II. WAVE FUNCTIONS AND WAVE EQUATIONS

What is the mathematical tool with which we can model an electron which is actually a wave? With a wave function. Waves are described using a wave function, i.e., their amplitude as a function of space and time. For instance it is easy to write a wave with frequency $\nu$ and wave length $\lambda$:

$$\psi(x, t) = e^{i(2\pi x/\lambda - 2\pi \nu t)} = e^{ikx - i\omega t}$$  \hspace{1cm} (23)

What I would like to do now, is reverse engineer an equation that would tell me what the wave function is. With light, we had only one thing to work with: $\lambda \nu = c$, or, the dispersion relation in the form:

$$\omega = ck$$  \hspace{1cm} (24)

Which connects the wave-length and the frequency. We need to modify a bit before we can actually use it. The wave we are trying to describe is propagating in some direction. Above, it is the x direction, but in 3d world it could have been any direction. So we can write:

$$\psi(\vec{r}, t) = e^{i\vec{k} \cdot \vec{r} - i\omega t}$$  \hspace{1cm} (25)

But what is the dispersion relation now?

$$\omega^2 = c^2 \vec{k}^2.$$  \hspace{1cm} (26)

To extract $\omega$ and $\vec{k}$ from the wave function, we can extract the angular frequency and the wave number by differentiation:

$$\frac{1}{i} \frac{\partial}{\partial x} \psi = k_x \psi, \quad \frac{1}{i} \nabla \psi = \vec{k} \psi$$  \hspace{1cm} (27)

and

$$-\frac{1}{i} \frac{\partial}{\partial t} \psi = \omega \psi$$  \hspace{1cm} (28)

And from these we can put together a nice partial differential equation:

$$\frac{\partial^2 \psi}{\partial t^2} = c^2 \nabla^2 \psi$$  \hspace{1cm} (29)

which is indeed the wave equation. For light.

A. The Schrödinger equation

What about for electrons? What would be the equivalent dispersion relation for electrons? A dispersion equation connects the angular frequency, which we connected with the energy, with the wave number - which we connected with the momentum. For an electron, how do these connect?

$$E = \frac{p^2}{2m}$$  \hspace{1cm} (30)

Can we make these into an equation? sure!

$$-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = \frac{1}{2m} \left( \frac{\hbar}{i} \nabla \right)^2 \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi$$  \hspace{1cm} (31)

This is the free particle Schrödinger equation.

Suppose the electrons are moving in a potential $V(\vec{r})$ what would be the equation? The energy gets modified to:

$$E = \frac{p^2}{2m} + V(\vec{r})$$  \hspace{1cm} (32)

So we can modify the Schrödinger equation as well:

$$\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r}) \psi.$$  \hspace{1cm} (33)
B. elementary solutions and baby Fourier transform

Let’s not complicate things. Let’s start thinking about the Schrödinger equation without an external potential.

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi \]  

(34)

This is a linear partial differential equation. The linearity is quite important. What does linearity guarantee? The superposition principle. If \( \psi_1(x,t) \) and \( \psi_2(x,t) \) are solutions, so is:

\[ \psi(x,t) = \psi_1(x,t) + \psi_2(x,t). \]  

(35)

Luckily, the equation also has constant coefficients. Nevertheless, it is a partial differential equation. What is our number one weapon when engaging with partial differential equations? Guessing. Let’s guess some solutions.

The first thing that comes to mind is constant: \( \psi = 1 \) say. Let’s do a bit better. Let’s try the usual wave equation favorite:

\[ \psi(x,t) = e^{ikx - i\omega t}. \]  

(36)

Putting this in the Schrödinger equation, we get:

\[ \hbar \omega e^{ikx - i\omega t} = \frac{\hbar^2 k^2}{2m} e^{ikx - i\omega t}. \]  

(37)

The dependence on \( x \) and \( t \) drops off, and we get the dispersion relation:

\[ \hbar \omega = \frac{\hbar^2 k^2}{2m}. \]  

(38)

But does this solution make sense? In terms of the frequency-wave number relation, it certainly does. It easily demonstrates both the Planck and De-Broglie rules:

\[ E = \hbar \omega = h\nu \quad p = \hbar k = h/\lambda. \]  

(39)

This is the way we constructed it - so no surprise there. But when we stop and think, we must confront the question: where is the particle? No one point in space in this solution is preferred to any other. Before plunging into the existential questions that arise in quantum mechanics, we can simply resolve this question by avoiding it for a second. If we can make a localized solution as well, something that resembles a localized entity, as we think a particle is, we can at least defer the question by a little bit.

As mentioned above, the Schrödinger equation is linear. So in fact we can make a rather crazy superposition of solutions:

\[ \psi(x,t) = \int \frac{dk}{2\pi} \phi(k) e^{ikx - i\hbar k^2 t/2m}. \]  

(40)

You can verify by substitution that this would work. In particular, we can consider the wave function at \( t = 0 \), which we choose as the starting time for the problem we consider:

\[ \psi(x,0) = \int \frac{dk}{2\pi} \phi(k) e^{ikx}. \]  

(41)

Does this remind you of anything? This is what is known as a Fourier transform. It turns out that any function can be described this way. Let’s look at an example: a good function for describing a particle is probably a Gaussian:

\[ \psi(x,0) = e^{-x^2/4\Delta x^2} \]  

(42)

We can generate it by choosing \( \phi(k) \) to be a Gaussian:

\[ \phi(k) = e^{-k^2/4\Delta k^2}. \]  

(43)

Let’s do the integral, and see how \( \Delta k \) and \( \Delta x \) correspond to each other:

\[ \psi(x,0) = \int \frac{dk}{2\pi} e^{-k^2/4\Delta k^2 + i k x}. \]  

(44)
This we can reasonably easily do by completing the square:

\[
\int \frac{dk}{2\pi} e^{-\frac{1}{4\Delta k^2} (k-2ix\Delta k)^2 - x^2 \Delta k^2} = \sqrt{2\pi} \Delta k e^{-x^2 \Delta k^2}
\]  

(45)

and we obtain:

\[
\Delta k \Delta x = \frac{1}{2}.
\]

(46)