3. 1 WAVEPACKETS

Objective: Find the wavefunction y (*x*,*t*) of a free particle in one dimension.

Properties that must be satisfied by $\psi(x,t)$:

- Ø Normalizable, single valued, smooth, continuous
- Ø Complex function that satisfies the time-dependent Schrödinger equation (TDSE).
- Ø Must satisfy the homogeneity requirement

$$|\psi'(x,t)|^2 = |\psi(x-a,t)|^2 = |\psi(x,t)|^2,$$

since observables (physical quantities) are independent of the origin of the coordinates.

TRIAL FUNCTION 1:

Complex harmonic function: $\psi(x,t) = Ae^{i(kx-\omega t)}$

One can show that this trial function satisfies the following requirements:

- Ø It is a single valued, smooth and continuous function.
- Ø It is a complex function that does satisfy the TDSE.
- Ø It does satisfy the homogeneity requirement.

The main problem of this trial function is that it does not satisfy the normalization condition, i.e.

$$\int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)dx = \int_{-\infty}^{\infty} |A|^2 dx \to \infty \ .$$

Therefore, complex harmonic waves do not satisfy the normalization requirement and can not represent a localized particle.

TRIAL FUNCTION 1:

Construct a spatially-localized function by adding together a large number of harmonic waves with different wavenumbers and different frequencies:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} A(k)e^{i(kx-\omega t)}dk$$

where $A(k)$ is called the amplitude function, or momentum state function.

Notes:

- Ø One must add infinite number of plane waves to describe spatially-localized particle.

- The amplitude function governs the mixture of plane harmonic waves.
- Each of the monochromatic waves has a phase velocity v_{ph}, defined as a velocity of constant phase:

$$kx - \omega t = \theta = const. \rightarrow kdx = \omega dt \rightarrow v_{ph} = \frac{dx}{dt} = \frac{\omega}{k}$$

- The propagation velocity is the velocity by which the peak of the wavepacket moves and is called group velocity:

$$v_{gr} = \left.\frac{d\omega}{dk}\right|_{k=k_0} \rightarrow \text{free particle} \rightarrow v_{gr} = \frac{\hbar k_0}{m}$$

  Free particle wavepackets with amplitude function peaked about k=k_0 evolve in such a way that the position of its center changes at a speed identical to that of a classical particle with same mass and momentum $\hbar k_0$. This is a proof of the correspondence principle.

The next goal is to find the function $\psi(x,t)$ that describes free electrons. We will use the knowledge that we already have for Gaussian functions, for which:

$$A(k) = \left(\frac{2\sigma^2}{\pi}\right)^{1/4} \exp\left(-(k-k_0)^2\sigma^2\right) \rightarrow \langle p \rangle = \hbar k_0, \Delta p = \frac{\hbar}{2\sigma}$$

$$\psi(x,0) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{ik_0 x} \exp\left(-\frac{x^2}{4\sigma^2}\right) \rightarrow \langle x \rangle = 0, \Delta x = \sigma$$

We want to find out what happens to the wavepacket for t>0. For this purpose, we need to calculate $\psi(x,t)$ at t>0:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{2\sigma^2}{\pi}\right)^{1/4} e^{-(k-k_0)^2\sigma^2} e^{i(kx-\omega t)} dk$$

$$= \left(\frac{1}{2\pi}\right)^{1/4} \frac{1}{\sqrt{\sigma\left(1 + i\hbar t / 2m\sigma^2\right)}} \exp\left[-\frac{(x - \hbar k_0 t / m)^2}{4\sigma^2\left(1 + i\hbar t / 2m\sigma^2\right)}\right] \exp\left(ik_0 x - i\hbar k_0^2 t / 2m\right)$$

This result was obtained by first introducing the change of variables u=k-k_0 and then using the following integral:

$$\int_{-\infty}^{\infty} \exp\left(-\alpha u^2 - \beta u\right) du = \sqrt{\frac{\pi}{\alpha}} \exp\left(\beta^2 / 4\alpha\right).$$

The probability for finding the particle at a given point x in space at time t is thus given by:

$$P(x,t)=\psi^*(x,t)\psi(x,t)=\left(\frac{1}{2\pi}\right)^{1/2}\frac{1}{\sigma\sqrt{1+\left(\hbar t/2m\sigma^2\right)^2}}\exp\left[-\frac{\left(x-\hbar k_0 t/m\right)^2}{2\sigma^2\left[1+\left(\hbar t/2m\sigma^2\right)^2\right]}\right]$$

We also have that:

$$P(x,0)=\psi^*(x,0)\psi(x,0)=\left(\frac{1}{2\pi}\right)^{1/2}\frac{1}{\sigma}\exp\left[-\frac{x^2}{2\sigma^2}\right]=\left(\frac{1}{2\pi}\right)^{1/2}\frac{1}{\Delta x}\exp\left[-\frac{x^2}{2(\Delta x)^2}\right]$$

Comparing these two expressions, we arrive at the following result:

$$\sigma'(t)=\sigma\sqrt{1+\left(\hbar t/2m\sigma^2\right)^2}\rightarrow\Delta x(t)=\Delta x(0)\sqrt{1+\left(\hbar t/2m\sigma^2\right)^2},$$

that suggests that the uncertainty in the particle's position increases with time. Since the integrated probability must be equal to 1, the peak of the wavepacket decreases.

Next, we want to find out the average particle position at some finite time t. By inspection, one easily arrives at the following result:

$$\langle x\rangle(t)=\frac{\hbar k_0}{m}t=v_{gr}t$$

i.e. the center of the wavepacket moves with the group velocity. The spreading of the wavepacket is accompanied with decrease in amplitude.

It is straightforward to show that the wavepacket satisfies the TDSE for free particle. This is left as an exercise to the reader.

3.2 CONSERVATION OF PARTICLES AND PROBABILITY CURRENT

The TDSE gives us:

- the state function $\psi(x,t)$
- it also allows us to address physical questions about the microworld.

For example, we might ask the following question: Is the total number of particles conserved, or can a particle be created or destroyed? In probabilistic terms, this question becomes a query about the position probability density: Is the probability of finding a particle anywhere in space independent of time?

The answer is the following one: The probability of finding a microscopic particle anywhere in space does not change with time, i.e. (non-relativistic) particles are neither created nor destroyed. Mathematically this is represented by:

$$\frac{d}{dt}P([-\infty,\infty],t)=\frac{d}{dt}\int_{-\infty}^{\infty}P(x,t)dt=0$$

Proof:

Start with the definition of the integrated probability density:

$$\frac{d}{dt}P([-\infty,\infty],t)=\frac{d}{dt}\int_{-\infty}^{\infty}P(x,t)dx=\frac{d}{dt}\int_{-\infty}^{\infty}\psi^{*}(x,t)\psi(x,t)dx$$
$$=\int_{-\infty}^{\infty}\left[\frac{\partial\psi^{*}}{\partial t}\psi(x,t)+\psi^{*}(x,t)\frac{\partial\psi}{\partial t}\right]dx$$

From the time-dependent Schrödinger wave equation, one has:

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

Substituting these two expressions into our initial expression gives:

$$\frac{d}{dt}P([-\infty,\infty],t)=\int_{-\infty}^{\infty}\left[-\frac{i\hbar}{2m}\frac{\partial^{2}\psi^{*}}{\partial x^{2}}\psi+\frac{i}{\hbar}\psi^{*}(x,t)V(x,t)\psi(x,t)\right.$$
$$\left.+\frac{i\hbar}{2m}\psi^{*}\frac{\partial^{2}\psi}{\partial x^{2}}-\frac{i}{\hbar}\psi^{*}(x,t)V(x,t)\psi(x,t)\right]dx$$
$$=-\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left[\frac{\partial\psi^{*}}{\partial x}\psi-\psi^{*}\frac{\partial\psi}{\partial x}\right]dx$$

The last result leads to the following two conclusions:

1. The integrated probability density does not depend on time, since

$$\frac{d}{dt}P([-\infty,\infty],t)=-\frac{i\hbar}{2m}\left[\frac{\partial\psi^{*}}{\partial x}\psi(x,t)-\psi^{*}(x,t)\frac{\partial\psi}{\partial x}\right]_{-\infty}^{\infty}=0,$$

   where one uses the fact that for the wavefunction to be a proper wavefunction, it must vanish at infinity.

2. The second, and more interesting result that comes from the last expression can be obtained by equating the integrands on the left and on the righ-hand side, which leads to

$$\frac{\partial}{\partial t}\left(\psi^{*}\psi\right)=-\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\frac{\partial\psi^{*}}{\partial x}\psi(x,t)-\psi^{*}(x,t)\frac{\partial\psi}{\partial x}\right]$$

If one compares the last expression with the continuity equation for electrons, which in one dimension is of the form

$$\frac{\partial n(x,t)}{\partial t} = \frac{1}{q}\frac{\partial J}{\partial x},$$

it immediately follows that the quantum-mechanical probability current J_w can be calculated using:

$$J_w = -\frac{i\hbar q}{2m}\left[\frac{\partial \psi^*}{\partial x}\psi(x,t) - \psi^*(x,t)\frac{\partial \psi}{\partial x}\right].$$

Note:

1. The continuity equation is an alternative way of expressing conservation of particles in the system besides the time-independence of the integrated probability density.
2. If $\psi(x,t)$ is a representation of a single particle, then J_w must be related to the velocity of that particle. Otherwise, if $\psi(x,t)$ represents a large ensemble of particles, then the actual current is some average current taken over that ensemble.