CHAPTER 2 GENERAL PRINCIPLES OF QUANTUM MECHANICS

1. Continuum States

It is convenient in continuum cases when introducing a complete orthogonal set of basis vectors Φ_ξ to normalize them so that

$$(\Phi_{\xi'}, \Phi_\xi) = \rho(\xi)\delta_{\xi',\xi} \tag{1}$$

Then an arbitrary state can be expressed as a linear combination of basis states

$$\Psi = \sum_\xi \frac{(\Phi_\xi, \Psi)}{\rho(\xi)} \Phi_\xi \tag{2}$$

Any sum over ξ of a smooth function $f(\xi)$ can be expressed as an integral

$$\sum_\xi f(\xi) \mapsto \int f(\xi)\rho(\xi)\mathrm{d}\xi \tag{3}$$

Hence in this limit

$$\Psi = \int (\Phi_\xi, \Psi)\Phi_\xi \mathrm{d}\xi \tag{4}$$

Similarly,

$$(\Psi, \Psi') = \int (\Phi_\xi, \Psi)^*(\Phi_\xi, \Psi')\mathrm{d}\xi \tag{5}$$

Recall that the wave function is nothing but the scalar product

$$\psi(x) = (\Phi_x, \Psi) \tag{6}$$

Delta function: In Fourier Transformation

$$f(x) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k)e^{ikx}\mathrm{d}k \tag{7}$$

and

$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{-ikx}\mathrm{d}x \tag{8}$$

Together,

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}x' f(x') \int_{-\infty}^{\infty} \mathrm{d}k\, e^{ik(x-x')} \tag{9}$$

we also know that

$$f(x) = \int \delta(x - x')f(x')\mathrm{d}x \tag{10}$$

So we can take

$$\delta(x - x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{ik(x-x')} \tag{11}$$

2. Observables

If we introduce a complete orthogonal set of basis vectors Φ_i, we can represent any linear operator A by a matrix A_{ij}, given by

$$A_{ij} \equiv \langle\Phi_i|A|\Phi_j\rangle \tag{12}$$

The expectation value of this observable in a state represented by a normalized vector Ψ is the sum over allowed values, weighted by the probability of each

$$\langle A\rangle_\Psi = \sum_r a_r|\langle\Psi_r|\Psi\rangle|^2 = \sum_r\langle\Psi|A|\Psi_r\rangle\langle\Psi_r|\Psi\rangle = \langle\Psi|A|\Psi\rangle \tag{13}$$

For some operators A, we may define a number called the *trace*, written $\mathrm{Tr}\, A$.

$$\mathrm{Tr}\ A = \sum_i\langle\Psi_i|A|\Psi_i\rangle \tag{14}$$

The trace has some properties

$$\mathrm{Tr}\ A^\dagger = (\mathrm{Tr}\ A)^* \quad \& \quad \mathrm{Tr(AB)} = \mathrm{Tr(BA)} \tag{15}$$

Operators can be constructed form state vectors. We may define a linear operator $|\Psi\rangle\langle\Omega|$ known as a ***dyad***. In particular, if Φ is a normalized state vector, then the dyad $|\Phi\rangle\langle\Phi|$ is an Hermitian operator equal to its own square:

$$(|\Phi\rangle\langle\Phi|)^2 = |\Phi\rangle\langle\Phi| \tag{16}$$

Such operators are called *projection operators*.

$$\sum_i|\Phi_i\rangle\langle\Phi_i| = \hat{\mathbf{1}} \tag{17}$$

Probabilities can enter in quantum mechanics not only because of the probabilistic nature of state vectors, but also ***because we may not know the state of a system***. A system may be in any one of a number of states, represented by state vectors Ψ_n that are normalized but *not necessarily orthogonal*, with probabilities P_n satisfying $\sum_n P_n = 1$.

In such cases, it is often convenient to define a ***density matrix*** as a sum of projection operators, with coefficients equal to the corresponding probabilities

$$\rho \equiv \sum_n P_n |\Psi_n\rangle\langle\Psi_n| \tag{18}$$

Thus

$$\langle A\rangle = \sum_n P_n \langle\Psi_n|A|\Psi_n\rangle = \mathrm{Tr}\{A\rho\} \tag{19}$$

It is sometimes convenient to express the degree to which the state of a system differs from a single pure state by the *von Neumann entropy*

$$S[\rho] \equiv -k_B \mathrm{Tr}(\rho \ln \rho) \tag{20}$$

3. Symmetry

Historically, it was classical mechanics that provided quantum mechanics with a menu of observable quantities and with their properties. But much of this can be learned from ***fundamental principles of symmetry***, without recourse to classical mechanics.

A symmetry principle is a statement that, ***when we change our point of view in certain ways, the laws of nature do not change. In particular, symmetry transformations must not change transition probabilities.***

$$P(\Psi \mapsto \Phi_i) = |\langle\Phi_i|\Psi\rangle|^2 \tag{21}$$

Thus symmetry transformations must leave all $|\langle\Phi|\Psi\rangle|^2$ invariant.

One way to satisfy this condition is to suppose that a symmetry transformation takes general state vectors Ψ into other state vectors $U\Psi$, where U is a linear operator satisfying the condition of *unitarity*.

$$\langle\Phi|U^\dagger U|\Psi\rangle = \langle\Phi|\Psi\rangle \tag{22}$$

Thus

$$U^\dagger U = \hat{\mathbf{1}} \tag{23}$$

We limit ourselves to symmetry transformations that have inverses which undo the effect of the transformation.

$$U^{-1} U = \hat{\mathbf{1}} \tag{24}$$

Hence $U^\dagger = U^{-1}$.

We are entitled to require that symmetry transformations ***map rays into rays***.

There are just only two ways due to **Eugene Wigner** theorem.

1. U is linear and unitary
2. U is anti-linear and anti-unitary

$$U(\alpha|\Psi\rangle + \alpha'|\Psi'\rangle) = \alpha^* U|\Psi\rangle + \alpha'^* U|\Psi'\rangle \tag{25}$$

   and

$$\langle\Phi|U^\dagger U|\Psi\rangle = \langle\Phi|\Psi\rangle^* = \langle\Psi|\Phi\rangle \tag{26}$$

We will mostly be concerned with symmetries represented by linear unitary operators.

The operator $\hat{\mathbf{1}}$ represents a trivial symmetry, that does nothing to state vector. If U_1 and U_2 both represent symmetry transformations, then so does $U_1 U_2$. This property, together with the existence of inverses and a trivial transformation $\hat{\mathbf{1}}$, means that the set of all operators representing symmetry transformations forms a ***group***.

There is a special class of symmetries represented by linear unitary operators - those for which U can be arbitrarily close to $\hat{\mathbf{1}}$. Any such symmetry operator can conveniently be written

$$U_\epsilon = \hat{\mathbf{1}} + i\epsilon T + O(\epsilon^2) \tag{27}$$

where ϵ is an arbitrary real infinitesimal number, and T is some ϵ-independent operator. The unitary condition is

$$\left(\hat{\mathbf{1}} - i\epsilon T^\dagger + O(\epsilon^2)\right)\left(\hat{\mathbf{1}} + i\epsilon T + O(\epsilon^2)\right) = \hat{\mathbf{1}} \tag{28}$$

or

$$T = T^\dagger \tag{29}$$

Thus Hermitian operators arise naturally in the presence of infinitesimal symmetries. If we take $\epsilon = \theta/N$ and then carry out the symmetry transformation N times and let N go to infinity, we find a transformation represented by the operator

$$[\hat{\mathbf{1}} + i\theta T/N]^N \to \exp(i\theta T) = U(\theta) \tag{30}$$

The operator T is known as the ***generator*** of the symmetry. *Many if not all of the operators representing observables in quantum mechanics are generators of symmetries.*

Under a symmetry transformation $\Psi \mapsto U\Psi$, the expectation value of any observable A is subjected to the transformation

$$\langle\Psi|A|\Psi\rangle \mapsto \langle\Psi|U^\dagger A U|\Psi\rangle = \langle\Psi|U^{-1} A U|\Psi\rangle \tag{31}$$

Thus

$$A \mapsto U^{-1}AU = A - i\epsilon[T, A] + O(\epsilon^2) \tag{32}$$

Transformations of this type are called *similarity transformation*.

4. Space Translation and Time Translation

Let us consider the symmetry under spatial translation: ***the laws of nature should not change if we shift the origin of our spatial coordinate system.***

So any particle coordinate $\mathbf{X}_n$ is transformed to $\mathbf{X}_n + \mathbf{a}$, where $\mathbf{a}$ is an arbitrary three-vector. It follows that:

$$U^{-1}(\mathbf{a})\mathbf{X}_n U(\mathbf{a}) = \mathbf{X}_n + \mathbf{a} \tag{33}$$

In particular, for $\mathbf{a}$ infinitesimal, we can write with an Hermitian three-vector operator $-\mathbf{P}/\hbar$

$$U(\mathbf{a}) = 1 - i\mathbf{P}\cdot\mathbf{a}/\hbar + O(\mathbf{a}^2) \tag{34}$$

Then

$$i[\mathbf{P}\cdot\mathbf{a}, \mathbf{X}_n] = \mathbf{a} \tag{35}$$

and therefore

$$[X_{ni}, P_j] = i\hbar\delta_{ij} \tag{36}$$

For finite translations we have

$$U(\mathbf{a}) = \exp(-i\mathbf{P}\cdot\mathbf{a}/\hbar) \tag{37}$$

Then we have

$$\text{If} \quad \Phi_{\mathbf{x}} \equiv U(\mathbf{X})\Phi_0 \quad \text{then} \quad \mathbf{X}\Phi_{\mathbf{x}} = \mathbf{x}\Phi_{\mathbf{x}} \tag{38}$$

From Eq.36 we can infer that

$$P_j\Phi_{\mathbf{x}} = i\hbar\frac{\partial}{\partial x_j}\Phi_{\mathbf{x}} \tag{39}$$

so the scalar product of this state with a state $\Psi_{\mathbf{p}}$ of definite momentum is

$$\langle\Psi_{\mathbf{p}}|\Phi_{\mathbf{x}}\rangle = \exp(-i\mathbf{p}\cdot\mathbf{x})\langle\Psi_{\mathbf{p}}|\Phi_0\rangle \tag{40}$$