Fundamentals of quantum mechanics

Quantum behaviour of particles

Experiment with bullets:

In the experimental setup, we have

- a machine gun that shoots (rather sprays) ‘‘classical’’ bullets, randomly over a fairly large angular direction,
- a wall that has two holes, large enough to allow only one bullet to pass through at a time,
- another wall behind the first wall in which the bullets are embedded after passing through the first wall.
- The first wall is impenetrable i.e. the bullets reach the second wall only and only if they pass through the holes in the first wall.
- The bullets are indestructible i.e. bullets do not shatter while passing through the first wall. Therefore, either a full bullet reaches the second wall or nothing reaches at all. There is no case of a partial bullet reaching the second wall.
- There is a detector in the second wall which records the arrival of the bullets and their position on the second wall. Therefore, the total number of bullets and their positions on the second wall can be determined.

The experimental setup is shown in Fig. 1. The holes in the first wall can be opened or closed as wished.

While passing through the holes, the bullets might hit the edges of the holes and scatter. Therefore, we observe a spread of the possible positions of arriving bullets on the second wall. Therefore, only a probability for the arrival of

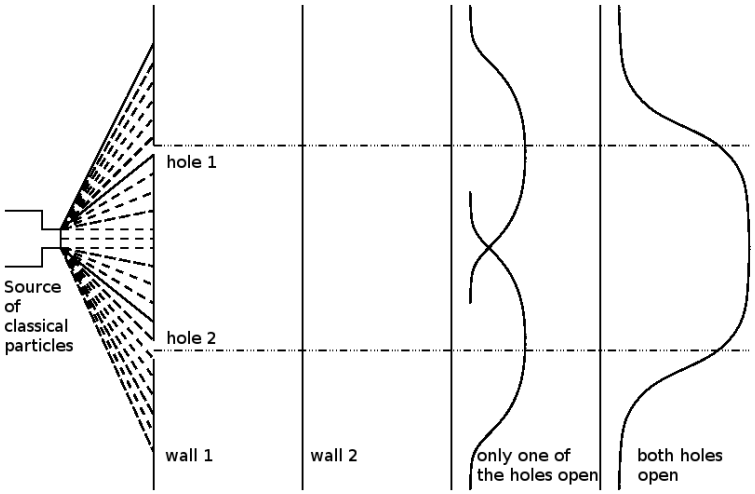

Figure 1: A schematic for the experiment with classical particles. The curves on the right show the spatial distribution of particles.

the bullets between two positions x and x+dx can be defined. This is given as the count of the total number of bullets between x and x+dx divided by the total number of bullets arriving the second wall during the entire experiment. We define the probabilities as follows:

P(1) = probability that the bullet reached the second wall when only hole 1 was open,

P(2) = probability that the bullet reached the second wall when only hole 2 was open,

P(12) = probability that the bullet reached the second wall when both holes 1 and 2 were open.

Since the bullets in this experiment are classical particles, a bullet will pass through wall 1 either through hole 1 or through hole 2. This is further confirmed as the bullets always reach in lumps. Due to this reason, we redefine P(12) as

P(12) = probability that the bullet reached the second wall passing either through hole 1 or through hole 2.

From the law of probability we get,

$$P(12) = P(1) + P(2) \tag{1}$$

The above equation shows that the bullets do not show ‘‘interference’’. The path followed by a bullet while passing through a particular hole is independent of the state (open or close) of the second hole.

Experiment with waves:

We use a similar apparatus as described for the experiment with bullets except that we use a source of waves instead of classical particles. The following differences are noteworthy:

- The detector measures intensity of the waves reaching wall 2. Intensity is proportional to the square of the amplitude of the wave.
- The intensity of the wave can have any value governed by the wave generator. Therefore, unlike the experiments with classical particles, the waves are not restricted to reach the second wall in lumps.

Figure 2 shows the setup for experiment with waves and the corresponding wave intensities.

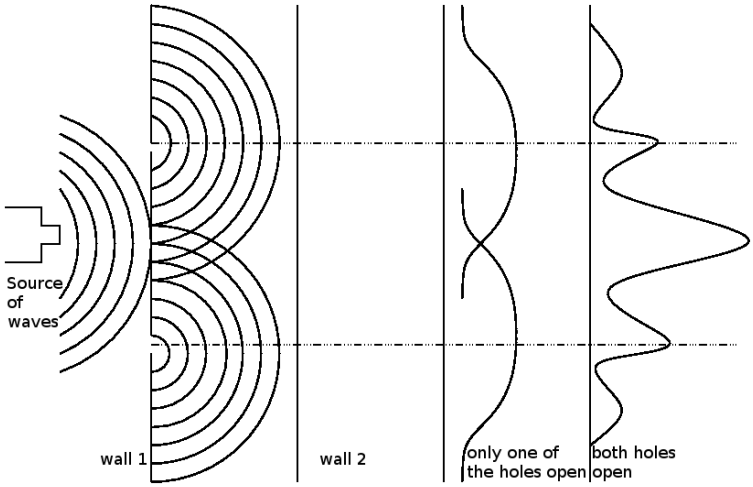

Figure 2: A schematic for the experiment with waves. The curves on the right show the intensity of the waves.

The intensities for this system are defined as follows.

I(1) = intensity detected at wall 2 when only hole 1 was open
I(2) = intensity detected at wall 2 when only hole 2 was open

I(12) = intensity detected at wall 2 when both holes were open

We have the following relations.

$$\exp(\pm ix) = \cos(x) \pm i\sin(x)$$

A cosine wave with an amplitude 'h' is given as

$$y = h\cos(\omega t) = hRe[\exp(i\omega t)]$$

Therefore, for the amplitudes of the waves passing through different holes in different states can be written as

Instantaneous height of the wave passing through hole 1 = $h_1 Re[\exp(i\omega t)]$
Instantaneous height of the wave passing through hole 2 = $h_2 Re[\exp(i\omega t)]$
Instantaneous height of the wave when both hole 1 and hole 2 are open = $(h_1+h_1)Re[\exp(i\omega t)]$

Further for a system with normalizable proportionality constant, I(1) = $|h_1(t)|^2$, I(2) = $|h_2(t)|^2$ and I(12) = $|h_1(t)+h_1(t)|^2$. Therefore,

$$I(12) = [h_1 Re(\exp(iwt)) + h_2 Re(\exp(iwt + i\delta))]^2$$

$$I(12) = h_1^2 Re(\exp(2i\omega t)) + h_2^2 Re(\exp(2i\omega t + 2i\delta)) + 2h_1 h_2 Re(\exp(i\omega t) Re(\exp(i\omega t + i\delta)))$$

$$I(12) = I(1) + I(2) + 2\sqrt{I(1)I(2)}\cos\delta \tag{2}$$

where δ is the phase difference between the waves arriving at any point on wall 2 from hole 1 and hole 2.

The term $2\sqrt{I(1)I(2)}\cos\delta$ is called the interference term. It is this term which makes the wave behaviour different from a particle behaviour. The particles do not show any interference.

0.0.1 Experiment with electrons:

The experimental setup used for the previous two experiments is used again except that now a source of electrons is used instead of a source of classical particles or waves. Following the classical concept considering electrons as particles, probability distributions identical to that of bullets must be obtained. However, probability distributions similar to that shown in Fig. 2 are observed. Fig. 3

shows the distributions observed with electrons. While the experiment was done, the following conditions were ensured:

- A sharp click at the detector is observed and there does not exist anything like a partial click. Therefore, either a complete electron arrives at wall 2 or nothing arrives at all.
- The above behaviour is similar to the behaviour of the bullets. Therefore, we must obtain a probability distribution for the arrival of electrons as a function of the position on second wall.
- The rate of emission of electrons could be controlled. Therefore, it could be ensured that a single (i.e. complete) electron arrived the second wall and the electrons therefore showed lumpiness as the bullets did.

In spite of the above, the probability distribution obtained for electrons resembled the bahaviour showed by the waves and not that by the particles. This is in contrast with the experimental procedure which ensured that the electrons followed particle-like behaviour.

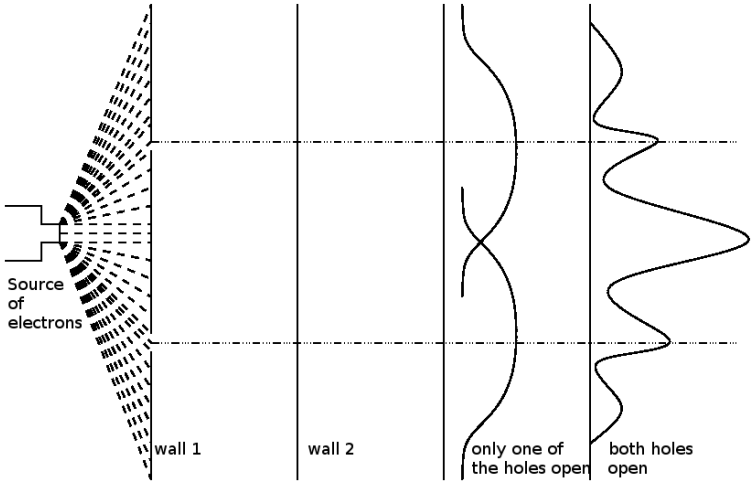

Figure 3: A schematic for the experiment with electron with the probability distributions on the right.

Proposition 1: Since during the experiment we observed that the electrons arrived the detector in lumps, it is proposed that the electron goes either through hole 1 or through hole 2.

If the above proposition is correct then the overall effect observed by opening both the holes must be the resultant of the individual effects. To establish this, the experiment is repeated by closing one of the holes and the probability distributions P(1) and P(2) are obtained.

Following the above proposition, P(12) = P(1) + P(2). However, it can be seen from the figure that

$$P(12) \neq P(1) + P(2) \tag{3}$$

Therefore, the two processes of passing through holes 1 and 2 are not mutually exclusive. This shows the presence of interference.

Proposition 2: It is now proposed that the electron goes through either hole 1 or hole 2 but not following a simple path. Rather, it may take a complicated path passing through hole 1 returning back, passing through hole 2, etc.

If the electrons follow such tortuous paths then closing of one of the holes changes the chance of arrival of electron at a particular point and, therefore, the probability distribution changes. However, if we analyze the probability distributions, we observe that on opening both the holes, there are regions where the probability of arrival of electrons has reduced compared to distribution corresponding to the case when only one hole is open. This means that the probability decreases for certain regions on opening both the holes. But at the center, probability is higher than the individual probabilities when both the holes are open. This means that closing of one hole decreased the probability of arrival of electrons which comes from the second hole. These two observations are contradictory and, therefore, the proposition of complicated paths can not be correct.

Experiment to test propositions by ‘‘watching’’ electrons:

The proposition was that the electron either goes through hole 1 or goes through hole 2. To test this, we modify the setup and put a light source between the two walls and the two holes as shown in Fig. 4. Since electric charges scatter light, the electrons will scatter light during their travel and we can find out the hole from which it passed. The following observations were made.

- Every time an electron is detected at wall 2, a flash is observed either

near hole 1 or near hole 2. Flash and detection are never at the same time. Further, flashes are not observed at both the holes at the same instant. This means that the electron either goes through hole 1 or through hole 2.

- Now we construct the probability distribution. $P'(1)$ is obtained by keeping a track of electrons passing through hole 1. This probability distribution is same as the probability distribution obtained with hole 2 closed. Similarly, probability distribution is obtained for electrons passing through hole 2 and the combined probability distribution. The resultant probability distribution is no more that of the electrons which were not observed (wave-like). The probability distribution is

$$P'(12) = P'(1) + P'(2) \tag{4}$$

This means that ''watching'' the electrons changes the probability distribution.

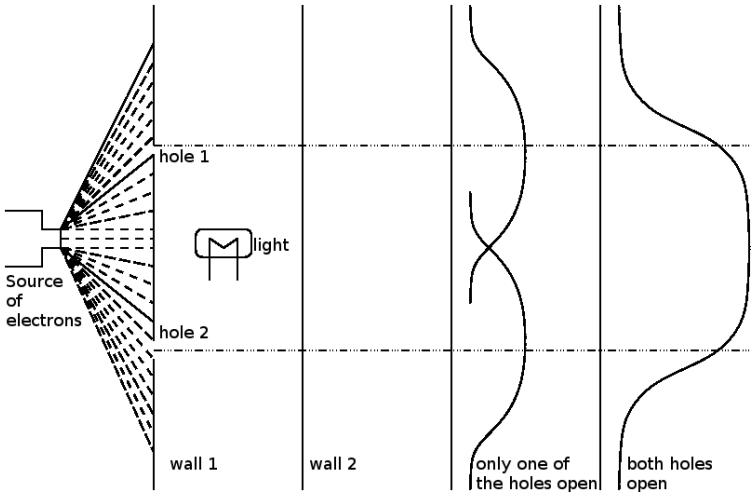

Figure 4: A schematic for the experiment with electron with a light source to detect the hole through which the electron has passed and the resultant probability distributions on the right.

The interaction of light with the electron may affect its motion thereby changing the probability distribution. This may be the reason behind not observing the wave-like behaviour. To overcome this problem, we make the following changes to the experimental setup.

- Use of light source of lesser intensity: With is change in setup, it is observed that the flashes on scattering do not get weaker. However, flashes

are not always observed whenever an electron is detected at wall 2. This is because making the light dimmer decreases the photon flux but keeps the energy of photons the same. As a result, the electrons may pass through the hole unobserved by the light source. However, the same amount of energy interacts with the electron as in the previous case causing the same disturbance to the motion. Therefore, with this modification also, wave-like pattern disappears.

- To observe electrons without disturbing their motion, we can use light of lesser frequency. However, with this setup, we are essentially using longer wavelength which makes the distinction between two spots in space separated by a distance of the order of wavelength of the radiation impossible. Therefore, this modification can also not be be used.

- We turn back to the previous modification where we had used a light source of lesser intensity. We now tabulate separately the cases where both flash and electron were detected and where only electrons was detected with no flash. The probability distribution constructed using this data will show that whenever electrons passed unobserved, interference is observed and whenever electrons were detected, the probability distribution corresponded to that of no-interference case.

To conclude, observation of motion of electron changes the probability distribution. One can comment whether the electron went through hole 1 or hole 2 only when one has observed the electron. However, when no observation has been made, we can no more comment upon the way electron takes a path between the source and the detector. This is in contrast to the nature of classical particles. Further, it is not the inability of to devise an experimental setup. This is the inherent quantum nature of electrons which can not be explained on the basis of classical senses.

Interfering alternatives and probability amplitude

In all the experiments described previously, the two holes provided two alternatives to the electron to move between the source and the detector. Whenever the electron was not observed, the alternatives always interfered. The resultant probability distribution for interfering alternatives can be developed as follows.

- A wave amplitude can be represented by a complex number called probability amplitude.
- Resulting amplitude from an experiment having a number of alternatives is the sum of amplitudes of the alternatives.
- Probability is the absolute square of the probability amplitude.

The above can be laid down mathematically as follows.

- For hole 1, probability amplitude = $\Phi_1(x)$
- Probability distribution for hole 1 = P(1) = $|\Phi_1(x)|^2$
- For hole 2, probability amplitude = $\Phi_2(x)$
- Probability distribution for hole 2 = P(2) = $|\Phi_2(x)|^2$
- Probability amplitude for interfering 1 and 2 = $\Phi_1(x) + \Phi_2(x)$
- Probability distribution for interfering 1 and 2 = P(12) = $|\Phi_1(x) + \Phi_2(x)|^2$

Note that the first step is the summation of all the interfering probability amplitudes. The resultant probability amplitude is then squared to get the probability distribution. The probability amplitude of an overall process is the sum of individual probability amplitudes.

The conclusion of the process (detection at the second wall in this case) is important. If any event/process disturbs the original process before its conclusion then the overall probability amplitude is destructed and we can no longer observe the interfering amplitude.

Now consider a setup in which more than two holes are present and additional screens are inserted. The resultant probability amplitude will be the sum of probability amplitudes of all the alternatives. Corresponding to the motion of

electron between the source and the detector following any path, a probability amplitude can be written and all such amplitudes have to be summed up and squared to get the resultant probability distribution.

If the number of holes in any screen is so large that nothing is left in the screen then the path of the electron must be specified by height as a function of x. A pair of heights x_D and x_E must be specified for the path passing through D and E. For all the possible heights, the amplitudes corresponding to each height must be integrated (instead of summation as x is now a continuous variable). Similar procedure has to be adopted for different possible screens along y-direction.

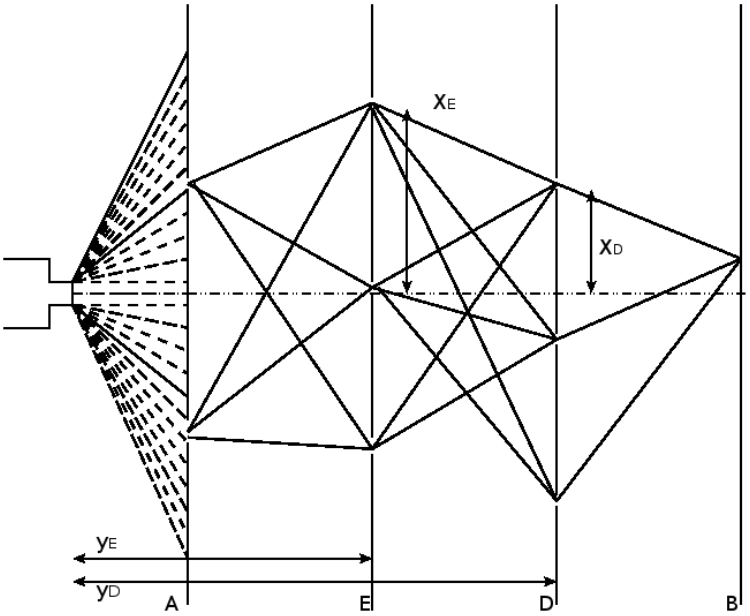

Figure 5: Path of an electron between the source and the detector conceived as a path consisting of a large number of screens each having a large number of holes.

Figure 5 shows a sharp contrast between the motion of a classical particle and the motion of a quantum particle between two points in space. For a classical particle, a deterministic trajectory can be drawn following Newton's laws of motion. In contrast, a quantum particle sees the path to destination to consist of an infinite number of screens with infinite number of holes. As a result, the contribution of all the possible paths are to be taken into account. The resultant motion of a quantum particle is a collection of different trajectories, each with some probability amplitude associated with it.

Analysis of motion of quantum particles using path integrals

For each possible trajectory between two points 'a' and 'b' in space and time interval t_b-t_a, a probability amplitude can be written which is a complex number. The trajectory of the particle is given as x(t) with $x(t_a) = x_a$ and $x(t_b) = x_b$.

Instead of a single trajectory between a and b observed for a classical particle, a collection of a large number of trajectories exists for a quantum particle. A single entity for the collection of trajectories satisfying the boundary conditions and the given time interval is called kernel (or propagator). The kernel K(b,a) gives the sum of contributions from all the probability amplitudes for the trajectories possible between a and b in a given time interval.

Principle of least action:

For every possible trajectory between a and b and a given time interval, it is possible to write an action defined as follows.

$$S = \int_{t_a}^{t_b} L(\dot{x}, x, t)dt \tag{5}$$

where L($\dot{x}$,x,t) is the Lagrangian for the system, defined as

$$L(\dot{x}, x, t) = \frac{1}{2}m\dot{x}^2 - V(x, t) \tag{6}$$

V(x,t) is the potential energy function and the dot over the quantities denotes the time derivative. The classical trajectory is the one for which the action is stationary i.e. $\delta S = 0$, subject to the conditions $\delta x(t_a) = \delta x(t_b) = 0$ i.e. the end points remain unchanged. Only one trajectory is observed for a classical particle whereas all the possible trajectories contribute to the motion of a quantum particle.

Relation between action and probability amplitude: For a given set of end points a and b and time interval t_b-t_a, a large number of trajectories can be written. An action can be computed for each trajectory. Every trajectory contributes equally to the motion of a quantum particle but the contributions may be at different phases. The kernel can be developed as follows.

- Relation between action and probability amplitude

$$\Phi[x(t)] = \text{constant} \cdot \exp[(i/\hbar)S(x, t)] \tag{7}$$

- Relation between probability amplitude and kernel

$$K(b,a) = \sum_{\text{all possible paths}} \Phi[x(t)] \tag{8}$$

- Relation between kernel and probability distribution

$$P(b,a) = |K(b,a)|^2 \tag{9}$$

All the paths between a and b can be seen to contribute equally but at different phases. For a classical particle, only one path, the classical path, seems to contribute and other paths do not appear. This can be understood as follows.

Contribution of a particular trajectory is given by $\Phi[x(t)]$. This involves the ratio $S/\hbar$. For a classical particle, $S/\hbar >> 1$. Therefore, the phase of the contribution of this particular value of $S/\hbar$ is very large. Changes in the trajectory introduce changes in S and the phase fluctuates rapidly with sines and cosines involved in rapidly oscillating phase. As a result, the average contribution of different trajectories is zero except for the contribution from the classical trajectory. For the classical trajectory, the action is stationary. Therefore, small changes in the trajectory do not change the action and, therefore, the only observed contribution is that from the classical trajectory.

Evaluation of sum over paths: Determination of the kernel using 8 requires the evaluation of the sum over all possible paths. A method can be devised to evaluate the sum as follows.

Area under a curve is proportional to the sum of all its ordinates. For a discretized set of abscissae, the area can be approximated as

$$A \sim \sum_i f(x_i)$$

where $f(x_i)$ is a set of discretized ordinates. This can be seen in Fig. 6. The area A can be defined as the limit of the sum by making the interval h smaller and smaller. We get the area as the Riemann integral.

$$\int_a^b f(x)dx = h \sum_i f(x_i) \tag{10}$$

This procedure can be used to construct the sum over paths. The procedure is given below. With reference to Fig. 7,

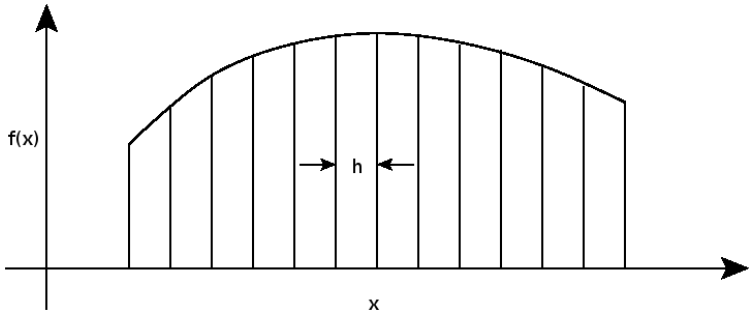

Figure 6: Evaluation of integrals by discretization.

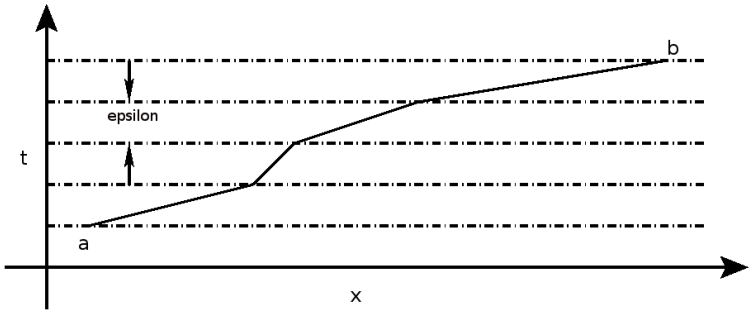

Figure 7: Discretization of path to evaluate sum over all paths.

- A path from a to b among the possible paths is chosen.
- The time interval is discritized into equal steps of interval ϵ. The initial time is t_a and the final time is t_b.
- The set (x_i,t_i) is generated corresponding to the chosen path.
- The path is generated by joining the points by straight lines as shown in the figure.
- This path is one of the possible paths from a to b with a given time interval t_b - t_a.
- A straight line path between x_i and x_{i+1} is described by a probability amplitude. However, x_i is only one of the possible points chosen. It is required to be integrated to obtain all the possible paths.

$$K(b,a) = \frac{1}{A^N} \int \int \dots \int [\Phi(x(t))] dx_1 dx_2 \dots dx_{N-1} \tag{11}$$

where $N\epsilon = t_b - t_a$, $\epsilon = t_{i+1} - t_i$, and $1/A^N$ = normalization constant. Further, $t_0 = t_a$, $t_N = t_b$, $x_0 = x_a$, and $x_N = x_b$. Note that the integration does not involve dx_0 or dx_N as the end points a and b are fixed. With $\Phi[x(t)] = \text{constant} \cdot \exp[(i/\hbar)S(x,t)]$, Eq. 11 can be written as

$$K(b,a) = \lim_{\epsilon \to 0} \frac{1}{A} \int \int \dots \int \exp[(i/\hbar)S(x(t))] \frac{dx_1}{A} \frac{dx_2}{A} \dots \frac{dx_{N-1}}{A} \tag{12}$$

Events occurring in succession: A compact notation for sum over all paths between a and b, irrespective of the method of integration is given below:

$$K(b,a) = \int_a^b \exp[(i/\hbar)S(b,a)] \mathcal{D}x(t) \tag{13}$$

The above equation signifies the ‘‘path integral’’, denoted by the letter $\mathcal{D}$ to distinguish it from the ordinary integral.

Consider the motion of a particle from a to b via c. Motion between a and c, and between c and b take place in succession. In such a case, the action can be written as

$$S(b,a) = S(b,c) + S(c,a)$$

The corresponding kernel becomes

$$K(b,a) = \int_a^b \exp[(i/\hbar)S(b,c) + (i/\hbar)S(c,a)] \mathcal{D}x(t) \tag{14}$$

In the above discussion, succession means that the particle goes from a to c and then from c to b. The event of motion from a to c also involves a large number of possible paths as shown in Fig. 8.

To describe a single event a$\rightarrow$b as two events in succession a$\rightarrow$c$\rightarrow$b, all paths between a and c are considered and all paths between c and b are considered. Now if point c itself can vary, then the result has to be integrated over all possible values of x_c.

Integration over all paths between a and c, keeping those between c an b constant gives

$$K(b,a) = \int_{-\infty}^{+\infty} \int_c^b \exp[(i/\hbar)S(b,c)] K(c,a) \mathcal{D}x(t) dx_c \tag{15}$$

The integration is carried out over all paths from a to c and all possible x_c. Now, the integration of all paths between c and b and arbitrary x_c gives

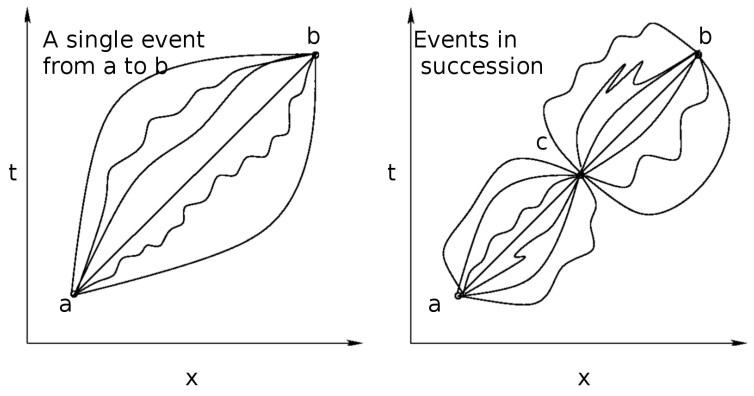

Figure 8: A single event and events taking place in succession.

$$K(b,a) = \int_{-\infty}^{+\infty} K(b,c)K(c,a)dx_c$$

From the above equation, it is clear that the amplitude for an event of succession of events is the product of the amplitudes of the individual events. This can be generalized for a series of events occurring in succession as

$$K(b,a) = \int_{x_{N-1}} \dots \int_{x_2} \int_{x_1} K(b,N-1)K(N-1,N-2)\dots K(1,a)dx_1dx_2\dots dx_{N-1} \qquad (16)$$

Evaluation of path integrals:

Consider a generalized Lagrangian given below.

$$L = a(t)\dot{x}^2 + b(t)\dot{x}x + c(t)x^2 + d(t)\dot{x} + e(t)x + f(t)$$

The kernel corresponding to the above Lagrangian is given as the path integral

$$K(b,a) = \int_a^b \exp[(i/\hbar)\int_{t_a}^{t_b} L(\dot{x},x,t)dt]\mathcal{D}x(t)$$

Consider the following situation. We imagine the existence of a classical path between (x_a,t_a) and (x_b,t_b). Any possible trajectory can be expressed as the sum of the classical path and a deviation from it.

$$x(t) = \overline{x}(t) + y(t)$$

where $\overline{x(t)}$ is the classical classical trajectory and y(t) is the deviation from the classical trajectory. The situation can be visualized in Fig. 9

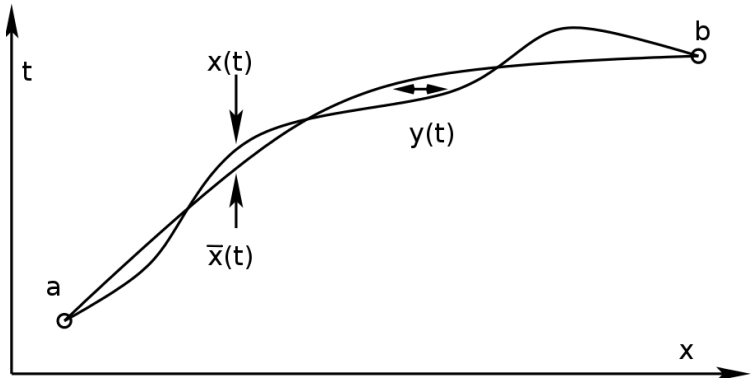

Figure 9: Realization of a quantum trajectory as a deviation from classical trajectory.

The action for the classical path is $S[\overline{x}(t)] = S_{Cl}(b,a)$. The quantum and classical actions can be related as

$$S[x(t)] = S[\overline{x}(t) + y(t)]$$

$$S[x(t)] = \int_{t_a}^{t_b} [a(t)(\dot{\overline{x}}^2 + 2\dot{\overline{x}}\dot{\overline{y}} + \dot{\overline{y}}^2) + \ldots]dt$$

The terms in the previous equation containing only $\overline{x}(t)$ result in the classical action. Therefore,

$$S[x(t)] = S_{Cl}(b,a) + \int_{t_a}^{t_b} [a(t)\dot{y}^2 + b(t)y\dot{y} + c(t)y^2]dt$$

where the subscript Cl signifies the classical action. The first order terms in y in the above equation vanish as y is a deviation variable and the integration will give zero. Therefore, the kernel can be written as

$$K(b,a) = \exp[(i/\hbar)S_{Cl}(b,a)] \int_0^0 [\exp[(i/\hbar) \int_{t_a}^{t_b} [a(t)\dot{y}^2 + b(t)y\dot{y} + c(t)y^2]dt]\mathcal{D}y(t) \qquad (17)$$

Note that the deviation variable $y(t)$ at (x_a,t_a) and (x_b,t_b) is zero. Therefore, the path integral in the above equation has both lower and upper limits as zero. Since it is a path integral whose value depends upon the path, its value is not zero even if the lower and upper limits are both zero. The above equation can, therefore, be written as

$$K(b,a) = \exp[(i/\hbar)S_{Cl}(b,a)]F(t_a,t_b)$$

Therefore, the evaluation of the path integral requires a knowledge of classical action and the kernel depends exponentially on the classical action. The function $F(t_a,t_b)$ must be determined case to case from the properties of the system. Consider a particle in potential V(x). The following Taylor series expansion can be written.

$$V(x) = V(\bar{x}+y) = V(\bar{x}) + yV'(\bar{x}) + \frac{y^2}{2!}V''(\bar{x}) + \frac{y^3}{3!}V'''(\bar{x})\dots$$

The differentiation in the above equation has been carried out with respect to x, and y has been taken as the differential variation from $\bar{x}$. For very small deviations, y^3 and higher orders can be neglected. Therefore,

$$V(x) = V(\bar{x}) + yV'(\bar{x}) + \frac{y^2}{2!}V''(\bar{x})$$

Since the action is stationary for a classical path, only the term second order in y will remain. Therefore, $S = S_{Cl}$ + terms second order in y. This approximation, accurate when the dependence on third and higher order terms is negligible, is called WKB (Wentzel-Kramers-Brillouin) approximation.

Multivariable and separable systems: Consider the motion of a particle in three dimensions. The particle is not subjected to any potential. In such a case,

$$S = \int_{t_a}^{t_b} \frac{m}{2}[\dot{x}^2(t) + \dot{y}^2(t) + \dot{z}^2(t)]dt$$

$$K(x_b, y_b, z_b, t_b; x_a, y_a, z_a, t_a) = \int_a^b \exp[(i/\hbar)\int_{t_a}^{t_b} \frac{m}{2}\left(\dot{x}^2(t) + \dot{t}^2(t) + \dot{z}^2(t)\right)dt]\mathcal{D}x(t)\mathcal{D}y(t)\mathcal{D}z(t) \tag{18}$$

Now consider two particles at x_1 and x_2 where x_1 and x_2 now represent the vectors of the coordinates of particles 1 and 2, respectively. The combined action contains the kinetic and potential energies of both the particles. Consider a special case where the combined action can be written as the sum of the individual actions.

$$S(x_1, x_2) = S(x_1) + S(x_2)$$

$$K(x_{1b}, x_{2b}, t_b; x_{1a}, x_{2a}, t_a) = \int_a^b \exp\left[\frac{i}{\hbar}[S(x_1) + S(x_2)]\right]\mathcal{D}^3x_1(t)\mathcal{D}^3x_2(t) \tag{19}$$

Note that $\mathcal{D}^3x_i(t)$ denotes path integral in three dimensions with $x_i(t)$ as a vector.

$$K(x_{1b}, x_{2b}, t_b; x_{1a}, x_{2a}, t_a) = \int_a^b \exp\left[\frac{i}{\hbar}[S(x_1)]\right] \mathcal{D}^3x_1(t) \int_a^b \exp\left[\frac{i}{\hbar}[S(x_2)]\right] \mathcal{D}^3x_2(t)$$

$$K(x_{1b}, x_{2b}, t_b; x_{1a}, x_{2a}, t_a) = K_{x_1}(x_{1b}, t_b; x_{1a}, t_a) K_{x_2}(x_{2b}, t_b; x_{2a}, t_a) \tag{20}$$

It can be seen from Eq. 20 that the kernel of a separable two-particle system is equal to the product of the individual kernels. Such a case is possible only if the particles are non-interacting. Therefore, for an N-particle non-interacting system,

$$K_{N-\text{particle}} = \prod_{i=1}^{N} K_{i(\text{one particle})} \tag{21}$$

Now consider a two-particle system with coordinate vectors x_1 and x_2 interacting with a potential $V(x_1,x_2)$. For such a system,

$$S(x_1, x_2) = \int_{t_1}^{t_2} \left[\left(\frac{m}{2}\right)\dot{x}_1^2 + \left(\frac{m}{2}\right)\dot{x}_2^2 - V(x_1, x_2)\right] dt$$

$$K(x_{1b}, x_{2b}, t_b; x_{1a}, x_{2a}, t_a) = \int_a^b \exp\left[\frac{i}{\hbar}\int_{t_1}^{t_2} \left[\left(\frac{m}{2}\right)\dot{x}_1^2 + \left(\frac{m}{2}\right)\dot{x}_2^2 - V(x_1, x_2)\right] dt\right] \mathcal{D}x_1(t)\mathcal{D}x_2(t) \tag{22}$$

Due the presence of $V(x_1,x_2)$ term in the above equation, the system may not be separable. In general, interacting systems may not be separable. Consider the interaction of a particle with a harmonic oscillator. Assume the coordinate vector for the particle be x and for the oscillator to be X. The action for such a system in the absence of oscillator, in the absence of the particle, and for the combined system can be written as

$$S(x) = \int_{t_a}^{t_b} \left[\left(\frac{m}{2}\right)\dot{x}^2 - V(x, t)\right] dt$$

$$S(X) = \int_{t_a}^{t_b} \left[\left(\frac{M}{2}\right)(\dot{X}^2 - \omega^2 X^2)\right] dt$$

$$S(x, X) = \int_{t_a}^{t_b} g[x(t), t]X(t)dt$$

g[x(t),t] can be regarded as the coupling coefficient signifying the interaction between the two systems.

$$K(b,a) = \int_a^b \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}\left(\left(\frac{m}{2}\right)\mathring{x}^2 - V(x,t)\right)dt + \int_{t_a}^{t_b}\left(\left(\frac{M}{2}\right)(\mathring{X}^2 - \omega^2 x^2)\right)dt + \int_{t_a}^{t_b} g[x(t),t]X(t)dt\right] \mathcal{D}x(t)\mathcal{D}X(t) \tag{23}$$

To carry out the above integration, we first carry out integration over all paths X(t).

$$K(b,a) = \int_a^b \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}\left(\frac{m}{2}\right)\mathring{x}^2 dt\right) T[x(t)]\mathcal{D}x(t)$$

where,

$$T[x(t)] = \int_a^b \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}\left(\frac{M}{2}(\mathring{X}^2 - \omega^2 X^2) + g[x(t),t]X(t)\right)dt\right]\mathcal{D}x(t) \tag{24}$$

Eq. 24 is call a functional as its value depends upon a function i.e. it is a function of a function. The form of Eq. 24 is same as the path integral required for generating a kernel. Therefore, the functional T[x(t)] can be regarded as the amplitude of the oscillator alone in interaction with the particle keeping the particle fixed.

For a given x(t), the functional T[x(t)] is evaluated. All possible paths for the oscillator for this given x(t) is obtained by the integral given as T[x(t)] in in Eq. 24. However, the paths of the particle, x(t), are also to be identified and T[x(t)] has to be evaluated for every single possible x(t). This further requires a path integral and the kernel resulting from both X(t) and x(t) is given by Eq. 23 with integration with respect to X(t) and x(t) signified by $\mathcal{D}X(t)$ and $\mathcal{D}xt$.

Summary and important observations from path integral formulation:

- Any disturbance before the completion of the motion of a quantum particle leads to non-observance of the interference of alternatives. This is referred to as the collapse of the wave function.
- A classical particle follows a unique trajectory, called the classical trajectory, which is determined as the trajectory with a stationary action. Since alternatives always interfere, the path between two points in space is seen by a quantum particle as a collection of an infinite number of alternatives obtained by a large number of highly porous screens placed between the two points in space. All the possible trajectories contribute equally to the motion of the quantum particle.

- Kernel signifies the knowledge of all the possible trajectories between two points in space subject to the constraint of the given time interval. Square of the kernel gives the probability. The calculations can be done in a step-wise manner as follows.

  - Initial (x_a,t_a); final (x_b,t_b).

  - Calculate kinetic energy and potential energy for a given path.

  - Calculate the Lagrangian for that path, L($\mathring{x}$,x,t) = KE - PE

  - Calculate the action for that path, S = $\int_a^b L(\mathring{x}, x, t)dt$

  - Calculate the probability amplitude, $\Phi[x(t)] = \text{constant} \cdot \exp[(i/\hbar)S]$

  - Kernel K(b,a)=$\sum \Phi[x(t)]$ over all possible paths

  - Probability P(b,a) = $|K(b,a)|^2$

Schrödinger's cat

This is a very famous thought experiment put forward by Schrdinger to describe the quantum behaviour of particles. Consider a cat placed in an opaque box. The cat is alive when put in the box. The box contains a capped bottle of poison. On the top of the bottle suspends a heavy hammer which may fall on the bottle and the bottle may break and the cat may lick the poison. However, the hammer is suspended by a pulley. The motion of the pulley is governed by triggering of a sensor by spontaneous emission of radiation by a radioactive material kept inside the box. Therefore, the events that that place inside the box may be as follows. The radioactive material ''may'' emit radiation owing to which the sensor ''may'' trigger due to which the hammer ''may'' fall on the bottle braking open the bottle. The cat thus ''may'' lick the poison. The question posed by Schrödinger was, ''is the cat dead or alive inside the box?'' The box is perfectly opaque and there are a lot of uncertainties associated with the events taking place inside the box. Therefore, any comment on the state of the cat (dead or alive) can be made only upon opening the box. When the box is opened, the cat is found either dead or alive. However, as long as the box is closed, one can not comment upon the state as the language is insufficient to describe a state of the cat which may or may not be alive. Exactly same is the situation with quantum particles.

Heisenberg uncertainty principle

In order to accurately determine the hole through which the electron goes, a modification in the experimental setup is made. The first wall is now supported by a pair of movable rolls such that the wall is free to move vertically. The motion of the wall is in a direction opposite to the direction of motion of the electron after leaving the wall.

When the electron is deflected while moving through a hole, the vertical component of its momentum changes. If the electrons reach the same point in wall 2 but come from different holes then they may have undergone different changes in momenta. The change in momentum of the electron can be measured by a change in the momentum of the wall, which in turn can be measured by the change in the velocity of the wall. If the electron goes through hole 1 and the change in momentum is $\delta \mathrm{P}_1$ and it is $\delta \mathrm{P}_2$ if the electron goes through hole 2 then an accurate determination of the difference in change of momenta ($\delta \mathrm{P} = \delta \mathrm{P}_1 - \delta \mathrm{P}_2$) will give the information whether the electron has gone through hole 1 or through hole 2.

The setup described above will again result in the probability distribution similar to the particle behaviour and the interference patterns will be lost.

In order to construct the probability distribution, an accurate knowledge of the position of arrival of electrons is required. But to know the hole through which the electron passes, an accurate knowledge of the position of the holes is also required. The position of the holes is governed by the momentum of the wall. Therefore, a simultaneous knowledge of both position as well as momentum of the electron is required.

Consider the interference pattern shown in Fig. 11. In order to capture this pattern, the measurements of positions must be made with an accuracy of at least d/2.

If the measurement of the position can not be made with an accuracy better than d/2 owing to the limitations of the instrument, the data for the position will result in an averaging owing to which a particle-like pattern will be obtained.

Consider Fig. 11 showing the interference of the waves. The first maxima will occur when the path difference BD-AD is equal to one wavelength. Let this point be D at a distance of d from the center (actually D is the position of second maxima with the first at center O). The condition for interference can be deduced

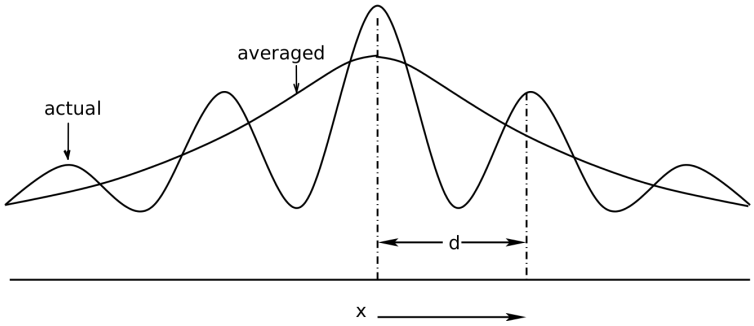

Figure 10: Measurement of position of electron from the interference pattern.

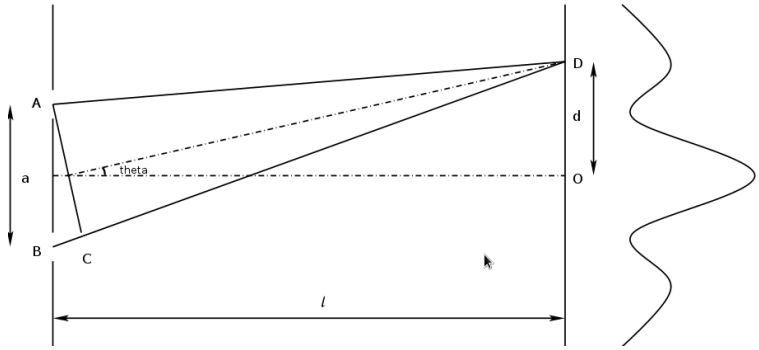

Figure 11: Figure showing different length scales involved in interference.

as $\lambda = \mathrm{asin}\theta$. For very small angle θ, $\mathrm{sin}\theta \approx \mathrm{tan}\theta$. Therefore,

$$\mathrm{tan}\theta = \frac{\mathrm{d}}{\mathrm{l}}$$

$$\lambda = \mathrm{a} \cdot \left(\frac{\mathrm{d}}{\mathrm{l}}\right)$$

$$\frac{\mathrm{a}}{\mathrm{l}} = \frac{\lambda}{\mathrm{d}} \tag{25}$$

For very small deflection angles, the deflection angle can be approximated as $|\delta \mathrm{P}|/|\mathrm{P}|$. Further, it can be shown that $|\delta \mathrm{P}_1 + \delta \mathrm{P}_2|/|\mathrm{P}|$ can be approximated as a/l. Therefore,

$$\frac{\delta \mathrm{P}}{\mathrm{P}} = \frac{\mathrm{a}}{\mathrm{l}}$$

$$\frac{\delta \mathrm{P}}{\mathrm{P}} = \frac{\lambda}{\mathrm{d}} = \frac{\mathrm{h}}{\mathrm{P} \cdot \mathrm{d}}$$

Since the uncertainty in measurement δx is of the order of d/2

$$\delta P \cdot \delta x \geq \frac{h}{2} \tag{26}$$

Eq. 26 gives the mathematical definition of Heisenberg uncertainty principle. According to this principle, it is impossible to determine simultaneously the position and momentum of a quantum particle with infinite precision. It is to be noted that the limit imposed on simultaneous measurements is inherent nature of the particles and it is not a limitation of the experimental setup. Further, this analysis only gives a motivation for the origins of uncertainty using path integrals and only an order of magnitude expression is obtained. For exact expression, h in Eq. 26 must be replaced by $\bar{h}$.

Schrödinger equation from path integrals

The kernel $K(x_b, t_b; x_a, t_a)$ can be used to determine the probability of finding a particle at x_b at time t_b given that the particle was present at x_a at time t_a. Now consider a special case where we define a quantity $\Psi(x, t)$ which, similar to the kernel, signifies the probability amplitude of finding the particle but without reference to its previous path. This amplitude is called the wave function of the particle. Thus, the absolute square of the wave function gives the probability of finding the particle in a given space without reference to its motion in the past. Therefore, the wave function is also called total amplitude.

Wave functions of a particle at two points (x_b, t_b) and (x_c, t_c) are related as

$$\Psi(x_b, t_b) = \int_{-\infty}^{+\infty} K(x_b, t_b; x_c, t_c)\Psi(x_c, t_c)dx_c$$

The above equation is a consequence of the resultant kernel of events in succession. $\Psi(x_c, t_c)$ gives the amplitude of the particle at (x_c, t_c) arrived following the definition of wave function. Amplitude to go from (x_c, t_c) to (x_b, t_b) is given by the kernel $K(x_b, t_b; x_c, t_c)$. Integration of the product over all the possible values of x_c will give the wave function at x_b.

Consider the relation between the wave functions at (x_a, t_a) and (x_b, t_b).

$$\Psi(x_b, t_b) = \int_{-\infty}^{+\infty} K(x_b, t_b; x_a, t_a)\Psi(x_a, t_a)dx_a$$

If the time t_a and t_b differ only infinitesimally i.e., $t_b - t_a = \epsilon$ then the kernel is approximated as

$$K(i+1,i) = \frac{1}{A}\exp\left[\frac{i}{\hbar}\epsilon L\left(\frac{x_{i+1}-x_i}{\epsilon}, \frac{x_{i+1}+x_i}{2}, \frac{t_{i+1}+t_i}{2}\right)\right]$$

where A is a normalization constant. Generally.

$$K(b,a) = \frac{1}{A}\exp\left[\frac{i}{\hbar}S(b,a)\right]$$

The above equations can be obtained as follows. For an infinitesimal $t_b - t_a, \mathring{x} \approx \frac{x_{i+1}-x_i}{\epsilon}$ and x can be evaluated at $(x_{i+1}+x_1)/2$ and t can be evaluated at $(t_{i+1}+t_i)/2$. Therefore,

$$\Psi(x,t+\epsilon) = \frac{1}{A}\int_{-\infty}^{+\infty} \exp\left[\frac{i}{\hbar}\epsilon L\left(\frac{x-y}{\epsilon}, \frac{x+y}{2}\right)\right]\Psi(y,t)dy \tag{27}$$

Now consider a particle moving in one dimension subject to a potential energy V(x,t)

$$L = \frac{1}{2}m\mathring{x}^2 - V(x,t)$$

$$L = \frac{m}{2\epsilon^2}(x-y)^2 - V\left(\frac{x+y}{2}, t\right)$$

$$\Psi(x,t+\epsilon) = \frac{1}{A}\int_{-\infty}^{+\infty} \exp\left[\frac{i}{\hbar}\epsilon\frac{m(x-y)^2}{2\epsilon^2} - \frac{i\epsilon}{\hbar}V\left(\frac{x+y}{2}, t\right)\right]\Psi(y,t)dy$$

$$\Psi(x,t+\epsilon) = \frac{1}{A}\int_{-\infty}^{+\infty} \exp\left[\frac{i}{\hbar}\frac{m(x-y)^2}{2\epsilon}\right]\exp\left[-\frac{i}{\hbar}\epsilon V\left(\frac{x+y}{2}, t\right)\right]\Psi(y,t)dy \tag{28}$$

Consider the differential quantity $\eta = y - x$ for a very small difference between x and y. Substitution of $y = x + \eta$ in Eq. 28 gives

$$\Psi(x,t+\epsilon) = \frac{1}{A}\int_{-\infty}^{+\infty} \exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right)\exp\left[-\frac{i}{\hbar}\epsilon V\left(x+\frac{\eta}{2}, t\right)\right]\Psi(x+\eta,t)d\eta \tag{29}$$

In the above equation, the phase is zero for $\eta = 0$ and is it equal to 1 rad for $\eta = \sqrt{2\hbar\epsilon/m}$. Therefore, η lies in this range for contribution to the integral. Thus, an order ϵ change corresponds to order η^2 change in the integral.Eq. 29 can be expanded in terms of power series.

$$\Psi(x,t+\epsilon) = \Psi(x,t) + \epsilon\left(\frac{\partial\Psi}{\partial t}\right)_{x,t}$$

$$\Psi(x,t+\epsilon) = \frac{1}{A}\int_{-\infty}^{+\infty} \exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right)\left[1 - \frac{i}{\hbar}\epsilon V(x,t)\right]\left[\Psi(x,t) + \eta\left(\frac{\partial\Psi}{\partial x}\right)_{x,t} + \frac{\eta^2}{2}\left(\frac{\partial^2\Psi}{\partial x^2}\right)_{x,t}\right]d\eta$$

$$\frac{1}{A}\int_{-\infty}^{+\infty} exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right) d\eta = \frac{1}{A}\left(\frac{2\pi i\hbar\epsilon}{m}\right)^{1/2} \tag{30}$$

The comparison of coefficients of $\Psi(x,t)$ in the above two equations gives

$$A = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{1/2}$$

Further,

$$\frac{1}{A}\int_{-\infty}^{+\infty} \eta exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right) d\eta = 0$$

$$\frac{1}{A}\int_{-\infty}^{+\infty} \eta^2 exp\left(\frac{im\eta^2}{2\hbar\epsilon}\right) d\eta = \frac{i\hbar\epsilon}{m}$$

Therefore, Eq. 30 becomes

$$\Psi(x,t) + \epsilon\left(\frac{\partial\Psi}{\partial t}\right)_{x,t} = \Psi(x,t) - \frac{i}{\hbar}\epsilon V\Psi(x,t) + \frac{i\hbar\epsilon}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}\right)_{x,t}$$

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial t^2}\Psi(x,t) + V(x,t)\Psi(x,t) \tag{31}$$

Eq. 31 is known the Schrödinger equation. It is the most fundamental equation of quantum mechanics. We will elaborate on its importance in a later chapter.
Eq. 31 can be rearranged as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left(\frac{-i\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\Psi(x,t) \tag{32}$$

The quantity $\frac{-i\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$ is called the Hamiltonian operator, denoted by $\hat{H}$. Thus,

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi \tag{33}$$

Chapter references and further reading:

[1] Feynman and Hibbs, Quantum Mechanics and Path Integrals, Dover Publications, Emended edition, 2010.
[2] Feynman, Leighton and Sands, The Feynman Lectures on Physics, Volume 3. Narosa Publishing House, 2007.