

# Quantum Mechanics

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# Chapter 1

## Mathematical Foundations of Quantum Mechanics

### 1.1 Introduction

First problem of quantum Theory: explanation of discrete values of energies of atomic levels. Thus, need appropriate math.

1. Postulate that some function only yields discrete values from a given set (Bohr).
2. Observables are defined by roots of some algebraic equations (Heisenberg).
3. Observables are eigenstates of some differential operator (Schrödinger).

Methods of modern Quantum Mechanics are based on properties of linear operators defined on Hilbert spaces.

### 1.2 Mathematical Formulation of Superposition Principle

Theorem (superposition principle): Any wave function  $\Psi(q, t)$  can be expanded in a terms of complete, orthonormalized set of functions:  $\Psi_1(q, t)$ ,  $\Psi_2(q, t)$ , ...,  $\Psi_k(q, t)$

4CHAPTER 1. MATHEMATICAL FOUNDATIONS OF QUANTUM MECHANICS

In order to prove it, let's recall the following:

$$\text{subset} \exists \Psi(q, t) \in [a, b]; \int_a^b dx \Psi_m^*(x) \Psi_n(x) = \delta_{mn} \quad (1.1)$$

For any function  $\Psi(x)$ :

$$\int_a^b |\Psi(x)|^2 dx \geq \sum_{k=1}^n |C_k|^2 \quad (1.2)$$

Where

$$C_k = \int_a^b dx \Psi^*(x) \Psi_k(x) \equiv \langle \Psi | \Psi_k \rangle \quad (1.3)$$

Let's introduce

$$\epsilon_n^2 = \frac{1}{b-a} \left( \int_a^b |\Psi(x)|^2 dx - \sum_{k=1}^n |C_k|^2 \right) \quad (1.4)$$

Indeed, if  $n \rightarrow \infty$  one gets a series expansion. Thus,  $\epsilon \rightarrow 0$  get closure relation

$$\int_a^b dx |\Psi(x)|^2 = \sum_{k=1}^{\infty} |C_k|^2 \quad (1.5)$$

where  $|c_k|^2 = C_k^* C_k$

Then:

$$\int_a^b dx |\Psi(x)|^2 = \int_a^b dx \Psi^*(x) \Psi(x) = \sum_{k=1}^{\infty} |C_k|^2 = \sum_{k=1}^{\infty} C_k^* \int_a^b dx \Psi^*(x) \Psi_k(x) \quad (1.6)$$

Change  $\sum$  and  $\int$  : series must be uniformly convergent, true for all physical systems

$$= \int_a^b dx \Psi^*(x) \sum_{k=1}^{\infty} C_k \Psi_k(x) \quad (1.7)$$

Thus, from 1.6 and 1.7

$$\Psi(x) = \sum_{k=1}^{\infty} C_k \Psi_k(x) \quad (1.8)$$

This is true for any number of dimensions

$$\Psi(\vec{r}) = \sum_{k=1}^{\infty} C_k \Psi_k(\vec{r}); C_k = \int d^3 \vec{r} \Psi^*(\vec{r}) \Psi_k(\vec{r}) \quad (1.9)$$

Theorem (completeness)

If for every  $\Psi(x)$  and a set of functions,  $\Psi_k(x)$  one can form a closure relationshipt ( $\Delta$ )

Then: this set of functions is complete.

Proof: Lets assume that this is not so, i.e.  $\exists \Psi_o(x)$ : it is orthogonal to  $\Psi_k(x)$ .

Then:  $\int dx \Psi_o^*(x) \Psi_m(x) = 0$ ,  $m = 1, 2, \dots, n$

But: since  $\Psi(x)$  is arbitrary: can take  $\Psi = \Psi_o$ !

Then:  $\int dx |\Psi_o(x)|^2 = \sum_k |C_k|^2 = \sum_k |\int dx \Psi_o^*(x) \Psi_k(x)|^2 = 0!!$

Thus,  $\boxed{\Psi_o(x) \equiv 0}$ , such a function does not exist and the set is complete.

### 1.3 Expectation values. Measurements

Consider finite motion.

$$\int_{-\infty}^{\infty} |\Psi(\vec{r})|^2 d\vec{r} = \sum_{k=1}^{\infty} |C_k|^2 = 1 \quad (1.10)$$

note:  $\Psi(\vec{r}) \longrightarrow 0$  as  $\vec{r} \longrightarrow \infty$

This is the probability of finding an object anywhere in space.

Then:  $|C_n|^2$  is the probability of finding our quantum system in a state described by  $\Psi_n(\vec{r})$ !

So: if  $f$  is some physical quantity described by  $\Psi(\vec{r})$ . Then  $f_n$  is realized with amplitude of probability  $\underline{C_n}$

### 1.4 Hilbert spaces. Operators

Definition: A set of vectors  $\vec{E}$  is called a linear space if:

1.  $\forall x \in \vec{E} \exists \lambda \in I : \lambda x \in \vec{E}$
2.  $\forall [x, y] \in [\vec{E}] : x + y \in [\vec{E}]$
3.  $\exists \vec{o} \in [\vec{E}]$

Let us define a set of functions  $[\Psi_i \vec{r}]$

$i = 1, \dots, n$  can be finite or infinite.

Definition: For any two functions  $\Psi(\vec{r})$  and  $\Psi_1(\vec{r})$ :

6 CHAPTER 1. MATHEMATICAL FOUNDATIONS OF QUANTUM MECHANICS

$$(\Psi, \phi) \equiv \langle \Psi | \phi \rangle = \int d\vec{r} \Psi^*(\vec{r}) \phi(\vec{r})$$

is called the scalar (inner) product.

Thus, any vector space with  $(*)$  is called an inner-product space.

Thus, if  $\Psi = \phi$ ; then  $(\Psi, \Psi) = \langle \Psi | \Psi \rangle = \|\Psi\|^2 = \int d\vec{r} \Psi^*(\vec{r}) \Psi(\vec{r})$

called a norm.

Definition: A Hilbert space  $\vec{H}$  is an inner product space that is complete \*wrt the norm defined by an inner product.

QM:

$$\Psi(\vec{r}) = \sum_k C_k \Psi_k(\vec{r}) \tag{1.11}$$

where  $C_k$  is the cosine of angles between  $\Psi(\vec{r})$  and  $\Psi_k(\vec{r})$

Prove: That  $\vec{H}$  is a linear space.

hint: Use the superposition principle.

Analogy:

Need some object to do “rotation”

Definition: An object that maps  $[\Psi_E] \xrightarrow{U} [\phi_i]$  is called an operator.

Ex:  $\frac{d}{dx}$  (consider polynomial space)

Definition: A linear operator is an operator for which:

$\forall [\Psi_1, \Psi_2] \in [\Psi_i]$  and  $\forall \alpha, \beta \in C$ :

$$\hat{L}(\alpha\Psi_1 + \beta\Psi_2) = \alpha\hat{L}\Psi_1 + \beta\hat{L}\Psi_2$$

i.e., *LHS* and *RHS* map onto the same element of  $[\phi_i]$

Some general properties of operators:

1.  $\hat{A} = \hat{B} \cdot \hat{C} : \forall \Psi : \hat{A} \Psi \equiv \hat{B} (\hat{C} \cdot \Psi)$
2. Commutator  $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} ; [\hat{A}, \hat{B}] = \hat{A}\hat{B} + \hat{B}\hat{A}$   
If  $[\hat{A}, \hat{B}] = 0 \implies$  commute.
3. Unit Operator:  $\hat{1}\Psi = \Psi, (\hat{A} \cdot \hat{A}^{-1})\Psi = (\hat{A}^{-1} \hat{A})\Psi = ?$

Recall that an operator can be written in intergral form:

$$\hat{L}\Psi = \int L(x, \xi) \Psi(\xi) d\xi \tag{1.12}$$

or simply by defining a rule (“explicit form”):

$$\hat{q}\Psi(x) = x\Psi(x)$$

## 1.5. MAIN PROPERTIES OF OPERATORS IN QUANTUM MECHANICS 7

$$\hat{d}\Psi(x) = \frac{d}{dx}\Psi(x)$$

$$\hat{P}\Psi(x) = \Psi(-x), \text{ and so on}$$

If  $\hat{L}\Psi = \lambda\Psi$ ;  $\lambda \in C$ :  $\Psi$  is eigenfunction,  $\lambda$  is eigenvalue of  $\hat{L}$ .

Example: Show that a product of two operators is a linear operator which can be written in the form 1.12.

$$\exists \hat{L}_1 \& \hat{L}_2: \hat{L} = \hat{L}_1 \cdot \hat{L}_2 \quad \exists \Psi:$$

$$\hat{L}_2(x)\Psi(x) = \int dy L_2(x, \xi)\Psi(\xi) \quad (1.13)$$

$$\begin{aligned} \hat{L}(x)\Psi(x) &= \hat{L}_1(x)(\hat{L}_2(x)\Psi(x)) = \int dy L_1(x, \zeta) \int dy L_2(\zeta, \xi)\Psi(\xi) \\ &= \int dy \int d\zeta L_1(x, \zeta)L_2(\zeta, \xi)\Psi(\xi) = \int d\xi L(x, \xi)\Psi(\xi) \end{aligned}$$

$$L(x, y) = \int dy L_1(x, \zeta)L_2(\zeta, \xi) \quad (1.14)$$

Ex. 2 Unit Operator:  $\hat{1}\Psi(x) = \Psi(x)$ . integral form:  $\hat{1}\Psi(x) = \int d\xi \delta(x - \xi)\Psi(\xi)$

## 1.5 Main properties of operators in Quantum Mechanics

As was mentioned, all operators of quantum mechanics must be linear (superposition principle)

In quantum mechanics, every physical quantity,  $F$ , can be represented by an operator (linear operator)  $\hat{F}$ :

$$\bar{F} = \langle F \rangle = \int_{-\infty}^{\infty} d^3\vec{r} \Psi^*(\vec{r})\hat{F}\Psi(\vec{r}) \quad (1.15)$$

where  $\langle F \rangle$  is the expectation value of  $F$

Operators of interest (related to  $\hat{F}$ ):

- Transposed operator:

$$\text{If } \int d^3\vec{r} \phi \hat{F}\Psi = \int d^3\vec{r} \Psi(\hat{F}^T, \phi)$$

Then:  $\hat{F}^T$  is called transposed of  $\hat{F}$ .

- Conjugated operator:

$$\text{consider } (\int d^3\vec{r} \Psi^*(\vec{r})\hat{F}\Psi(\vec{r}) = \int d^3\vec{r} \Psi^*(\vec{r})(\hat{F}^*)^T\Psi(\vec{r}), (\hat{F}^*)^T \text{ is } \Psi^t$$

$$\hat{F}^t \equiv (\hat{F}^*)^T \quad (1.16)$$

8CHAPTER 1. MATHEMATICAL FOUNDATIONS OF QUANTUM MECHANICS

- If  $\boxed{\hat{F}^t = \hat{F}}$   $\implies \hat{F}$  is called self-conjugated or Hermitian.

Properties of Hermitian operators:

1.  $(\hat{F} + \hat{G})^t = \hat{F}^t + \hat{G}^t$
2.  $\hat{L} = \hat{A} + \hat{B}$ :  $\hat{A} = \frac{1}{2}(\hat{L} + \hat{L}^*, \hat{B} = \frac{i}{2}(\hat{L} - \hat{L}^t)$
3.  $(\hat{F} \cdot \hat{G})^t = \hat{G}^t \hat{F}^t$  (note order)

Proof:  $\int d^3\vec{r}\Psi^*(\hat{F}\hat{G})^t\Psi = \int d^3\vec{r}\Psi^*\hat{G}^t\hat{F}^t\Psi = \int d^3\vec{r}(\hat{G}\Psi)^*\hat{F}^t\Psi = \int d^3\vec{r}\Psi^*\hat{G}^t\hat{F}^t\Psi$

corollary: A product of two Hermitian operators is Hermitian if and only if they commute.

4. Very important!

Hermitian operators have real eigenfunctions, i.e.  $\forall \hat{F} : \hat{F}^t = \hat{F}$  we have  $\hat{F}\Psi_n = \lambda_n\Psi_n$  (or  $\hat{F}|n\rangle = \lambda_n|n\rangle$ ) with  $\lambda_n \in \mathfrak{R}$ !

Proof:  $\int d^3\vec{r}\Psi_n^*\hat{F}\Psi_n \equiv \langle n|\hat{F}|n\rangle = \lambda \langle n|n\rangle = (\langle n|\hat{F}^t|n\rangle)^* = \lambda_n^* \langle n|n\rangle$

$$\lambda_n = \lambda_n^* \tag{1.17}$$

5. Eigen functions that correspond to different eigen values are orthogonal

Proof:  $\hat{F}\Psi_n = \lambda_n\Psi_n$  &  $\hat{F}\Psi_m = \lambda_m\Psi_m$

then:  $\langle m|\hat{F}|n\rangle = \lambda_m \langle m|n\rangle$

$\langle m|\hat{F}^t|n\rangle = (\langle n|\hat{F}|m\rangle)^* = \lambda_m \langle m|n\rangle$

$(\lambda_m - \lambda_n) \langle m|n\rangle = 0 \implies \langle m|n\rangle = 0$

These are exactly the properties needed to describe a system with discrete spectrum!

Lets put together some notions that we have discussed so far.

$\Psi(\vec{r}) = \sum_k C_k \Psi_k(\vec{r}), C_k = \int d^3\vec{r} \Psi_k^*(\vec{r}) \Psi(\vec{r})$

$C_k$  is the amplitude of probability to realize state which corresponds to  $F = f_k$

$\Psi_k$  is the state that describes when some physical quantity  $F$  is said to have a definite value.

How we can find  $\Psi_k^*$  which corresponds to  $\hat{F}$ ?

Recall **\*\*\***matens definition of expectation value (mean value):

$$\langle F \rangle = \sum_k |C_k|^2 f_k \quad (1.18)$$

where  $|C_k|$  is probability for  $F$  to take  $F_k$  and  $f_k$  us definite values of  $F$   
 Thus,  $\int d^3\vec{r} \Psi^* \hat{F} \Psi(\vec{r}) = \sum_k C_k^* C_k f_k = \int d^3\vec{r} \Psi^*(\vec{r}) \sum_k C_k f_k \Psi_k(\vec{r}) =$

$$\hat{F} \Psi(\vec{r}) = \sum_n C_n f_n \Psi_n(\vec{r}) \quad (1.19)$$

Now, if we want to find a state where  $F$  takes on definite value:  $\Psi(\vec{r}) \longrightarrow \Psi_m(\vec{r})$

Thus,  $\Psi_m(\vec{r}) = \sum_n C_n \Psi_n(\vec{r})$  works only if  $m = n$ , i.e.:

$$C_n = \begin{cases} 1, & n = m \\ 0, & \text{otherwise} \end{cases}$$

$$\hat{F} \Psi_m(\vec{r}) = f_m \Psi_m(\vec{r}) \quad (1.20)$$

is the eigen function equation for discrete spectrum

Example: Let  $\hat{F} = \hat{H}$  (Hamiltonian)

Thus,  $f_m = E_m$  (energy levels)

$$\hat{H} \Psi_m(\vec{r}) = E_m \Psi_m(\vec{r}) \quad (1.21)$$

\*Does it make sense (as far as physics is concerned) to talk about sum of operators??? what about product???

## 1.6 Compatible and Incompatible Observables

Take  $\hat{F}$  &  $\hat{G}$  that correspond to  $F$  &  $G$ .

If  $F$  &  $G$  can be simultaneously measured  $\Leftrightarrow \hat{F}$  &  $\hat{G}$  have the same set of eigen functions.

Recall: "correspond" to observable a Hermitian operator ( $L : \hat{L} \Psi_{qc} = L \Psi_{qc}$ )

or: Hermitian part of operator.

**Theorem 1** *If two physical quantities (observables) can be simultaneously measured then the operators that correspond to those observables commute.*

Proof: Let  $F \longrightarrow \hat{F}\Psi_n = f_n\Psi_n$  and  $G \longrightarrow \hat{G}\Psi_n = g_n\Psi_n$

We need to prove that  $[\hat{F}, \hat{G}] = 0$

Let's act with  $\hat{F}\hat{G}$  on  $\Psi_n$ :

$$\hat{F}\hat{G}\Psi_n = \hat{F}(\hat{G}\Psi_n = \hat{F}g_n\Psi_n = g_n f_n\Psi_n \quad (1.22)$$

Similarly, let's act with  $\hat{G}\hat{F}$  on  $\lambda_n$ :

$$\hat{G}\hat{F}\Psi_n = \hat{G}(\hat{F}\Psi_n = \hat{G}f_n\Psi_n = f_n g_n\Psi_n \quad (1.23)$$

Subtract 1.23 from 1.22:

$$\hat{F}\hat{G}\Psi_n - \hat{G}\hat{F}\Psi_n = [\hat{F}, \hat{G}]\Psi_n = g_n f_n\Psi_n - f_n g_n\Psi_n = 0 \quad (1.24)$$

Thus,  $[\hat{F}, \hat{G}] = 0$

**Theorem 1** *If  $\hat{F}$  and  $\hat{G}$  commute;  $[\hat{F}, \hat{G}] = 0$ , then corresponding observables can be simultaneously measured.*

Proof:  $\forall[\hat{F}, \hat{G}] = 0$  Prove that

$$\text{same set}|\Psi_m\rangle = \begin{cases} \hat{F}\Psi_n = f_n\Psi_n \\ \hat{G}\Psi_n = g_n\Psi_n \end{cases}$$

$\Psi_n$  are eigen functions (eigenstates) of  $\hat{F}$ ;

$$\hat{F}\Psi_n = f_n\Psi_n \quad (1.25)$$

Let's act with  $\hat{G}$  on both side of equation 1.25:

$$\hat{G}\hat{F}\Psi_n = (as[\hat{F}, \hat{G}] = 0) = \hat{F}(\hat{G}\Psi_n)$$

and =

$$\hat{G}f_n\Psi_n = f_n(\hat{G}\Psi_n) \quad (1.26)$$

Thus: if  $\Psi_n$  is an eigen vector of  $\hat{F}$  then  $\hat{G}\Psi_n$  is an eigen vector too.

But: the eigen system of  $\hat{F}$  must be unique! Thus,  $\hat{G}\Psi_n = \text{constant } \Psi_n$ ; where constant =  $g_n$  from the form of eigen value problem.

Thus:  $\hat{F}$  &  $\hat{G}$  have the same set of eigen functions. (This is a simultaneous eigen function of  $\hat{F}$  &  $\hat{G}$ )

Definition: If  $[\hat{F}, \hat{G}] = 0$  then the corresponding observables are called compatible.

If  $[\hat{F}, \hat{G}] \neq 0 \Leftrightarrow$  incompatible.

**Theorem 1** *Eigen functions corresponding to physical observables of community operators form a orthonormalized system.*

Proof: given  $\hat{F}, \hat{G}, \hat{L} \dots$

- a)  $[\hat{F}, \hat{G}] = [\hat{F}, \hat{L}] = \dots = 0$
- b)  $\hat{F} = \hat{F}^t, \hat{G} = \hat{G}^t, \dots$

Prove for two operators, the rest is obvious.

Thus, for  $[\hat{F}, \hat{G}] = 0$  :  $\Psi_n$  is a simultaneous eigen function.

$$\text{Theorem I } \left\{ \begin{array}{l} \hat{F}\Psi_{nm} = f_n \Psi_{nm} \\ \hat{G}\Psi_{nm} = g_n \Psi_{nm} \end{array} \right\}$$

Also:  $\hat{F}^* \Psi_{n'm'}^* = f_{n'} \Psi_{n'm'}^*$

$$\hat{G}^* \Psi_{n'm'}^* = g_{m'} \Psi_{n'm'}^*$$

( $f_n^* = f_n$  as Hermitian operator)

Intergrate (\*) with  $\int \Psi_{n'm'}^*$ :

$$\int d^3\vec{r} \Psi_{n'm'}^* \hat{F} \Psi_n = f_n \int d^3\vec{r} \Psi_{n'm'}^* \Psi_{nm}$$

same for (\*, \*):

$$\int d^3\vec{r} \Psi_{nm} \hat{F}^* \Psi_{n'm'}^* = f_{n'} \int d^3\vec{r} \Psi_{n'm'}^* \Psi_{nm}$$

where;  $\int d^3\vec{r} \Psi_{nm} \hat{F}^* \Psi_{n'm'}^* = \int d^3\vec{r} (\Psi_{n'm'}^*, \hat{F}^t) \Psi_{nm}$

Subtract:  $\int d^3\vec{r} \Psi_{n'm'}^* (\hat{F} - \hat{F}^t) \Psi_{nm} = (f_n - f_{n'}) \int d^3\vec{r} \Psi_{n'm'}^* \Psi_{nm} = 0$ , as  $\hat{F} = \hat{F}^t$

$$\left\{ \begin{array}{l} f_n - f_{n'} \int d^3\vec{r} \Psi_{n'm'}^* \Psi_{nm} = 0 \\ g_n - g_{n'} \int d^3\vec{r} \Psi_{n'm'}^* \Psi_{nm} = 0 \end{array} \right.$$

Consider four separate cases:

1.  $n \neq n', m \neq m'$

Thus, (I) and (II) :  $\int d^3\vec{r} \Psi_{n'm'}^* \Psi_{nm} = 0$ ,  $f_n \neq f_{n'}, g_n \neq g_{n'}$

2.  $n = n', m \neq m'$  (I) :  $\int d^3\vec{r} \Psi_{n'm'}^* \Psi_{nm} = \frac{0}{0}$ , but:

$$(II) \int d^3\vec{r} \Psi_{n'm'}^* \Psi_{nm} = 0!$$

3. same for  $n \neq n', m = m'$

4.  $n = n', m = m'$ : (I) and (II) give %...

but: normalization of  $\Psi$  implies  $\int_{-\infty}^{infy} |\Psi_{nm}|^2 d^3\vec{r} = 1$  so ...

$$\int d^3\vec{r} \Psi_{n'm'}^* \Psi_{nm} = \delta_{nn'} \delta_{mm'} \quad (1.27)$$

## 1.7 Unitary operators: Unitary equivalent observables

**Definition 1**  $\hat{U}$  is called unitary operator if  $\boxed{\hat{U}\hat{U}^\dagger = \hat{U}^*\hat{U} = 1}$

Properties of unitary operators:

1. For  $U|\Psi\rangle = \lambda|\Psi\rangle$ :  $|\lambda|^2 = 1$   
Proof:  $\langle\Psi|U^\dagger U|\Psi\rangle = \lambda\langle\Psi|U^\dagger|\Psi\rangle = \lambda\lambda^*\langle\Psi|\Psi\rangle$   
 thus,  $\lambda\lambda^* = 1$
2. If  $\hat{U}$  and  $\hat{V}$  are unitary, then  $\hat{W} = \hat{U}\hat{V}$  is also unitary  
 $\hat{W}^\dagger = \hat{V}^\dagger\hat{U}^\dagger$   
 thus,  $\hat{W}^\dagger\hat{W} = \hat{V}^\dagger\hat{U}^\dagger\hat{U}\hat{V} = \hat{1} \Rightarrow \text{unit.}$

**Definition 1**  $\hat{U}$  is unitary. A transformation  $\phi = \hat{U}^\dagger\hat{\Psi}\hat{N} = \hat{U}^\dagger\hat{L}U$  for  $\hat{L}\hat{\Psi}$  is called unitary transformation. ( $\hat{N}$  and  $\hat{L}$  are unitary equivalent observables)

Properties:

1. Commut. rel. are “conserved”:  
 $[\hat{L}, \hat{M}] = \hat{N} : \hat{L}' = \hat{U}^\dagger\hat{L}\hat{U}, \hat{M}' = \hat{U}^\dagger\hat{M}\hat{U}, \dots$   
 Thus,  $[\hat{L}', \hat{M}'] = \hat{N}'$
2. Conserves “hermicity” if  $\hat{L} = \hat{L}^\dagger \Rightarrow \hat{L}' = \hat{L}'^\dagger$
3. Important: conserves eigen values:  
 $\hat{L}\Psi = \lambda\Psi : \hat{U}^\dagger\hat{L}\Psi = \lambda U^\dagger\Psi$   
 thus,  $\hat{U}^\dagger\hat{L}U U^\dagger\Psi = \lambda U^*\Psi$   
 with,  $\hat{U}^\dagger\hat{L}U = \hat{L}'$  and  $U^\dagger\Psi = \phi$   
 thus,  $\hat{L}'\phi = \lambda\phi$

## 1.8 General properties of continuous spectrum

So far: mostly discrete spectrum of eigenstates (realized on finite motion)

But: There are examples of observables with continuous eigenvalues.

example: momentum operator  $\hat{p}$  eigenvalues  $p$  take  $(-\infty, \infty)$ .

Expect that normalization condition for wave functions could be different. In order to study continuous spectrum we need to empty  $\delta$ -function.

Mathematics aside Properties of  $\delta$ -function

Recall definition: kernel of  $\hat{1}$  operator.

Basic Properties:

1.

$$\delta(x) = \begin{cases} \infty, & x = 0; \\ 0, & x \neq 0. \end{cases}$$

$$\int_{-\infty}^{\infty} dx \delta(x) = 1$$

2.  $\int_{-\infty}^{\infty} dx f(x) \delta(x) = f(0)$

Show this for particular “representation” of  $\delta$ -function:

$$\delta(x) = \lim_{\Delta \rightarrow 0} \frac{1}{\sqrt{\pi\Delta^2}} e^{-\frac{x^2}{\Delta^2}}:$$

$$\int_{-\text{infy}}^{\infty} f(x) \delta(x) dx = \lim_{\Delta \rightarrow 0} \frac{1}{\sqrt{\pi\Delta^2}} \int_{-\text{infy}}^{\infty} dx e^{-\frac{x^2}{\Delta^2}} f(x) = \text{mean value theorem}$$

$$\lim_{\Delta \rightarrow 0} \frac{1}{\sqrt{\pi\Delta^2}} e^{-\frac{x^2}{\Delta^2}} f(0) \int_{-\text{infy}}^{\infty} dx e^{-\frac{x^2}{\Delta^2}} = \frac{f(0)}{\pi}$$

$$\text{other reps: } \delta(x) = \frac{1}{\pi} \frac{x}{x^2 + \Delta^2}, \delta(x) = \frac{1}{\pi i} \frac{\sin^2 \Delta x}{\Delta^2 x^2}$$

3.  $\delta(-x) = \delta(x)$ :

$$\int_{-\infty}^{\infty} \delta(-x) dx = - \int_{+\infty}^{-\infty} \delta(y) dy = \int_{-\infty}^{\infty} \delta(y) dy = 1 = \int_{-\infty}^{\infty} \delta(x) dx = \delta(-x) = \delta(x).$$

4.  $\delta(-x) = \delta(x)$ :

$$\int_{-\infty}^{\infty} \delta(-x) dx = - \int_{+\infty}^{-\infty} \delta(y) dy = \int_{-\infty}^{\infty} \delta(y) dy = 1 = \int_{-\infty}^{\infty} \delta(x) dx$$

Thus,  $\delta(-x) = \delta(x)$

5.  $\delta(\alpha x) = \frac{1}{|\alpha|} \delta(x)$

$$(a) \alpha > 0: \int_{-\infty}^{\infty} \delta(\alpha x) dx = \frac{1}{\alpha} \int_{-\infty}^{\infty} \delta(x) dx = \int_{-\infty}^{\infty} \frac{1}{|\alpha|} \delta(x) dy$$

$$(b) \alpha < 0: \int_{-\infty}^{\infty} \delta(\alpha x) dx = -\frac{1}{|\alpha|} \int_{+\infty}^{-\infty} \delta(y) dy = \int_{-\infty}^{\infty} \frac{1}{|\alpha|} \delta(x) dx$$

6. “Integral representation”:

$$f(x) = \int_{-\infty}^{\infty} f(\beta) e^{i\beta x} d\beta = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\beta \int_{-\infty}^{\infty} dx' f(x') e^{-i\beta x'} e^{i\beta x} = \int_{-\infty}^{\infty} dx' f(x') \frac{1}{2\pi} \int_{-\infty}^{\infty} d\beta e^{i\beta(x-x')}$$

and  $\delta(x - x')$  by definition:  $f(x) = \int dx \delta(x - x')$  Thus;

$$\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\beta e^{i\beta(x-x')} \tag{1.28}$$

Generalize to 3 dimensions:  $\delta^{(3)}(\vec{r} - \vec{r}') = \frac{1}{(2\pi)^3} \int d^3\vec{p} e^{i\vec{p}(\vec{r} - \vec{r}')}$

$$\delta^{(3)}(\vec{r}) = \delta(x)\delta(y)\delta(z)$$

$\delta(\phi(f) - \phi(f')) = ?$

If  $\phi(f)$  is continuous

takes  $\Delta f : f - f' \ll f, f'$ :

Then:  $\phi(x) = \phi(f') + \left. \frac{d\phi}{df} \right|_{f=f'} (f - f') + \dots$

Thus,  $\delta(\phi(f) - \phi(f')) = \delta\left(\left. \frac{d\phi}{df} \right|_{f=f'} (f - f')\right) = \frac{1}{\left| \left. \frac{d\phi}{df} \right|_{f=f'} \right|} \delta(f - f')$

In general:

$$\delta(\phi(f) - \phi(f')) = \sum_{i=1}^n \frac{1}{\left| \left. \frac{d\phi}{df} \right|_{f=f_i} \right|} \delta(f - f') \quad (1.29)$$

### 7. "Convolution of $\delta$ -function"

$$\int_{-\infty}^{\infty} \delta(a - x)\delta(x - b)dx = \delta(a - b)$$

multiply both sides by  $f(a)$  and integrate over  $\int_{-\infty}^{\infty} da$ :

$$\int_{-\infty}^{\infty} f(a) \int_{-\infty}^{\infty} \delta(a - x)\delta(x - b)dx da = \int_{-\infty}^{\infty} dx f(x)\delta(x - b) \equiv \int_{-\infty}^{\infty} da f(a)\delta(a - b)$$

### Continuous Spectrum(cont.)

Consider  $\hat{F}\Psi_f(q) = f\Psi_f(q)$ ,  $f$  is a continuous value  
what about closure, normalization, and other conditions?

Take the "limiting procedure" :  $\sum_n \longrightarrow \int df$

Thus;

$$\int_{-\infty}^{\infty} |\Psi(q)|^2 dq = \int df |a(f)|^2 \quad (1.30)$$

$$a(f) = \int_{-\infty}^{\infty} dq \Psi(q) \Psi_f^*(q) \quad (1.31)$$

Use this to plug in  $a^*$  in completeness relation:

$$\int_{-\infty}^{\infty} dq \Psi^*(q) \Psi(q) = \int df a(f) \int_{-\infty}^{\infty} dq \Psi^*(q) \Psi_f(q) dq = \int_{-\infty}^{\infty} dq \Psi^*(q) \underbrace{\int df a(f) \Psi_f(q)}_{(1.32)}$$

$$\Psi(q) = \int df a(f) \psi_f(q) \quad (1.33)$$

lets substitute 1.33 into 1.31:

$$a(f) = \int_{-\infty}^{\infty} dq \Psi_f^*(q) \int df' a(f') \Psi_f(q) = \int df' a(f') \underbrace{\int_{-\infty}^{\infty} dq \Psi_f^*(q) \Psi_f(q)}_{\text{must be } \delta(f - f')!}$$

$$\int_{-\infty}^{\infty} dq \Psi_f^*(q) \Psi_{f'}(q) = \delta(f - f') \quad (1.34)$$

This is a normalizing condition for wave functions of continuous spectrum.

Another relation: plug 1.31 into 1.33:

$$\Psi(q) = \int df a(f) \Psi_f(q) = \int \Psi(q') \underbrace{\int \Psi_f^*(q') \Psi_f(q) df}_{\delta(q' - q)} dq'$$

Thus:

$$\int df \Psi_f^*(q') \Psi_f(q) = \delta(q' - q) \tag{1.35}$$

Example: Find eigenfunction of the coordinate operator in coordinate representation

Definition: Coordinate representation” of a wave function is such a representation that the wave function describes the probability distribution in coordinate space.

$$dw(q) = |\Psi(q)|^2 dq \tag{1.36}$$

Define coordinate operator:

$$1. \langle q \rangle = \int_{-\infty}^{\infty} q dw(q) = \int_{-\infty}^{\infty} dq q \Psi^*(q) \Psi(q) = \int_{-\infty}^{\infty} dq \Psi^*(q) q \Psi(q)$$

$$2. \text{ But: } \langle q \rangle = \int_{-\infty}^{\infty} dq \Psi^*(q) \hat{q} \Psi(q)$$

compare: in coordinate representations

$$\hat{q} = q \tag{1.37}$$

Let’s find eigenfunctions:

$$\hat{q} \Psi_{q_o}(q) = q_o \Psi_{q_o}(q) \tag{1.38}$$

from equation 1.37 ;  $q \Psi_{q_o}(q) = q_o \Psi_{q_o}(q)$

This equation holds if:

- (a)  $q \neq q_o$  :  $\Psi_{q_o}(q) = 0$
- (b)  $q = q_o$  :  $\Psi_{q_o}(q) = \Psi_{q_o}(q)$

use normalization:

$$\int_{-\infty}^{\infty} dq \Psi_{q_o}^*(q) \Psi_{q_o}(q) = \delta(q_o - q_o) \tag{1.39}$$

The only form consistent with (a) and (b) is

$$\Psi_{q_o}(q) = A \delta(q - q_o) \tag{1.40}$$

Thus,  $\int_{-\infty}^{\infty} dq A * A \delta(q - q'_o) = [\textit{useconvolution}]$   
 $= |A|^2 \delta(q_o - q'_o) = \delta(q_o - q_o)$ , by normalizing,  $|A|^2 = 1$

$$\Psi_{q_o}(q) = \delta(q - q_o) \tag{1.41}$$