Lecture 4: Quantum Dynamics and Schroedinger Equation

November 18, 2020

1 Time Evolution of Quantum System

In the previous section we identified the complex vector states in the Hilbert space with the quantum states and we introduced the definition of a quantum mechanical observable and corresponding Hermitian operator.

In this respect we completed the "Still Life" description of the quantum reality. However anything to be right it should be predictable and to predict anything one needs to describe its time evolution.

Thus to achieve the complete description of the quantum system one needs both the "Still Life" description and its time evolution.

The discussions and developments that follow will be strictly within the scope of the *three* corresponding principles and we will avoid to make any additional assumptions on that matter.

1.1 The State Vector and the Time

What is the quantum system at the given *time*?
We will try to follow the correspondence principle. According to which time is a classical observable therefore it should be an observable in the quantum domain with its own eigenvalue and eigenstate.

This allows us to follow Schoedinger's prescription that the state vector that defines the quantum state of the system at the given time is an eigenstate of the time operator $\hat{t}$: Thus $\mid \psi(t)\rangle$ is the probability amplitude that the give state vector is identified at the time t.

Once such a state vector is defined we can discuss the time evolution of such a state by using the correspondence principle (II). According to the latter the state vector at any other time t can be defined as

$$\mid \psi(t)\rangle = \hat{U}(t, t_0) \mid \psi(t_0)\rangle. \tag{1}$$

where by t_0 we identified the current time.

Using the normalization of the state vector:

$$\langle \psi(t) \mid \psi(t)\rangle = \langle \psi(t_0) \mid \hat{U}^{\dagger}(t, t_0)\hat{U}(t, t_0)\psi(t_0)\rangle = \langle \psi(t_0) \mid \psi(t_0)\rangle = 1 \tag{2}$$

we conclude that the time translate operator is a unitary operator:

$$\hat{U}^{\dagger}(t,t_0) = \hat{U}^{-1}(t,t_0) = \hat{U}(t_0,t), \tag{3}$$

Since U is a continuous transformation, we can introduce a generator of the transformation in the form of

$$\hat{U}(t,t_0) = e^{-i\hat{K}(t-t_0)}, \tag{4}$$

where K is the generator of time translation. Because U is a unitary operator then according to the theorem of Lecture 3, Seciotn 3 Eq.57 the operator K is a hermitean operator. From Eq.4 it follows that:

$$\lim_{t\to 0}\frac{d}{dt}\hat{U}(t,t_0) = -i\hat{K}(t_0). \tag{5}$$

Using the unitarity of operator U one obtains

$$\frac{d}{dt}\hat{I} = \lim_{t\to 0}\frac{d}{dt}\left[\hat{U}(t,t_0)^{\dagger}\hat{U}(t,t_0)\right] = i\left[K^{\dagger}(t_0) - \hat{K}(t_0)\right] = 0 \tag{6}$$

from it follows that $\hat{K}^{\dagger}(t_0) = \hat{K}(t_0)$ is a Hermitean operator:

Let us consider an operator which does not have an explicit time dependence $\hat{A}$ and consider it for the quantum state at time t: $\mid \psi(t)\rangle$. Using above defined operator K we can calculate the time derivative of the expectation value of the operator $\hat{A}$ for the given time of t_0 as follows:

$$\begin{aligned}\frac{d}{dt}\langle\hat{A}\rangle &= \lim_{t\to 0}\frac{d}{dt}\left\langle\psi(t)\mid\hat{A}\mid\psi(t)\right\rangle = \lim_{t\to 0}\frac{d}{dt}\left\langle\psi(t_0)\left|\hat{U}(t,t_0)^{\dagger}\hat{A}\hat{U}(t,t_0)\right|\psi(t_0)\right\rangle \\ &= i\left\langle\psi(t_0)\left|\hat{K}(t_0)\hat{A} - \hat{A}\hat{K}(t_0)\right|\psi(t_0)\right\rangle = i\left\langle\psi(t_0)\left|[\hat{K}(t_0),\hat{A}]\right|\psi(t_0)\right\rangle\end{aligned} \tag{7}$$

In particular we can apply Eq.8 to the operators of momentum p_i and coordinate q_i to obtain:

$$\begin{aligned}\frac{d}{dt}\langle\hat{p}_i\rangle &= i\left\langle\psi(t_0)\left|[\hat{K}(t_0),\hat{p}_i]\right|\psi(t_0)\right\rangle \\ \frac{d}{dt}\langle\hat{q}_i\rangle &= i\left\langle\psi(t_0)\left|[\hat{K}(t_0),\hat{q}_i]\right|\psi(t_0)\right\rangle\end{aligned} \tag{8}$$

Referring to the third statement of the corresponding principle that the time evolution of the expectation values of operators follow the classical laws we expect that the r.h.s. of Eq.(9) should satisfy the classical Hamilton's equations:

$$\begin{aligned}\frac{d}{dt}\langle\hat{p}_i\rangle &= -\frac{\partial H_{cl}}{\partial q_i} \\ \frac{d}{dt}\langle\hat{q}_i\rangle &= \frac{\partial H_{cl}}{\partial p_i},\end{aligned} \tag{9}$$

where H_{cl} is the classical Hamiltonian. SInce H_{cl} is an observable, we can now use the first statement of the corresponding principle to relate:

$$\begin{aligned} \frac{\partial H_{cl}}{\partial q_i} &= \langle \frac{\partial \hat{H}}{\partial \hat{q}_i} \rangle \\ \frac{\partial H_{cl}}{\partial p_i} &= \langle \frac{\partial \hat{H}}{\partial \hat{p}_i} \rangle \end{aligned} \tag{10}$$

where $\hat{H}$ we call the Hamiltonian operator.

Comparing Eqs.(10,11) and (9) we arrive at:

$$\begin{aligned} \frac{\partial \hat{H}}{\partial \hat{q}_i} &= -i[\hat{K}(t), \hat{p}_i] \\ \frac{\partial \hat{H}}{\partial \hat{p}_i} &= i[\hat{K}(t), \hat{q}_i]. \end{aligned} \tag{11}$$

Our next task is to solve the above equations to find $\hat{K}$.

However to do so we need some knowledge about the operator $\hat{H}$.

Hamiltonian operator $\hat{H}$: Main basis for guessing the structure of the hamiltonian is that since it is a hermitean operator it should correspond to the classical observable (as it was discussed earlier). This allows us to make some assumtion to the analytic form of the operator $\hat{H}$.

Suppose

$$\hat{H} = \alpha \sum_i \hat{p}_i^2 \tag{12}$$

Then using this relation in Eq.(12) we observe that these equations have solutions only if momentum and coordinate operators satisfy the following commutating relations:

$$[\hat{q}_i, \hat{p}_j] = ic\delta_{ij} \tag{13}$$

with the solution

$$\hat{K} = \hat{H}/c \tag{14}$$

where c is the constant that should be determined from the "outside" condition of the problem.

It can be shown that same is true if we assume:

$$\hat{H} = \beta \sum_i \hat{q}_i^2 \tag{15}$$

More general statement is that for $\hat{H}$ having general polinomial dependence of $\hat{p}$ and $\hat{q}$ will result to the solution of Eqs.(13) and (14).

One naturally should assume that the classical observable of operator $\hat{H}$ should correspond to the classical Hamiltonian function. This assumption is important since it allows us to construct the quantum mechanical Hamiltonian based on our knowledge of the classical Hamiltonian function. In

other words if classical hamiltonian is described by function $F(q,p)$ one assume that the quantum mechanical Hamiltonian operator has a form

$$\hat{H} = F(\hat{q}, \hat{p}). \tag{16}$$

Note however that due to nonzero commutation relation of Eq.(13) such a correspondence has ambiguity related to the terms proportional to product of q and p. In this case while in classical mechanics the position of p and q in the product is not important, in quantum mechanics $\hat{q}\hat{p}$ and $\hat{p}\hat{q}$ are different due to Eq.(13). The convention is that if one constructs the $\hat{H}$ operator from the classical counterparts then one positions $\hat{p}$ after $\hat{q}$ to avoid the action of momentum operator on the result of $\hat{x} \mid \psi\rangle$.

The most common form of the quantum mechanical hamiltonian is in the form that resembles sum of kinetic and potential energies:

$$\hat{H} = \frac{\sum\limits_i \hat{p}_i^2}{2m} + V(\hat{r}) \tag{17}$$

Summarizing the above discussion we note that the time evolution of the quantum state $\mid \psi\rangle$ is defined by the hamiltonian operator $\hat{H}$ such that

$$\begin{aligned} c\frac{d}{dt} \mid \psi(t)\rangle &= -i\hat{H} \mid \psi(t)\rangle \\ [\hat{q}_i, \hat{p}_j] &= ic\delta_{ij} \end{aligned} \tag{18}$$

1.1.1 The Canonical Commutation Relations

To match the dimensions of left and right hand sides of Eq.(19) one observes that the coefficient c should have dimension of the action: [L]^2[M]/[T]. This constant can be defined numerically only by application of the Eq.(19) to the quantum mechanical problem in which the actual measurements have been made. We will see in the coming section that this constant can be unambiguously identified with the Planck constant h:

$$c \equiv \hbar \equiv \frac{h}{2\pi} = 1.054 \times 10^{-27} erg \cdot sec = 6.58^{-27} Mev \cdot sec \tag{19}$$

after which Eq..(19) reads:

$$\begin{aligned} i\hbar\frac{d}{dt} \mid \psi(t)\rangle &= \hat{H} \mid \psi(t)\rangle \\ [\hat{q}_i, \hat{p}_j] &= i\hbar\delta_{ij} \end{aligned} \tag{20}$$

where the firs of the above two equations called Schrödinger equation. The above presented magnitude of $\hbar$ sets the scale at which quantum effects become important in the system. It also follows that the classical limit can be achieved with considering $\hbar \to 0$ limit.

2 Quantum Dynamics

2.1 The Time-Translation Operator

$$| \psi(t)\rangle = \hat{U}(t, t_0) \mid \psi(t_0)\rangle \tag{21}$$

$$i\hbar \frac{d}{dt}\hat{U}(t, t_0) \mid \psi(t_0)\rangle = \hat{H}(t)U(t, t_0) \mid \psi(t_0)\rangle \tag{22}$$

$$i\hbar \frac{d}{dt}\hat{U}(t, t_0) = \hat{H}(t)U(t, t_0) \tag{23}$$

Solution of above equation with the boundary condition:

$$\hat{U}(t, t_0) = I - \frac{i}{\hbar}\int_{t_0}^{t} \hat{H}(t')\hat{U}(t', t_0)dt' \tag{24}$$

The above equation have a simple solution if $\hat{H}$ is constant. Then

$$\hat{U}(t, t_0) = e^{-\frac{i}{\hbar}\hat{H}\cdot(t-t_0)} \tag{25}$$

The above discussion is refereed as **Schrödinger Picture**.

2.2 The Heisenberg Picture

3 The Uncertainty Principle

Let $\hat{A}$ is an operator of any observable A and $\langle A\rangle$ is the expectation value of the operator for some state $| \psi\rangle$, i.e.

$$\langle A\rangle = \langle \psi \mid \hat{A} \mid \psi\rangle. \tag{26}$$

If $| \psi\rangle$ is an eigenstate of $\hat{A}$ with the eigenvalue A, then $\langle A\rangle = A$.

Now let us define quantum mechanical *variance*:

$$\sigma_A^2 = \langle \psi \mid (\hat{A} - \langle A\rangle)^2 \mid \psi\rangle \equiv \langle \psi \mid \Delta A^2 \mid \psi\rangle \tag{27}$$

which can be interpreted as a *standard deviation* in the spread of the measurements of the observable A for the quantum system which is characterized by the state $| \psi >$. Here $\Delta A = \hat{A} - \langle A\rangle$.

After these definitions we now consider two non-cummuting operators $\hat{A}$ and $\hat{B}$ corresponding to A and B observables for which we will prove the General Uncertainty Principle, according to which:

$$\sigma_A^2\sigma_B^2 \geq -\frac{1}{4}\langle \psi \mid [\hat{A}, \hat{B}] \mid \psi\rangle^2 \tag{28}$$

Remember that if two operators does not commute then there is no quantum state which can be

eigenstate for both operators. Or in other way one can say there is no one state in which two observables have eigenvalues.

To prove Eq.(**??**) one needs to obtain an inequity relation that contains $\sigma_A^2\sigma_B^2$. For this we consider an operator $\hat{C}$ defined as:

$$\hat{C} = \Delta A + i\tau\Delta B \tag{29}$$

where τ is a real parameter. Not that operator $\hat{C}$ is a linear combination of the $\hat{A}$ and $\hat{B}$ operators and as such operates in the Hilbert space. Therefore one can state

$$f(\tau) \equiv \langle\psi \mid \hat{C}^\dagger\hat{C} \mid \psi\rangle \geq 0, \tag{30}$$

where because of $\hat{A}$ and $\hat{B}$ being Hermitean operators

$$\hat{C}^\dagger = \Delta A - i\tau\Delta B. \tag{31}$$

Using Eqs.(29) and (31) one obtains

$$\hat{C}^\dagger\hat{C} = \Delta A^2 + \tau^2\Delta B^2 + i\tau[\Delta A, \Delta B] = \Delta A^2 + \tau^2\Delta B^2 + i\tau[A, B], \tag{32}$$

where in the last part of the above equation we used the relation:

$$[\Delta A, \Delta B] = \Big((\hat{A} - \langle A\rangle), (\hat{B} - \langle B\rangle)\Big) = [\hat{A}\hat{B}] \tag{33}$$

which follows from the fact that $\langle A\rangle)$ and $\langle B\rangle)$ are numbers and they commute.

Inserting Eq.(32) into Eq.(30) one obtains:

$$f(\tau) = \langle\psi \mid \Delta A^2 + \tau^2\Delta B^2 + i\tau[\hat{A}, \hat{B}] \mid \psi\rangle \geq 0, \tag{34}$$

It is worth noting that $[\hat{A}, \hat{B}]$ is an imaginary quantity by proving that

$$\langle\psi \mid [\hat{A}, \hat{B}] \mid \psi\rangle^* = \langle\psi \mid [\hat{A}, \hat{B}]^\dagger \mid \psi\rangle = -\langle\psi \mid [\hat{A}, \hat{B}] \mid \psi\rangle, \tag{35}$$

therefore Eq.(34) is a real function.

Since $f(\tau)$ function is real and positive one can obtaine the inequity relations by minimizing it. For this we find the extremum of of $f(\tau)$ estimating its first derivative by τ.

$$f'(\tau) = \langle\psi \mid 2\tau\Delta B^2 + i[\hat{A}\hat{B}] \mid \psi\rangle = 0, \tag{36}$$

which yields

$$\tau_0 = -\frac{i\langle\psi \mid [\hat{A}\hat{B}] \mid \psi\rangle}{2\langle\psi \mid \Delta B^2 \mid \psi\rangle} \tag{37}$$

Inserting this into Eq.(34) one obtains

$$f(\tau_0) = \langle\psi \mid \Delta A^2 \mid\rangle + \frac{1}{4}\frac{\langle\psi \mid [\hat{A}\hat{B}] \mid \psi\rangle^2}{\langle\psi \mid \Delta B^2 \mid \psi\rangle} \geq 0. \tag{38}$$

Note that τ_0 corresponds to the minimum of the function $f(\tau)$ which can be seems from the fact that $f'' = 2\langle\psi \mid \Delta B^2 \mid\rangle > 0$.

Using the inequity of Eq.(38) we obtain the relation:

$$\langle\psi \mid \Delta A^2 \mid\rangle \cdot \langle\psi \mid \Delta B^2 \mid \psi\rangle \geq -\frac{1}{4}\langle\psi \mid [\hat{A}\hat{B}] \mid \psi\rangle^2, \tag{39}$$

which represents the generalized uncertainty principle of Eq.(28).

Heisenberg Uncertainty Relation :

Choosing $\hat{A} = \hat{p}_i$ and $\hat{B} = \hat{r}_i$ and commutator relation $[r_i, p_j] = i\hbar\delta_{ij}$ one obtains the Heinsenberg's uncertainty relation in the better known form:

$$\sigma_{p_i}\sigma_{r_i} \geq \frac{1}{2}\hbar \tag{40}$$

3.1 Eigenstates of Position and Momentum

The position, x of quantum system of an object is an observable therefore one should be able to associate with this observable operator $\hat{x}$ and eigenstate $\mid \psi_x\rangle$ such that

$$\hat{x}\psi_x = x\psi_x. \tag{41}$$

This relation can be generalized for three-dimensional case in the form of

$$\hat{r}\psi_r = \vec{r}\psi_r. \tag{42}$$

These eigenstates describe the quantum states being in the position of x (or $\vec{r}$).

In the similar manner, since momentum is an observable we can define also the operator $\hat{p}$ and eigenstate of momentum $\mid \phi_p\rangle$ such that

$$\hat{p}_x\phi_{p_x} = p_x\phi_{p_x}, \tag{43}$$

with three-dimensional generalization as:

$$\hat{p}\phi_p = \vec{p}\phi_p. \tag{44}$$

These eigenstates describe the quantum states having momentum p_x (or $\vec{p}$).

If one accepts that the position and the momentum are continues observables, then the above defined state vectors represent the continuum state and satisfy the conditions discussed in the previous lecture as:

$$\langle\psi_{x'} \mid \psi_x\rangle = \delta(x' - x) \quad \text{and} \quad \int_{-\infty}^{\infty} \mid \psi_x\rangle\langle\psi_x \mid dx = 1 \tag{45}$$

The similar relations can be written for the momentum eigenstates:

$$\langle \phi_{p'_x} \mid \phi_{p_x} \rangle = \delta(p'_x - p_x) \quad \text{and} \quad \int_{-\infty}^{\infty} \mid \phi_{p_x} \rangle \langle \phi_{p_x} \mid dp_x = 1 \tag{46}$$

These relations can be easily generalized for 3-dimensional case.

3.2 Momentum and Space Translation

Definition of the position eigenstates allows to define the properties of space translation in Quantum domain. Remind that space translation in classical physics was defined as an operation having the following property [1]:

$$T(a)x = x + a \quad \text{and} \quad T(a)p = p \tag{47}$$

Using the general principle of symmetry operation in quantum domain we now define space translation as an operator acting on the quantum state. The appropriate quantum state in this case is the eigenstate of the position and momentum for which the operation of space translation will be defined as

$$T(a) \mid \psi_x \rangle = e^{\alpha(x)} \mid \psi_{x+a} \rangle \tag{48}$$

and

$$T(a) \mid \phi_{p_x} \rangle = e^{\beta(p_x)} \mid \phi_{p_x} \rangle \tag{49}$$

From the uniformity of space one can show that phase factors α and β are constants (independent of the position and momentum) therefore can be absorbed in the definition of the state vectors. It is worth mentioning several properties of the operator $\hat{T}$ discussed in the previous sections.

$$T^{-1}(a) = \hat{T}(-a) \tag{50}$$

$$\hat{T}(a)^n = \hat{T}(na) \tag{51}$$

3.2.1 Space translation of position eigenstates

We first observe that due to space uniformity the matrix elements $\langle \psi_{x'} \mid \psi_{x''} \rangle$ should be invariant with respect to the space translations, i.e.

$$\langle \psi_{x'} \mid \psi_{x''} \rangle = \langle \psi_{x'+a} \mid \psi_{x''+a} \rangle. \tag{52}$$

Since, on the other hand

$$\langle \psi_{x'+a} \mid \psi_{x''+a} \rangle = \langle \psi_{x'} \mid T^{\dagger}(a)T(a) \mid \psi_{x''} \rangle \tag{53}$$

the relation in Eq.(52) indicates that the operator of space translation is unitary operator

$$T^{\dagger}T = I \tag{54}$$

[1] For the sake of simplicity we are discussing one-dimensional case which later will be generalized to three-dimension

Note that the very same Eq.(52) indicates that if the space translation generates an additional phase factor $\alpha(x)$ as in Eq.(48) the it should not depend on x thus being constant that can be chosen to be 0. With the similar approach to the eigenstates of momenta $\mid \phi_{p_x}$ one can see that β too should be constant thus eliminated from Eq.(49).

We now try to see how above rules of the transformation of the states translates to the relationship between the operator of space translation $\hat{T}$ and position $\hat{x}$.

For position operator $\hat{x}$ the matrix element between two eigenstates is defined as:

$$\langle \psi_{x'} \mid \hat{x} \mid \psi_{x''} \rangle = x'' \langle \psi_{x'} \mid \psi_{x''} \rangle. \tag{55}$$

Using this relation for the matrix element of between two space translated states one obtains:

$$\langle \psi_{x'+a} \mid \hat{x} \mid \psi_{x''+a} \rangle = (x'' + a) \langle \psi_{x'+a} \mid \psi_{x''+a} \rangle = \langle \psi_{x'+a} \mid \hat{x} + a\hat{I} \mid \psi_{x''+a} \rangle \tag{56}$$

Using the space translation operator the same matrix element we can present as:

$$\langle \psi_{x'+a} \mid \hat{x} \mid \psi_{x''+a} \rangle = \langle \psi_{x'} \mid \hat{T}(-a)\hat{x}\hat{T}(a) \mid \psi_{x''} \rangle. \tag{57}$$

By comparing Eqs.(56) and (57) we obtain the following relation between the space and translation operators:

$$\hat{T}(-a)\hat{x}\hat{T}(a) = \hat{x} + a\hat{I}. \tag{58}$$

This equation can be further elaborated noting that the space transformation is a continuous transformation and for infinitesimal transformations can be expressed through the generator of the transformation in the form:

$$T(\epsilon) = I - i\hat{K}_x\epsilon. \tag{59}$$

Inserting this equation into Eq.(58 and keeping up to the linear terms of ϵ one obtains:

$$(1 + i\hat{K}_x\epsilon)\hat{x}(1 - i\hat{K}_x\epsilon) = \hat{x} + i\hat{K}_x\hat{x}\epsilon - i\hat{x}\hat{K}_x\epsilon = \hat{x} + i\epsilon[\hat{K}_x\hat{x}] = \hat{x} + \epsilon\hat{I}. \tag{60}$$

Solving above equation for the commutator $[\hat{x}\hat{K}]$ one obtains:

$$[\hat{x}\hat{K}_x] = i \tag{61}$$

3.2.2 Space translation of momentum eigenstates

We now consider the space translation of the momentum eigenstates trying to relate the momentum operator $\hat{p}_x$ to the $\hat{T}(a)$. For this using Eq.(49) for the matrix element of operator $\hat{p}_x$ for the momentum eigenstates one obtains

$$\langle \phi_{p'_x} \mid \hat{p}_x \mid \phi_{p_x} \rangle = \langle \phi_{p'_x} \mid \hat{T}(-a)\hat{p}_x\hat{T}(a) \mid \phi_{p_x} \rangle \tag{62}$$

which yields:

$$\hat{T}(-a)\hat{p}_x\hat{T}(a) = \hat{p}_x \quad \rightarrow \quad [\hat{p}_x\hat{T}(a)] = 0 \tag{63}$$

Using now Eq.(59) one obtains for the generator of space translation operator:

$$[\hat{p}_x \hat{K}_x] = 0. \tag{64}$$

The last relation together with Eqs.(63) and (61) should be solved to find $\hat{K}$. For this we use the relation of Eq.(**??**) which together with Eq.(61) result in

$$\hat{x}\hat{K}_x - \hat{K}_x\hat{x} = i = \hat{x}\frac{\hat{p}_x}{\hbar} - \frac{\hat{p}_x}{\hbar}\hat{x} \tag{65}$$

This together with Eq.(64) indicates that the general solution for $\hat{K}_x$ is

$$\hat{K}_x = \frac{\hat{p_x}}{\hbar} + \hat{C} \tag{66}$$

where $\hat{C}$ is an operator independence to $\hat{x}$ and $\hat{p}$. One can observe from Eqs.(59,**??**,**??**) that the operator $\hat{C}$ will produce a constant phase factor which one can absorb in the definition of the state vector. Or in other words $\hat{C}$ can be arbitrary for which we can choose $\hat{C} = 0$. Thus we conclude that

$$\hat{K}_x = \frac{\hat{p}_x}{\hbar} \tag{67}$$

4 Wave Functions

In many problems of Quantum Mechanics the main question one is interested is the position of the given quantum system in the space. The question in this case can be formulated as *what is the probability amplitude* that the given quantum sate $\mid \psi\rangle$ is at the position x. As it was discussed above the x being an observable is characterized by and Hermitean operator $\hat{x}$ and eigenstate $\mid \psi_x\rangle$. Therefore we are now in the position of defining the probability amplitude as

$$\psi(x) = \langle \psi_x \mid \psi \rangle \tag{68}$$

which represents the component of the state vector $\mid \psi\rangle$ projected on the "orth" $\mid \psi_x\rangle$. This "component" is called *wave function* which is an important object for considering the "position" of the quantum state.

If we consider a given quantum state $\mid \psi\rangle$ normalized to unity, then using the properties of coordinate eigenstates from Eq.(45) one obtains

$$1 = \langle \psi \mid \psi \rangle = \int_{-\infty}^{\infty} \langle \psi \mid \psi_x \rangle \langle \psi_x \mid \psi \rangle dx = \int_{-\infty}^{\infty} \mid \psi(x) \mid^2 dx = 1. \tag{69}$$

This relation basically sates that total probability of finding quantum sate anywhere is unity. It also allows to interpret the quantity

$$\int_{x_1}^{x_2} \mid \psi(x) \mid^2 dx \tag{70}$$

as a probability for finding the quantum state between x_1 and x_2 and the integrant of the above expression is named *probability density*

$$\rho(x) = \psi(x)^*\psi(x) \tag{71}$$

The wave function $\psi(x)$ is the most appropriate "object" when we are dealing with the position of the quantum state. In further, many discussions will be carried out based on the notion of the wave functions. For this reason in many instances for any given operator $\hat{A}$ one will need to calculate the quantity

$$\langle \psi_x \mid \hat{A} \mid \psi \rangle. \tag{72}$$

Such a calculation can be performed if we notice that in studying the quantum sate through its hamiltonian operator $\hat{H}$ be borrow that classical mechanical principle according to which the classical hamiltonian is a function of the position r and momentum p. Using this and the concept of constructing quantum mechanical hamiltonian operator discussed in the above section we expect that any hamiltonian operator should be function of coordinate and momentum operator. For one dimensional case the statement is that :

$$\hat{H} \equiv \hat{H}(\hat{x}, \hat{p}) \tag{73}$$

Thus in this situation to complete the task of Eq.(72) we need to consider only

$$\langle \psi_x \mid \hat{x}^n \mid \psi \rangle \quad \text{and} \langle \psi_x \mid \hat{p}_x^m \mid \psi \rangle \tag{74}$$

for any arbitrary integer number of n and m.

We start with considering

$$\langle \psi_x \mid \hat{x} \mid \psi \rangle = x \langle \psi_x \mid \psi \rangle = x\psi(x) \tag{75}$$

where we used the fact that $\hat{x}$ is a hermitean operator and $\langle \psi_x \mid \hat{x} = x \langle \psi_x \mid$. From Eq.(75) and remembering the the product of two operators:

$$\hat{A}\hat{B} \mid \psi \rangle = \hat{A}(\hat{B} \mid \psi \rangle) \tag{76}$$

we arrive at

$$\langle \psi_x \mid \hat{x}^n \mid \psi \rangle = x^n \langle \psi_x \mid \psi \rangle. \tag{77}$$

If now we consider a function $f(\hat{x})$ such that it can be represented through a form containing the power of $\hat{x}$ then

$$f(\hat{x}) \mid \psi \rangle = f(x) \mid \psi \rangle \tag{78}$$

where x is the eigenvalue of $\hat{x}$.

Now we consider $\langle \psi_x \mid \hat{p} \mid \psi \rangle$ for which we use the fact that momentum operator represents a generator of space translation. We first consider:

$$\psi(x + \epsilon) = \langle \psi_x \mid T(-\epsilon) \mid \psi \rangle = \psi_x \mid I + i\epsilon \frac{\hat{p_x}}{\hbar} \mid \psi \rangle = \psi(x) + i\epsilon \langle \psi_x \mid \frac{\hat{p}_x}{\hbar} \mid \psi \rangle, \tag{79}$$

where in the first part of the equation we used $\langle\psi_{x+\epsilon}\mid=\langle\psi_x\mid\hat{T}(-\epsilon)\mid=(\mid T(\epsilon)\mid\psi_x)^\dagger$. One can solve Eq.(79) to obtain

$$\langle\psi_x\mid\hat{p}_x\mid\psi\rangle=-i\hbar\frac{(\psi(x+\epsilon)-\psi(x)}{\epsilon}\mid_{\epsilon\to 0}=-i\hbar\frac{\partial d\psi(x)}{\partial x}. \tag{80}$$

5 Momentum Space Wave Function

5.1 Eigenstate of the Momentum Operator

The eigenstates of momentum operator satisfy the equation:

$$\hat{p}\mid\phi_p\rangle=p\mid\phi_p\rangle. \tag{81}$$

We now try to see what is the space projection of the momentum eigenstate, which will represent the *momentum space wave function*, defined as

$$\psi_p(x)=\langle\psi_x\mid\phi_p\rangle. \tag{82}$$

To obtain the properties of $\psi_p(x)$ we project Eq.(81) to the coordinate space by considering:

$$\langle\psi_x\mid\hat{p}\mid\phi_p\rangle=p\langle\psi_x\mid\phi_p\rangle=p\psi_p(x). \tag{83}$$

Then using Eq.(80) one obtains:

$$-i\hbar\frac{d}{dx}\psi_p(x)=p\psi_p(x) \tag{84}$$

this is a simple differential equation which can be solved with the above defined normalization condition for continuos observables $\langle\phi_{p'}\mid\phi_{p''}\rangle=\delta(p'-p'')$, resulting to the solution:

$$\psi_p(x)=\frac{1}{\sqrt{2\pi\hbar}}e^{i\frac{p}{\hbar}x}. \tag{85}$$

The above result represents the wave function of one-dimensional momentum eigenstate.

One can naturally generalize it for the three-dimensional case for which the wave function is

$$\psi_{\vec{p}}(\vec{r})=\langle\psi_{\vec{r}}\mid\phi_{\vec{p}}\rangle=\frac{1}{(2\pi\hbar)^{\frac{2}{3}}}e^{i\frac{\vec{p}}{\hbar}\vec{r}}. \tag{86}$$

5.2 Momentum Space Wave Function

In the analogy with the wave function defined in Sec.4, which are naturally coordinate space wave functions we can defined also the *momentum space wave function.* For one dimensional case such a definition is

$$\phi(p_x)=\langle\psi_{p_x}\mid\psi\rangle \tag{87}$$

where $\mid \psi\rangle$ is the arbitrary quantun state and $\mid \psi_{p_x}\rangle$ is the eigenstate of the momentum operator $\hat{p}_x$.

Using the completeness condition of the coordinate space vector from Eq.(45) the momentum space wave function can be represented as follows:

$$\phi(p) = \langle \psi_{p_x} \mid \psi \rangle = \int_{-\infty}^{\infty} \langle \psi_{p_x} \mid \psi_x \rangle \langle \psi_x \mid \psi \rangle dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{ip_x x}{\hbar}} \psi(x) dx \tag{88}$$

where in the last part of the equation we used the general definition of the coordinate space wave function from Eq.(68) as well as coordinate space wave function of momentum operator in Eq.(85).

Above relation indicates that the coordinate space wave function is related to the momentum space wave function through the conventional Fourier transformation. This result can be generalized for 3-dimensional case as follows:

$$\phi(\vec{p}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}} \psi(\vec{r}) d^3r. \tag{89}$$

Using the properties of Fourier transformation one can naturally relate the coordinate space wave function to the momentum space wave function through the inverse Fourier transformation in the form:

$$\psi(\vec{r}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int e^{i\frac{\vec{p}\cdot\vec{r}}{\hbar}} \phi(\vec{p}) d^3p \tag{90}$$

5.3 Gaussian Wave Function

In many practical application the quantum system is described by a coordinate space wave function which has a gaussian form:

$$\psi(x) = Ae^{-\frac{a^2x^2}{2}} \tag{91}$$

Such a wave function is good example for calculating Fourier transformation as well as checking Heisenberg uncertainty relation.

6 Schrödinger Wave Equation

We learned above that space projection of the action of the momentum operator $\hat{p}$ on the given state vector $\mid \psi\rangle$ can be represented as a derivative of the wave function of the same state:

$$\langle \psi_r \mid \hat{p}_x \mid \psi \rangle = -i\hbar \frac{\partial \psi(r)}{\partial x}. \tag{92}$$

Using this relation one can consider the Schrödinger equation being projected to the coordinate eignenstate as follows:

$$i\hbar \langle \psi_x \mid \frac{d}{dt} \mid \psi \rangle = \langle \psi_x \mid \hat{H} \mid \psi \rangle. \tag{93}$$

To proceed with this equation we need an explicit expression for $\hat{H}$. For the particle with mass m with the potential energy $V(x)$ such an expression can be guessed based on the Correspondence Principle in the form:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{94}$$

To be able to calculate Eq.(93) we need to evaluate the following operators:

$$\begin{aligned} \langle \psi_x \mid \hat{p}^2 \mid \psi \rangle &= \langle \psi_x \mid \hat{p} \mid \phi \rangle = -i\hbar \frac{\partial \phi(x)}{\partial x} = -i\hbar \frac{\phi(x+\epsilon) - \phi(x)}{\epsilon} = -i\hbar \frac{\langle \psi_{x+\epsilon} \mid \hat{p} \mid \psi \rangle - \langle \psi_x \mid \hat{p} \mid \psi \rangle}{\epsilon} \\ &= -i\hbar \frac{-i\hbar \left(\frac{\partial \psi(x+\epsilon)}{\partial x} - \frac{\partial \psi(x)}{\partial x} \right)}{\epsilon} = -\hbar^2 \frac{\partial^2 \psi(x)}{\partial x^2} \end{aligned} \tag{95}$$

where in the intermediate state of derivation we introduced the state vector $\mid \phi \rangle = \hat{p} \mid \psi \rangle$. Next we consider:

$$\langle \psi_x \mid V(\hat{x}) \mid \psi \rangle = V(x) \langle \psi_x \mid \psi \rangle = V(x)\psi(x), \tag{96}$$

where we take into account the fact that $\mid \psi_x \rangle$ is the eigenstate of $\hat{x}$ and $V(\hat{x})$ can be expanded into the power series of operator $\hat{x}$, thus $V(\hat{x}) \mid \psi_x \rangle = V(x) \mid \psi_x \rangle$.

Using Eqs.(95) and (96) as well as the fact that $\mid \psi_x \rangle$ is time independent eigenstates, for Eq.(93) one obtains:

$$i\hbar \frac{d}{dt}\psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t). \tag{97}$$

This equation referred as em Schroedinger's Wave Equation. We can easily generalize the above equation for three-dimensional case in the following form:

$$i\hbar \frac{d}{dt}\psi(r,t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(r,t) + V(r)\psi(r,t). \tag{98}$$

6.1 Continuity Equation

One of the important property of Schroedinger Wave equation is the continuity equation for the probability density

$$\rho(r,t) = \psi(r,t)\psi(r,t). \tag{99}$$

The continuity equation solves the following apparent contradiction, According to Eq.(98) $\rho(r,t)$ is time dependent quantity while one expects that the normalization of the wave function is time independent. For example for the quantum system confined in the volume V

$$\int_V \rho(r,t) d^3r = 1. \tag{100}$$

Thus the time dependence of $\psi(r,t)$ should conspire to make the integral above time independent. To show this we consider the time dependence of $\rho(r,t)$ as it follows from Eq.(98). For this one

first consider the complex-conjugate of Eq.(98):

$$-i\hbar\frac{d}{dt}\psi^*(r,t) = -\frac{\hbar^2}{2m}\nabla^2\psi^*(r,t) + V^*(r)\psi(r,t)^*. \tag{101}$$

Multiplying Eq.(ShrWaveq3d) by $\psi(r,t)^*$ and Eq.(101) by $\psi(r,t)^*$ and subtracting from each other one obtains:

$$\frac{d\rho(r,t)}{dt} = -\vec{\nabla}\cdot\vec{j}(r,t) + \frac{ImV}{\hbar}\rho(r,t) \tag{102}$$

where we introduced probability current vector in the form:

$$\vec{j}(r,t) = \frac{i\hbar}{2m}\left[\psi(r)\vec{\nabla}\psi^*(r) - \psi^*(r)\vec{\nabla}\psi(r)\right] = \frac{\hbar}{m}Im(\psi^*(r)\vec{\nabla}\psi(r)). \tag{103}$$

For the case of real potential energy, which naturally follows from the correspondence principle one arrives at the continuity equation:

$$\frac{d\rho(r,t)}{dt} + \vec{\nabla}\cdot\vec{j}(r,t) = 0. \tag{104}$$

One now will show that the continuity equation solves the issue of time independence of Eq.(100). For this we substitute Eq.(104) to Eq.(100) and use the Gauss theorem to relate the divergence of the volume integration to the flux integral of the surface the encompasses the volume:

$$\frac{d}{dt}\int_V \rho(r,t)d^3r = \int_V \frac{d\rho(r,t)}{dt}d^3r = -\int_V \vec{\nabla}\cdot\vec{j}d^3r = -\int_S \vec{j}d\vec{\sigma}. \tag{105}$$

The RHS part of the equation represents the flux of the probability current from the surface that contains the volume V. Since according to our initial assumption the quantum system was confined in the volume V such a flux should be zero this proving that $\int_V \rho(r,t)d^3r$ is time independent. The continuity equation is the statement of the conservation of the probability density in the quantum mechanics. From this it follows that the probability density can change only if there is a flux of probability current into our out of the considered region. Note, that Eq.(105) is satisfied for any finite volume of $\rho(r,t)$ is time independent. In this case the RHS part of the equation states that the net flux from the considered volume is zero, that is the incoming and outgoing probability currents cancel each other.

Finally it is worth noting, that in practical quantum mechanical applications, in which one need to take into account the absorption effects, one can formally add the negative imaginary part to the potential energy V. Then according to Eq.(103) the negative imaginary part of the potential energy will imitate the decrease of the probability density $\rho(r,t)$ during the time that can be associated with the absorption effects.

7 Time-Dependent Free Particle Wave Function

We consider now a free particle in one dimension. According to above discussion, the Hamiltonian operator for the free particle can be written as:

$$\hat{H} = \frac{\hat{p}^2}{2m} \tag{106}$$

from which it follows that it will commute with the operator of the momentum $\hat{p}$:

$$[\hat{H}\hat{p}] = 0. \tag{107}$$

Therefore $\hat{H}$ and $\hat{p}$ should have common eigenstates, $\mid \psi_{E,p}(t)\rangle$ which satisfies the following equation:

$$\begin{aligned} \hat{p} \mid \psi_{E,p}\rangle &= p \mid \psi_{E,p}\rangle \\ \hat{H} \mid \psi_{E,p}\rangle &= E \mid \psi_{E,p}\rangle. \end{aligned} \tag{108}$$

In addition the time evolution of $\mid \psi_{E,p}\rangle(t)$ should be defined by the Schoedinger equation:

$$i\hbar \frac{d}{dt} \mid \psi_{E,p}\rangle = \hat{H} \mid \psi_{E,p}\rangle = E \mid \psi_{E,p}\rangle \tag{109}$$

where in the RHS part of the equation we used the fact that $\mid \psi_{E,p}(t)\rangle$ is an eigenstate of $\hat{H}$. Comparing Eqs.(108) and (109) we observe that the first depends on operator $\hat{p}$ while the second on t. Thus one can search for the solution of $\mid \psi_{E,p}\rangle$ in the separable form:

$$\mid \psi_{E,p}\rangle(t) = \Phi(t) \mid \phi_p\rangle \tag{110}$$

where $\mid \phi_p\rangle$ is the eigenstate of the operator $\hat{p}$. Inserting Eq.(110) into Eq.(109) for $\phi(t)$ one obtains:

$$i\hbar \frac{d}{dt}\phi(t) = E\phi(t) \tag{111}$$

which is first order differential equation which can be solved resulting to:

$$\phi(t) = Ce^{-i\frac{E}{\hbar}} \tag{112}$$

where $E = \frac{p^2}{2m}$, which is obtained by inserting Eq.(110) into Eq.(108). Using this in Eq.(110) one obtains:

$$\mid \psi_{E,p}\rangle(t)\rangle = e^{-i\frac{E}{\hbar}} \mid \phi_p\rangle, \tag{113}$$

where we choose $C = 1$ that allows the free state vector to be normalized according to the normalization condition of continues variables.

Using Eq.(113) we can calculate also the wave function of the free particle by projecting it to the eigenstate of the coordinate:

$$\psi_{E,p}(x,t) = \langle \psi_x \mid \psi_{E,p}\rangle(t)\rangle = e^{-i\frac{E}{\hbar}}\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i(p_x x - Et)}{\hbar}}, \tag{114}$$

where in the last part of the equation we used the definition of the wave function of the eigenstate of $\hat{p}_x$ from Eq.(85). The Eq.(114) can be generalized for three dimensional case in the form:

$$\psi_{E,p}(r,t) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} e^{\frac{i(\vec{p}\cdot r - Et)}{\hbar}}. \tag{115}$$

7.1 Some Properties of the Free Particle Wave Function

Eqs.(114) and (115) mathematically represent a plane waves in one and three dimensions with wave number $\vec{k} = \frac{\vec{p}}{\hbar}$ and angular frequency $\omega = \frac{E}{\hbar}$ respectively. If one use the expressions for k and E from above, then for the phase velocity of the wave in the $\hat{k}$ direction one obtains:

$$v_{phase} \equiv \frac{\omega}{\mid k \mid} = \frac{p}{2m}. \tag{116}$$

The above represents the half of the classical velocity $\frac{p}{m}$.

It is worth mentioning that even with such a "wrong" velocity the time derivative of the expectation value of the coordinate corresponds to the true classical velocity, i.e.:

$$\frac{d}{dt}\langle\hat{x}\rangle = \frac{p}{m} \tag{117}$$

To prove the above relation recall the expression for the time derivation of the expectation value of quantum mechanical observable A.

$$-i\hbar\frac{d}{dt}\langle\hat{A}\rangle = \langle[\hat{H}\hat{A}]\rangle, \tag{118}$$

and use this relation to consider operator $\hat{x}$:

$$-i\hbar\frac{d}{dt}\langle\hat{x}\rangle = \langle[\hat{H}\hat{x}]\rangle. \tag{119}$$

Now using the expression for the free particle hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m}$ and relation $(\hat{x}\hat{p} - \hat{p}\hat{x}) = i\hbar$ one obtains:

$$\begin{aligned} [\hat{H}\hat{x}] &= \frac{1}{2m}(\hat{p}^2\hat{x} - \hat{x}\hat{p}^2] = \frac{1}{2m}(\hat{p}^2\hat{x} - (i\hbar + \hat{p}\hat{x})\hat{p}) \\ &= \frac{1}{2m}(\hat{p}^2\hat{x} - (i\hbar\hat{p} + \hat{p}(i\hbar + \hat{p}\hat{x}))) = -i\hbar\frac{\hat{p}}{m} \end{aligned} \tag{120}$$

Using this relation in Eq.(119) one obtains

$$\frac{d}{dt}\langle\hat{x}\rangle = \frac{\langle\hat{p}\rangle}{m} = \langle\hat{v}\rangle. \tag{121}$$

The *second* interesting property of the free particle wave function is that the particles position is not localized in the space. According to our discussion above Eqs.(114) and (115 represent the

wave functions for the eigenstate of the one- and three- dimensional momentum. Thus they describe states with definitive magnitude for momentum p_x or $\vec{p}$. According to the uncertainty principle such a state should have infinite uncertainty for the position of the particle. This can be seen if we calculate the position density function ρ which results in (for 3d case):

$$\rho(r) = \frac{1}{(2\pi\hbar)^3}. \tag{122}$$

This results indicates that the probability density to find the free particle with momentum $\vec{p}$ is constant in all over the space, therefore its location is not determined.

7.2 Detection of the Free Quantum Particle - wave packet

The above discussed free particle wave function is spread all over the space with indefinite position. However the detection of the free particle assumes that we know the position of it in the confines of the detector. Therefore from the point of view of classical observer, what makes sense to discuss how such a particle discussed by the free wave function is detected.

The mathematical concept of the detection is that one detects the particle with finite resolution for its momentum and the process of detection is associated with the response of the detector $f(k)$ which peaks at value k_0 corresponding to the momentum $p_0 = k_0\hbar$ for which the detector is "tuned" (see e.g. Fig.). The response function also satisfies condition $\int f(k)dk = 1$. The result of such a measurement is a wave packed defined as:

$$\psi_{pck}(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-i(\omega t - kx)} f(k)dk. \tag{123}$$

Using the fact that $f(k)$ peaks at k_0 one can expand $\omega t - kx$ around k_0 using relations

$$\omega = \omega_0 + \frac{d\omega}{dk}(k-k_0) + \frac{1}{2}\frac{d^2\omega}{dk^2}(k-k_0)^2 + \cdots \tag{124}$$

where $\omega_0 = \omega(k_0)$. Writing $k = k_0 + (k - k_0)$ one obtains:

$$\omega t - kx = \omega_0 t - k_0 x + \left[\frac{d\omega}{dk} - x\right](k-k_0) + \frac{1}{2}(k-k_0)^2\frac{d^2\omega}{dk^2} + \cdots. \tag{125}$$

Inserting the above relation into the expression of the wave packet Eq.(**??**) and keeping only the first order derivative of $\omega(k)$ one obtains:

$$\begin{aligned} \psi_{pck}(x,t) &= \frac{1}{\sqrt{2\pi\hbar}} e^{-i(\omega_0 t - k_0 x)} \int e^{-i(v_g t - x)(k-k_0)} f(k)dk = \frac{1}{\sqrt{2\pi\hbar}} e^{-i(\omega_0 - k_0 v_g)t} \int e^{-i(v_g t - x)k} f(k)dk \\ &= e^{-i(\omega_0 - k_0 v_g)t} \psi_{pck}(x - v_g t). \end{aligned} \tag{126}$$

The above equation indicates that the measured wave packet propagates with the speed of

$$v_g = \frac{d\omega}{dk} = \frac{p}{m} = v, \tag{127}$$

which represents the group velocity of the wave and coincides with the classical velocity.

8 Ambiguities Related to the Explicit form of operator $\hat{H}$