Lecture 32: Klein-Gordon Equation – Wave Packet Construction

Physics 452
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32.1 Inner Product

As we learned in the lecture 31, the Klein-Gordon equation is more general than the Schrödinger equation in that it describes a wave function for a particle even at relativistic energies. For a free particle, the Klein-Gordon equation is given by

\[-\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} = m^2 c^4 \Psi - c^2 \hbar^2 \nabla^2 \Psi.\]  \hspace{1cm} (32.1)

As we saw before, this equation is satisfied by plane wave solutions:

\[\Psi_p(\vec{r},t) = A e^{i(\vec{p} \cdot \vec{r} - \omega t)/\hbar},\]  \hspace{1cm} where \(\vec{k} \equiv \vec{p}/h\) and \(\omega \equiv E/\hbar\). The Klein-Gordon equation enforces \(E^2 = m^2 c^4 + c^2 p^2\), so we see that \(E\) and \(p\) are not independent. In light of the probability density defined by (31.20) \(\rho(\vec{r}) = \int \rho d^3r\), we define the inner product between two different wave functions to be

\[\langle \Psi_1 | \Psi_2 \rangle = \int \frac{i\hbar}{2mc^2} \left[ \Psi_1^* \frac{\partial \Psi_2}{\partial t} - \Psi_2^* \frac{\partial \Psi_1}{\partial t} \right] d^3r.\]  \hspace{1cm} (32.2)

The expectation of an operator \(\hat{O}\) is then

\[\langle \Psi | \hat{O} \Psi \rangle = \int \frac{i\hbar}{2mc^2} \left[ \Psi^* \frac{\partial \hat{O} \Psi}{\partial t} - \hat{O} \frac{\partial \Psi^*}{\partial t} \right] d^3r.\]  \hspace{1cm} (32.3)

32.2 Normalization of the Klein-Gordon Plane Wave

Obviously, the plane wave \(\Psi_{p'}(\vec{r},t) = A e^{i(\vec{p'} \cdot \vec{r} - \omega t)/\hbar}\) is not normalizable in the traditional sense, since it fills the universe. We must use Dirac normalization. (This is not unique to the Klein-Gordon equation. We have to do this type of normalization also for plane waves satisfying the Schrödinger equation.) We choose the coefficient \(A\) such that

\[\langle \Psi_p(\vec{r},t) | \Psi_{p'}(\vec{r},t) \rangle = \delta^3(\vec{p} - \vec{p'}) \equiv \delta(p_x - p'_x) \delta(p_y - p'_y) \delta(p_z - p'_z).\]  \hspace{1cm} (Dirac normalization)  \hspace{1cm} (32.4)
The subscripts $\bar{p}'$ and $\bar{p}$ help us keep track of two distinct plane waves. Computing the inner product explicitly for the two plane waves, we have

$$\langle \Psi_{\bar{p}'}(\bar{r},t) | \Psi_{\bar{p}}(\bar{r},t) \rangle = \frac{i\hbar}{2mc^2} \int \left[ \left( A^* e^{-i(\bar{p}' - E')/\hbar} \right) \left( \frac{\partial}{\partial \bar{t}} A e^{i(\bar{p} - E)/\hbar} \right) \right] d^3 r$$

$$= \frac{i\hbar A^*}{2mc^2} \int \left[ \left( A^* e^{-i(\bar{p}' - E')/\hbar} \right) \left( -\frac{i}{\hbar} A e^{i(\bar{p} - E)/\hbar} \right) \right] d^3 r$$

$$= \frac{A A^* (E + E') e^{-i(E - E')/\hbar}}{2mc^2} \int e^{i(\bar{p}' - \bar{p})/\hbar} d^3 r$$

(32.5)

The final 3-D integral gives rise to delta functions:

$$\int e^{i(\bar{p}' - \bar{p})/\hbar} d^3 r = \int dx \int dy \int dz = (2\pi)^3 \delta(p_x - p_x') \delta(p_y - p_y') \delta(p_z - p_z')$$

(32.6)

Recall that $E$ depends on $\bar{p}$, so the delta functions force the two energies $E$ and $E'$ to be the same if we are to get a non-zero result. Also note $\delta((p_x - p_x')/\hbar) = h\delta(p_x - p_x')$.

Thus we have

$$\langle \Psi_{\bar{p}'}(\bar{r},t) | \Psi_{\bar{p}}(\bar{r},t) \rangle = |A|^2 \frac{E}{mc^2} (2\pi)^3 \delta(p_x - p_x') \delta(p_y - p_y') \delta(p_z - p_z')$$

(32.7)

For this to look like (32.4), we require

$$\frac{|A|^2 E}{mc^2} (2\pi)^3 = 1 \Rightarrow A = \frac{mc^2}{(2\pi)^3 E}$$ (plane wave normalizing coefficient) (32.8)

### 32.3 Superposition of Plane Waves

Consider a wave function constructed by superimposing many plane waves:

$$\Psi(\bar{r},t) = \int a(\bar{p}) \Psi_{\bar{p}}(\bar{r},t) d^3 \bar{p}$$

(32.9)

The inner product of this wave function with itself is

$$\langle \Psi(\bar{r},t) | \Psi(\bar{r},t) \rangle = \frac{i\hbar}{2mc^2} \int d^3 r \left[ \left( \int d^3 p' a^*(\bar{p}') \Psi_{\bar{p}'}(\bar{r},t) \right) \frac{\partial}{\partial \bar{t}} \int d^3 p a(\bar{p}) \Psi_{\bar{p}}(\bar{r},t) \right]$$

$$= \int d^3 p a(\bar{p}) \int d^3 p' a^*(\bar{p}') \left[ \int d^3 r \left( \Psi_{\bar{p}'}(\bar{r},t) \frac{\partial \Psi_{\bar{p}}(\bar{r},t)}{\partial \bar{t}} - \left( \frac{\partial \Psi_{\bar{p}}(\bar{r},t)}{\partial \bar{t}} \right) \Psi_{\bar{p}'}(\bar{r},t) \right) \right]$$

(32.10)
where we have utilized (32.2) in simplifying the final expression. We next install the Dirac normalization condition (32.4) for plane waves, which gives
\[ \langle \Psi(\vec{r},t) | \Psi(\vec{r},t) \rangle = \int d^3p a(\vec{p}) \int d^3p' a^*(\vec{p}') \delta(p_x - p'_x) \delta(p_y - p'_y) \delta(p_z - p'_z) \]
\[ = \int d^3p a(\vec{p}) a^*(\vec{p}) = \int d^3p |a(\vec{p})|^2 \]  
(32.11)

This tells us that we are able to construct a finite localized wave packet (with \( \langle \Psi(\vec{r},t) | \Psi(\vec{r},t) \rangle = 1 \)) out of the infinite plane waves. We just choose our coefficient \( a(\vec{p}) \) such that \( \int d^3p |a(\vec{p})|^2 = 1 \).

### 32.4 Example: Gaussian Wave Packet

Let us choose a Gaussian distribution of momentum centered around \( \vec{p}_o \)
\[ a(\vec{p}) = \xi \exp \left\{ -\frac{|\vec{p} - \vec{p}_o|^2}{2p_w^2} \right\} \]  
(32.12)

It is left as an exercise to show that \( \xi = (p_w \sqrt{\pi})^{-3/2} \) ensures that \( \langle \Psi(\vec{r},t) | \Psi(\vec{r},t) \rangle = 1 \).

With this choice for \( a(\vec{p}) \), our wave packet is computed as follows:
\[ \Psi(\vec{r},t) = \int a(\vec{p}) \Psi(\vec{r},t) d^3p = \frac{1}{(p_w \sqrt{\pi})^{3/2}} \frac{mc^2}{(2\pi)\hbar} \int \exp \left\{ -\frac{|\vec{p} - \vec{p}_o|^2}{2p_w^2} \right\} e^{i(\vec{p} \cdot \vec{r} - E(t)) / \hbar} d^3p \]
\[ = \frac{1}{(p_w \sqrt{\pi})^{3/2}} \frac{mc^2}{(2\pi)\hbar} \int e^{-|\vec{p} - \vec{p}_o|^2/(2p_w^2)} e^{i(\vec{p} \cdot \vec{r} - E(\vec{p})) / \hbar} \frac{1}{\sqrt{E(\vec{p})}} d^3p \]  
(32.13)

where \( d^3p \equiv dp_x dp_y dp_z \), \( E(\vec{p}) = \sqrt{m^2c^4 + p^2c^2} = \sqrt{m^2c^4 + (p_x^2 + p_y^2 + p_z^2)c^2} \),
\[ |\vec{p} - \vec{p}_o|^2 = (p_x - p_{ox})^2 + (p_y - p_{oy})^2 + (p_z - p_{oz})^2 = p_x^2 + p_y^2 + p_z^2 - 2(p_x p_{ox} + p_y p_{oy} + p_z p_{oz}) + p_o^2, \]
and \( \vec{p} \cdot \vec{r} = px x + py y + pz z \).

If we want to see our wave function evolve (i.e. move and spread in time), we must perform a 3-D integral for every different time \( t \) we want to see. Unfortunately, there isn’t an analytic solution, and this integration is numerically very challenging using a computer, especially given the oscillatory nature of the integrand. We will do the numerics on this wave packet at a later time. The computed wave packet is shown in Fig. 32.1 for an electron at rest (i.e. \( \vec{p}_o = 0 \)). The spherical Gaussian probability cloud expands rapidly outward as time progresses.
Fig. 32.1 A spherical Gaussian electron wave packet at rest (i.e. $\vec{p}_o = 0$) and spreading as a function of time. For this simulation, $p_w = 0.005m_ec$, which gives an initial wave-packet size of 1 Å at $t = 0$. The packets are evaluated at 25 fs and 100 fs, and the frames are 1 μm across.