Lecture 31: Introduction to Klein-Gordon Equation

Physics 452
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31.1 Review of De Broglie - Schrödinger

From the de Broglie relation, it is possible to ‘derive’ the Schrödinger equation, at least in the case of a free particle (i.e. \( V = 0 \)). From the de Broglie relation, we can find the corresponding dispersion relation as follows:

\[
p = \frac{h}{\lambda} = \hbar k \quad \text{(de Broglie)} \tag{31.1}
\]

\[
\Rightarrow m v_g = m \frac{d\omega}{dk} = \hbar k \Rightarrow d\omega = \frac{\hbar}{m} dk \tag{31.2}
\]

\[
\Rightarrow \hbar \omega = \frac{\hbar^2 k^2}{2m} \quad \text{(dispersion relation)} \tag{31.3}
\]

In the above analysis, it is important to realize that the particle momentum is related to the group velocity \( v_g \equiv d\omega/dk \), since a particle ought to travel at the speed of the wave packet associated with it.

The above dispersion relation results when a plane wave \( \Psi(\vec{r},t) = Ae^{i(\vec{k} \cdot \vec{r} - \omega t)} \) is plugged into the following differential equation:

\[
\frac{i\hbar}{\hbar} \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi \quad \text{(Schrödinger equation for free particle)} \tag{31.4}
\]

We conclude that (31.4) is the wave equation with solutions consistent with de Broglie’s hypothesis.

We have the following correspondence between momentum/energy and the derivatives in (31.4):

\[
h\omega \equiv E \leftrightarrow i\hbar \frac{\partial}{\partial t}, \quad \hbar k \equiv p \leftrightarrow -i\hbar \nabla. \tag{31.5}
\]

That is, these ‘operators’ when applied to \( \Psi \) tell you something about energy and momentum. In this language, the dispersion relation (31.3) may be written as \( E = \frac{p^2}{2m} \).

31.2 Review of Continuity Equation - Schrödinger

We next examine the time derivative of the following quantity
\[ \rho(\vec{r}, t) \equiv |\Psi(x, t)|^2. \quad \text{(Schrödinger probability density)} \quad (31.6) \]

With appropriate normalization of \( \Psi \), \( \rho \) is interpreted as a probability density. That is, the probability of finding the particle in a region of space is

\[ P = \int_{\text{region of space}} \rho(\vec{r}, t) d^3r. \quad (31.7) \]

Let us take the time derivative of this probability (to see how the probability of finding the particle in the region either increases or decreases with time):

\[
\frac{dP}{dt} = \int \frac{\partial \rho}{\partial t} d^3r = \int \left[ \frac{\partial \Psi^*}{\partial t} \Psi + \frac{\partial \Psi}{\partial t} \Psi^* \right] d^3r \\
\int \frac{1}{-i\hbar} \left( -\frac{\hbar^2}{2m} \nabla^2 \Psi \right) \Psi + \frac{\partial \Psi}{\partial t} \Psi^* + \Psi^* \frac{\partial \Psi}{\partial t} \left( -\frac{\hbar^2}{2m} \nabla^2 \Psi \right) d^3r \\
= -\int \frac{i\hbar}{2m} \left[ \Psi (\nabla^2 \Psi^*) - (\nabla^2 \Psi) \Psi^* \right] d^3r = -\int \nabla \cdot \left( \frac{i\hbar}{2m} \left[ \Psi (\nabla \Psi^*) - (\nabla \Psi) \Psi^* \right] \right) d^3r
\]

(31.8)

In the above expression, we have substituted from (31.4) and (31.6). We next define

\[ \vec{J}(\vec{r}, t) = \frac{i\hbar}{2m} \left[ \Psi \left( \nabla \Psi^* \right) - \left( \nabla \Psi \right) \Psi^* \right], \quad \text{(Schrödinger probability current)} \quad (31.9) \]

where we call the probability current. We can appreciate why it is named the probability current by applying the divergence theorem to (31.8):

\[
\frac{dP}{dt} = -\int_{\text{region of space}} \nabla \cdot \vec{J} d^3r = -\oint_{\text{surface}} \vec{J} \cdot \hat{n} da
\]

(31.10)

We see that the change in the probability of finding the quantum particle within a region of space is connected to the flow of \( \vec{J} \) through the surface containing the region. (Note that \( \hat{n} \) is the surface normal.)

Finally, can write (31.10) as

\[
\int \frac{dP}{dt} d^3r = -\int \nabla \cdot \vec{J} d^3r = \int \left[ \nabla \cdot \vec{J} + \frac{\partial \rho}{\partial t} \right] d^3r = 0
\]

(31.11)

Since the region of integration is arbitrary, the only way for (31.10) to be true is for the integrand to be zero everywhere. Thus we have

\[ \nabla \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0, \quad (31.11) \]
which is called a continuity equation.

3. De Broglie – Klein-Gordon

The preceding sections follow a non-relativistic scenario. In particular, (31.2) assumes 
\( p = mv_g \), which comes from Newtonian mechanics. If we want a wave equation that 
obey the principle of relativity, we must use

\[
p = \frac{mv_g}{\sqrt{1 - v_g^2/c^2}} = \hbar k 
\]

(31.13)

where we still use the de Broglie relation (31.1) to express the momentum in terms of 
wavelength. We will need to do some algebra to isolate \( v_g \). Starting from (31.13) we get

\[
\Rightarrow m^2 v_g^2 = \hbar^2 k^2 \left( 1 - v_g^2/c^2 \right) \Rightarrow \left( m^2 + \hbar^2 k^2/c^2 \right) v_g^2 \Rightarrow v_g = \frac{\hbar k}{\sqrt{m^2 + \hbar^2 k^2/c^2}}. 
\]

(31.14)

As before, we will use \( v_g = d\omega/dk \) and integrate

\[
\frac{d\omega}{dk} = \frac{\hbar k}{\sqrt{m^2 + \hbar^2 k^2/c^2}} \Rightarrow d\omega = \frac{c^2}{\hbar} \frac{\left( \hbar^2 k/c^2 \right)dk}{\sqrt{m^2 + \hbar^2 k^2/c^2}} \Rightarrow \hbar \omega = c^2 \sqrt{m^2 + \hbar^2 k^2/c^2} 
\]

(31.15)

We square this expression and arrive at

\[
\hbar^2 \omega^2 = m^2 c^4 + c^2 \hbar^2 k^2, 
\]

(31.16)

which is a dispersion relation. We get this relation when a plane wave \( \Psi(\vec{r}, t) = Ae^{i(k \cdot \vec{r} - \omega t)} \)
is plugged into the following equation:

\[
-\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} = m^2 c^4 \Psi - c^2 \hbar^2 \nabla^2 \Psi \quad \text{(Klein-Gordon equation for free particle)}
\]

(31.17)

We conclude that this is the wave equation governing particles, which is valid at 
relativistic speeds. This equation is harder to solve than the Schrödinger equation, since 
it is second order in time.

We may view the Schrödinger equation as a low-energy limit to the Klein-Gordon 
equation. We see this by noting (31.15) may be approximated at low energy as

\[
\hbar \omega = mc^2 \sqrt{1 + \hbar^2 k^2/m^2 c^2} = mc^2 \left( 1 + \hbar^2 k^2/2m^2 c^2 + \ldots \right) \equiv mc^2 + \hbar^2 k^2/2m, \text{ which agrees with (31.3)},
\]
except of a constant offset $mc^2$. In context of the Schrödinger equation, this rest energy merely alters the arbitrary zero point reference for the particle energy. This simply appends $e^{i(mc^2/h)t}$ to the wave function, which does not alter any observable.

Using the same correspondences as before (31.5), the dispersion relation (31.15) may be written as

$$E^2 = m^2c^4 + c^2 p^2.$$  \hfill (31.17)

It is common to write our plane wave solutions as

$$\Psi_{\vec{p}}(\vec{r},t) = A_{\vec{p}}e^{i(p \cdot r - \omega t)/\hbar},$$ \hfill (31.18)

where $\vec{k} = \vec{p}/\hbar$ and $\omega = E/\hbar$. The subscript $\vec{p}$ remind us that the wave is associated with a specific momentum. We may want to set the the normalizing factor $A_{\vec{p}}$ to different values depending on the momentum. According to (31.17), the energy $E$ is determined by the momentum through $E(p) = \pm \sqrt{m^2c^4 + c^2p^2}$, where we will tend to favor the positive root rather than the negative root, the latter corresponding to antiparticles.

### 4. Continuity Equation – Klein-Gordon

We would like to develop expressions for probability density and probability current similar to (31.6) and (31.9), but this turns out to be a little tricky. If we try

$$\rho(x,t) = |\Psi(x,t)|^2$$ (i.e., if we start with $d\rho/dt = \int \frac{\partial}{\partial t} |\Psi(x,t)|^2 \ d^3r = \int \left[ \frac{\partial \Psi^*}{\partial t} \Psi + \Psi^* \frac{\partial \Psi}{\partial t} \right] d^3r$ as in (31.8)), then we will not be able to proceed, since the Klein-Gordon equation does not have a first-order derivative that would enable a substitution. So let’s instead try working backwards from the current density (31.10) $J(\vec{r},t) = \frac{i\hbar}{2m} \left[ \Psi (\nabla \Psi^*) - (\nabla \Psi)^* \Psi^* \right]$ to see if we can find a corresponding probability density $\rho(\vec{r},t)$ that would satisfy the continuity equation.

Using our previous definition of current density, we have

$$\int \nabla \cdot J d^3r = \int \nabla \cdot \frac{i\hbar}{2m} \left[ (\nabla \Psi^*) \Psi - (\nabla \Psi)^* \right] d^3r = \int \frac{i\hbar}{2m} \left[ (\nabla^2 \Psi) \Psi^* - \Psi (\nabla^2 \Psi^*) \right] d^3r$$ \hfill (31.19)

Substitution from the Klein-Gordon equation (31.17) gives
\[ \Rightarrow \vec{\nabla} \cdot \int d^3 r = \int \frac{ih}{2mc} \left[ \Psi \left( \frac{1}{c^2} \frac{\partial^2 \Psi^*}{\partial t^2} + \frac{m^2 c^2}{\hbar^2} \Psi^* \right) - \left( \frac{1}{c^2} \frac{\partial^2 \Psi}{\partial t^2} + \frac{m^2 c^2}{\hbar^2} \Psi \right) \Psi^* \right] d^3 r \]

\[ = \int \frac{ih}{2mc} \left[ \Psi \left( \frac{\partial^2 \Psi^*}{\partial t^2} - \left( \frac{\partial^2 \Psi}{\partial t^2} \right) \Psi^* \right) \right] d^3 r = -\int \frac{\partial}{\partial t} \frac{ih}{2mc^2} \left[ \left( \frac{\partial \Psi}{\partial t} \right) \Psi^* - \Psi \left( \frac{\partial \Psi^*}{\partial t} \right) \right] d^3 r \]

(31.20)

Apparently, the probability density is

\[ \rho(\vec{r},t) = \frac{ih}{2mc^2} \left[ \left( \frac{\partial \Psi}{\partial t} \right) \Psi^* - \Psi \left( \frac{\partial \Psi^*}{\partial t} \right) \right], \quad (31.21) \]

instead of the familiar \(|\Psi|^2\). At least, this is what obeys the continuity equation (31.12)

\[ \frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0. \]

As an example, the probability density for a free-particle plane wave

\[ \Psi(\vec{r},t) = A e^{i(\vec{k} \cdot \vec{r} - \omega t)} \]

is

\[ \rho(\vec{r},t) = \frac{ih}{2mc^2} \left[ \left( \frac{\partial A e^{i(\vec{k} \cdot \vec{r} - \omega t)}}{\partial t} \right) A^* e^{-i(\vec{k} \cdot \vec{r} - \omega t)} - A e^{i(\vec{k} \cdot \vec{r} - \omega t)} \left( \frac{\partial A^* e^{-i(\vec{k} \cdot \vec{r} - \omega t)}}{\partial t} \right) \right] \]

(31.22)

\[ = \frac{ih}{2mc^2} \left[ -i\omega |A|^2 - i\omega |A|^2 \right] = \frac{\hbar \omega |A|^2}{mc^2} = \frac{E |A|^2}{mc^2} \]

In the low-energy limit (i.e., the non-relativistic limit), we have \(E \to mc^2\), so this reduces the same answer as we would expect, namely \(|A|^2\).