabla^2 \varphi(\mathbf{r}) + V(\mathbf{r}) \varphi(\mathbf{r}) = \hbar\omega \varphi(\mathbf{r})$$

This is the **stationary solution of the Schrödinger equation**, and we can get the possibility density $|\psi(\mathbf{r}, t)|^2 = |\varphi(\mathbf{r})|^2$, it is corresponding to a **well-defined energy** $E = \hbar\omega$ for a stationary state, according to the Plank-Einstein relations. We can also rewrite the equation as

$$\boxed{H\varphi(\mathbf{r}) = E\varphi(\mathbf{r})}$$

where

$$\boxed{H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})}$$

is a linear differential operator, and this is the **eigenvalue equation** of H , and **the allowed energies are therefore the eigenvalues of the operator H** , and only certain E can make $\varphi(\mathbf{r})$ square-integrable, which is the origin of **energy quantization**, and we denote each possible energy as E_n , and thus the solution can write as

$$\psi(\mathbf{r}, t) = \sum_n c_n \varphi_n(\mathbf{r}) e^{-iE_n t/\hbar}$$

where $\varphi_n(\mathbf{r})$ is the corresponding solution to

$$H\varphi(\mathbf{r}) = E_n \varphi(\mathbf{r})$$

1.4.2 One-dimensional “square” potentials. Qualitative study

We use it to represent schematically a potential energy $V(x)$ which actually has the shape shown in Figure ??, this only invalid when the particle has high energy and short wavelength. And it is like the particle in a gravitational potential energy, and move through a deep valley. In this case the eigenvalue equation becomes

$$\left[\frac{d^2}{dx^2} + \frac{2m}{\hbar^2} (E - V) \right] \varphi(x) = 0$$

and this remind us that in optics, for a transparent medium whose index n depends neither on \mathbf{r} nor on time, the electric field in it is independent of y and z and has the form

$$\mathbf{E}(\mathbf{r}, t) = E(x) e^{-i\Omega t} \hat{\mathbf{e}}$$

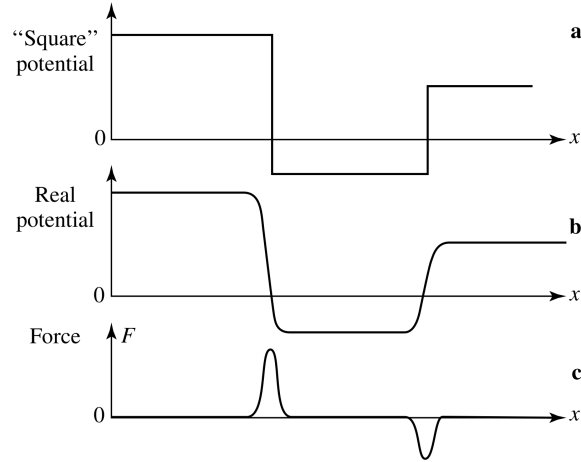


Figure 1.4: "Square" potential

where $\hat{\mathbf{e}} \perp \hat{\mathbf{x}}$, and $E(x)$ satisfies

$$\left[\frac{d^2}{dx^2} + \frac{n^2 \Omega^2}{c^2} \right] E(x) = 0$$

Thus if we let

$$n(\Omega) = \frac{1}{\hbar \Omega} \sqrt{2mc^2(E - V)}$$

also since the boundary condition of $E(x)$ and $\varphi(x)$ is the same (both the function and its derivative continuous), then we can use the conclusion in optics to explain this case.

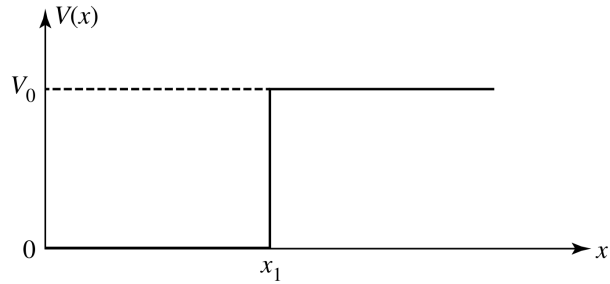


Figure 1.5: Potential step

Example 1 (Potential step). Consider the potential step in figure ??.

Solution. Consider the potential step as figure ?? shows, use the optics analogue, we get

$$n = \begin{cases} n_1 = \frac{c}{\hbar \Omega} \sqrt{2mE}, & x < x_1 \\ n_2 = \frac{c}{\hbar \Omega} \sqrt{2m(E - V_0)}, & x > x_1 \end{cases}$$

If $E - V_0 > 0$ and thus both n_1, n_2 are real, we know that in optics the light would split into a reflected wave and a transmitted wave, and this in QM means that the particle **has a certain probability \mathcal{P} of being reflected**, and probability $1 - \mathcal{P}$ to go to right.

If $E - V_0 < 0$, then n_2 is complex number, and since the existence of evanescent wave, we predict that the particle has a non-zero probability of being found in $x > x_1$. ■

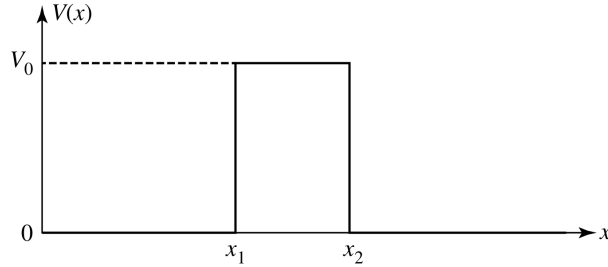


Figure 1.6: Potential barrier

Example 2 (Potential barrier). *Consider the potential step in figure ??.*

Solution. For $E < V_0$, a classical particle would turn back, but in optics, if the thickness is less than $1/\rho$, which is the range of evanescent wave $e^{-\rho x}$, then part of the incident wave is transmitted into the region $x > x_2$, and thus there is **a nonzero probability of the particle crossing the barrier**, this is called **tunnel effect**. ■

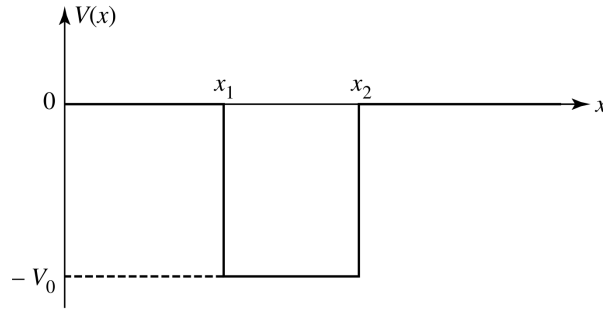


Figure 1.7: Potential well

Example 3 (Potential well). *Consider the Potential well in figure ??.*

Solution. In optics, if $-V_0 < E < 0$, both n_1, n_3 are imaginary, and this is like wave reflect between media, and only certain frequency can allow stable stationary wave, and others would destroy for interference. And in QM, this shows that **the negative energies are quantized**,

For $E > 0, n_1 = n_3 < n_2$, and this is like putting a layer of glass in air, multiple wave interferometer analogous to a Fabry-Perot, and there exists frequency s.t. the wave is entirely transmitted, and the corresponding energy in QM is called **resonance energies**. ■

Chapter 2

The mathematical tools of quantum mechanics

2.1 Space of the one-particle wave function

We have know that the interpretation of wave function $\psi(\mathbf{r}, t)$, $\psi(\mathbf{r}, t)d^3\mathbf{r}$ represents the probability of finding, at time t , the particle in a volume $d^3r = dx dy dz$ about the point \mathbf{r} . And also we have

$$\int |\psi(\mathbf{r}, t)|^2 d^3r = 1$$

Thus we need to study the set of **square-integrable** functions, which is L^2 , moreover, we want to study those are everywhere defined, continuous, and infinitely differentiable, have a bounded domain etc. We call \mathcal{F} the set of wave functions composed of sufficiently regular functions of L^2 .

2.1.1 Structure of the wave function space \mathcal{F}

- \mathcal{F} is a vector space.

Proof. For $\forall \psi_1(\mathbf{r}), \psi_2(\mathbf{r}) \in \mathcal{F}$, $\forall \lambda_1, \lambda_2 \in \mathbb{C}$, we say that $\psi(\mathbf{r}) = \lambda_1\psi_1(\mathbf{r}) + \lambda_2\psi_2(\mathbf{r}) \in \mathcal{F}$.

$$\begin{aligned} |\psi(\mathbf{r})|^2 &= (\lambda_1\psi_1(\mathbf{r}) + \lambda_2\psi_2(\mathbf{r}))(\lambda_1\psi_1(\mathbf{r}) + \lambda_2\psi_2(\mathbf{r}))^* \\ &= |\lambda_1|^2|\psi_1(\mathbf{r})|^2 + |\lambda_2|^2|\psi_2(\mathbf{r})|^2 + \lambda_1\lambda_2^*\psi_1(\mathbf{r})\psi_2^*(\mathbf{r}) + \lambda_1^*\lambda_2\psi_1^*(\mathbf{r})\psi_2(\mathbf{r}) \\ &\leq |\lambda_1|^2|\psi_1(\mathbf{r})|^2 + |\lambda_2|^2|\psi_2(\mathbf{r})|^2 + 2|\lambda_1||\lambda_2||\psi_1(\mathbf{r})||\psi_2(\mathbf{r})| \\ &\leq |\lambda_1|^2|\psi_1(\mathbf{r})|^2 + |\lambda_2|^2|\psi_2(\mathbf{r})|^2 + |\lambda_1||\lambda_2|(\psi_1^2(\mathbf{r}) + \psi_2^2(\mathbf{r})) \end{aligned}$$

So $\psi(\mathbf{r})$ is also square-integrable, and so $\psi(\mathbf{r}) \in \mathcal{F}$. □

- Scalar product.

Definition. For $\psi(\mathbf{r}), \phi(\mathbf{r}) \in \mathcal{F}$, the scalar product map the pair $(\phi(\mathbf{r}), \psi(\mathbf{r}))$ to a complex number:

$$(\phi, \psi) = \int d^3r \phi^*(\mathbf{r})\psi(\mathbf{r})$$

Property.

(a) **Linear** w.r.t. second and **antilinear** w.r.t. first.

$$\begin{aligned}(\varphi, \psi) &= (\psi, \varphi)^* \\(\varphi, \lambda_1 \psi_1 + \lambda_2 \psi_2) &= \lambda_1 (\varphi, \psi_1) + \lambda_2 (\varphi, \psi_2) \\(\lambda_1 \varphi_1 + \lambda_2 \varphi_2, \psi) &= \lambda_1^* (\varphi_1, \psi) + \lambda_2^* (\varphi_2, \psi)\end{aligned}$$

(b) $(\varphi, \psi) = 0 \iff \varphi$ and ψ is **orthogonal**.

(c) $(\psi, \psi) \in \mathbb{R}^+ \cup \{0\}$, it is zero iff. $\psi = 0$.

(d) **Schwarz inequality**:

$$|(\psi_1, \psi_2)|^2 \leq (\psi_1, \psi_1)(\psi_2, \psi_2)$$

- Linear operators.

Example 4.

(a) Parity operator Π :

$$\Pi\psi(x, y, z) = \psi(-x, -y, -z)$$

(b) Multiplication by x :

$$X\psi(x, y, z) = x\psi(x, y, z)$$

(c) Differential operator D_x :

$$D_x\psi(x, y, z) = \frac{\partial}{\partial x}\psi(x, y, z)$$

- Commutator.

For operator A and B , the **commutator** is

$$[A, B] = AB - BA$$

Example 5.

$$\begin{aligned}[X, D_x]\psi(\mathbf{r}) &= \left(x \frac{\partial}{\partial x} - \frac{\partial}{\partial x} x\right)\psi(\mathbf{r}) \\&= -\psi(\mathbf{r})\end{aligned}$$

2.1.2 Discrete orthonormal bases in $\mathcal{F} : \{u_i(\mathbf{r})\}$

Definition. Consider a countable set of functions in $\mathcal{F} : \{u_i(\mathbf{r})\}$, if it is both **orthonormal** and **complete**, which means

$$(u_i, u_j) = \int d^3r u_i^*(\mathbf{r})u_j(\mathbf{r}) = \delta_{ij}$$

and for $\forall \psi(\mathbf{r}) \in \mathcal{F}$, it can be expanded only one way in terms of $\{u_i(\mathbf{r})\}$:

$$\psi(\mathbf{r}) = \sum_i c_i u_i(\mathbf{r})$$

Components of wave function in basis.

$$\begin{aligned}
 (u_j, \psi) &= \left(u_j, \sum_i c_i u_i \right) \\
 &= \sum_i c_i (u_j, u_i) \\
 &= c_j
 \end{aligned}$$

and so we get

$$c_j = \int d^3r u_j(\mathbf{r})^* \psi(\mathbf{r})$$

Expression for the scalar product in terms of the components. Suppose we have

$$\begin{aligned}
 \psi(\mathbf{r}) &= \sum_j c_j u_j(\mathbf{r}) \\
 \varphi(\mathbf{r}) &= \sum_i b_i u_i(\mathbf{r})
 \end{aligned}$$

then

$$\begin{aligned}
 (\varphi, \psi) &= \sum_{i,j} b_i^* c_j (u_i, u_j) \\
 &= \sum_i b_i^* c_i
 \end{aligned}$$

and

$$(\psi, \psi) = \sum_i |c_i|^2$$

Closure relation.

$$\begin{aligned}
 \psi(\mathbf{r}) &= \sum_i c_i u_i(\mathbf{r}) \\
 &= \sum_i (u_i, \psi) u_i(\mathbf{r}) \\
 &= \sum_i \left[\int d^3r' u_i^*(\mathbf{r}') \psi(\mathbf{r}') \right] u_i(\mathbf{r}) \\
 &= \int d^3r' \left[\sum_i u_i^*(\mathbf{r}') u_i(\mathbf{r}) \right] \psi(\mathbf{r}')
 \end{aligned}$$

Then we get

$$\sum_i u_i^*(\mathbf{r}') u_i(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}')$$

since $\psi(\mathbf{r})$ is arbitrary, and vice versa.

2.1.3 “Bases” not belonging to \mathcal{F}

- Plane wave.

We know that the fourier transformation of a plane wave is

$$\begin{aligned}\psi(\mathbf{r}) &= \int d^3p \left(\frac{1}{2\pi\hbar} \right)^{3/2} \bar{\psi}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \\ \bar{\psi}(\mathbf{p}) &= \int d^3r \left(\frac{1}{2\pi\hbar} \right)^{3/2} \psi(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}\end{aligned}$$

Now consider function

$$v_{\mathbf{p}}(\mathbf{r}) = \left(\frac{1}{2\pi\hbar} \right)^{3/2} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$$

since $|v_{\mathbf{p}}(\mathbf{r})| = \left(\frac{1}{2\pi\hbar} \right)^{3/2}$ and so $v_{\mathbf{p}}(\mathbf{r}) \notin \mathcal{F}$, but consider set $\{v_{\mathbf{p}}(\mathbf{r})\}$ where the index p is continuous, then for $\forall \psi(\mathbf{r}) \in \mathcal{F}$, we have

$$\psi(\mathbf{r}) = \int d^3p \bar{\psi}(\mathbf{p}) v_{\mathbf{p}}(\mathbf{r})$$

where

$$\bar{\psi}(\mathbf{p}) = \int d^3r v_{\mathbf{p}}^*(\mathbf{r}) \psi(\mathbf{r}) = (v_{\mathbf{p}}, \psi)$$

and also

$$(\varphi, \psi) = \int d^3p \bar{\varphi}^*(\mathbf{p}) \bar{\psi}(\mathbf{p})$$

$$(v_{\mathbf{p}}, v_{\mathbf{p}'}) = \delta(\mathbf{p} - \mathbf{p}')$$

$$\int d^3p v_{\mathbf{p}}(\mathbf{r}) v_{\mathbf{p}}(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$$

- ”Delta function”.

We define

$$\xi_{\mathbf{r}_0}(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}_0)$$

and clearly $\xi_{\mathbf{r}_0}(\mathbf{r}) \notin \mathcal{F}$, but $\forall \psi(\mathbf{r}) \in \mathcal{F}$, we have

$$\begin{aligned}\psi(\mathbf{r}) &= \int d^3r_0 \psi(\mathbf{r}_0) \xi_{\mathbf{r}_0}(\mathbf{r}) \\ \psi(\mathbf{r}_0) &= (\xi_{\mathbf{r}_0}, \psi) = \int d^3r \xi_{\mathbf{r}_0}^*(\mathbf{r}) \psi(\mathbf{r})\end{aligned}$$

so the scalar product becomes

$$(\varphi, \psi) = \int d^3r_0 \varphi^*(\mathbf{r}_0) \psi(\mathbf{r}_0)$$

orthonormal and closure

$$\begin{aligned} \int d^3r_0 \xi_{\mathbf{r}_0}(\mathbf{r}) \xi_{\mathbf{r}'_0}^*(\mathbf{r}') &= \delta(\mathbf{r} - \mathbf{r}') \\ (\xi_{\mathbf{r}_0}, \xi_{\mathbf{r}'_0}) &= \delta(\mathbf{r}_0 - \mathbf{r}'_0) \end{aligned}$$

- Generalization: continuous “orthonormal” bases. Similarly we can obtain continuous bases w_α , summary in figure ??:

	Discrete basis $\{u_i(\mathbf{r})\}$	Continuous basis $\{w_\alpha(\mathbf{r})\}$
Ortho-normalization relation	$(u_i, u_j) = \delta_{ij}$	$(w_\alpha, w_{\alpha'}) = \delta(\alpha - \alpha')$
Closure relation	$\sum_i u_i(\mathbf{r}) u_i^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$	$\int d\alpha w_\alpha(\mathbf{r}) w_\alpha^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$
Expansion of a wave function $\psi(\mathbf{r})$	$\psi(\mathbf{r}) = \sum_i c_i u_i(\mathbf{r})$	$\psi(\mathbf{r}) = \int d\alpha c(\alpha) w_\alpha(\mathbf{r})$
Expression for the components of $\psi(\mathbf{r})$	$c_i = (u_i, \psi) = \int d^3r u_i^*(\mathbf{r}) \psi(\mathbf{r})$	$c(\alpha) = (w_\alpha, \psi) = \int d^3r w_\alpha^*(\mathbf{r}) \psi(\mathbf{r})$
Scalar product	$(\varphi, \psi) = \sum_i b_i^* c_i$	$(\varphi, \psi) = \int d\alpha b^*(\alpha) c(\alpha)$
Square of the norm	$(\psi, \psi) = \sum_i c_i ^2$	$(\psi, \psi) = \int d\alpha c(\alpha) ^2$

Figure 2.1: Bases summary

2.2

2.3

2.4

2.5

2.6