Lecture 7: Quantum Equations

I. Momentum and Energy Operators

From above de Broglie wave-function packet one can identify at $t = 0$ the functions

$$u_{\mathbf{p}}(\mathbf{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}\ ,\ \ \overline{u}_{\mathbf{p}}(\mathbf{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}$$

with the coordinate-momentum scalar products unfolded as

$$\mathbf{p}\cdot\mathbf{r} = p_x x + p_y y + p_z z$$

However, note the very intriguing fact that, while the wave-function in *momentum representation* takes the form associable with a (generalized) *functional scalar product*

$$\psi_0(\mathbf{p}) = \int_{(\infty)} \overline{u}_{\mathbf{p}}(\mathbf{r})\psi_0(\mathbf{r})d\mathbf{r} := \left(u_{\mathbf{p}}(\mathbf{r}), \psi_0(\mathbf{r})\right)$$

this is not the case of the wave-functio n in the *coordinate representation* since the integral performed on convoluted function belonging to different spaces (and representations):

$$\psi_0(\mathbf{r}) = \int_{(\infty)} u_{\mathbf{p}}(\mathbf{r})\psi_0(\mathbf{p})d\mathbf{p}\ .$$

Such striking situation is solved (explained) by the fact the function $u_{\mathbf{p}}(\mathbf{r})$ is not assimilated with ordinary wave-function because not obeys the normalization condition through providing a divergent square integral:

$$\int_{-\infty}^{+\infty} \left|u_{\mathbf{p}}(\mathbf{r})\right|^2 d\mathbf{r} = \int_{-\infty}^{+\infty} \overline{u}_{\mathbf{p}}(\mathbf{r})u_{\mathbf{p}}(\mathbf{r})d\mathbf{r} = \frac{1}{(2\pi\hbar)^3}\int_{-\infty}^{+\infty} d\mathbf{r} \to \infty\ ,$$

although being indefinite derivable respecting the space coordinates:

$$\frac{d^n}{dx^n} u_{\mathbf{p}}(\mathbf{r}) = \left(-\frac{i}{\hbar} p_x\right)^n u_{\mathbf{p}}(\mathbf{r})$$

and with finite norm in both zero- and *n*-th order of such derivation:

$$\left|u_{\mathbf{p}}(\mathbf{r})\right| = \frac{1}{(2\pi\hbar)^{3/2}}\ ,\ \left|\frac{d^n}{dx^n} u_{\mathbf{p}}(\mathbf{r})\right| = \left(\frac{p_x}{\hbar}\right)^n \frac{1}{(2\pi\hbar)^{3/2}}\ .$$

Such functions are called distributions, so being more general than the ordinary wave-functions since the chain spaces inclusion:

$$\underbrace{\mathscr{L}(\Re_{\mathbf{r}})}_{\int\limits_{(\infty)} f d\mathbf{r}<\infty} \subset \underbrace{\mathscr{L}^2(\Re_{\mathbf{r}})}_{\int\limits_{(\infty)} f^2 d\mathbf{r}<\infty} \subset \underbrace{\mathscr{D}(\Re_{\mathbf{r}})}_{\int\limits_{(\infty)} f^2 d\mathbf{r}\to\infty}$$

among the simple integrable (trial wave-functions), square integrable (true wave-functions) and square non-integrable (temperate distributions) functions to be used as describing quantum particles and events.

The fact the function $u_{\mathbf{p}}(\mathbf{r})$ is in fact a temperate distribution can be seen also from its inner scalar product

$$\left(u_{\mathbf{p}'}, u_{\mathbf{p}}\right) = \int\limits_{(\infty)} \overline{u}_{\mathbf{p}'}(\mathbf{r}) u_{\mathbf{p}}(\mathbf{r}) d\mathbf{r} = \delta(\mathbf{p} - \mathbf{p}'),$$

leading with another distribution function, the Dirac (delta) function, previously introduced.

Nevertheless, one fundamental consequence of dealing with $u_{\mathbf{p}}(\mathbf{r})$ as a generalized function is that it can be considering as patterning a special (generalized in the sense of resumed) wave-function abstracted from the de Broglie wave-packet, namely

$$\vartheta_t(\mathbf{r}) = u_{\mathbf{p}}(\mathbf{r}) e^{-\frac{i}{\hbar}Et} = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{r} - Et)}$$

leading with the basic identities

$$\frac{\partial}{\partial t}\vartheta_t(\mathbf{r}) = -\frac{i}{\hbar} E \vartheta_t(\mathbf{r}),$$

$$\frac{\partial}{\partial x}\vartheta_t(\mathbf{r}) = \frac{i}{\hbar} p_x \vartheta_t(\mathbf{r})$$

producing the *quantum operatorial* definitions for energy and momentum:

$$\hat{E}\bullet = i\hbar \frac{\partial}{\partial t}\bullet$$

$$\hat{p}_x \bullet = -i\hbar \frac{\partial}{\partial x}\bullet,$$

while the 3D-momentum operatorial definition will look like

$$\hat{\mathbf{p}}\bullet = -i\hbar\nabla\bullet$$

in terms of nabla-differential operator over the space coordinates:

$$\nabla = \partial_i \partial^i,\ \partial^i := \partial / \partial x_i,\ i = 1(\text{for } x), 2(\text{for } y), 3(\text{for } z).$$

These operators, along the multiplicative space-coordinate rules (equally for coordinates and vectors):

$$\hat{x}\bullet = x\bullet, \quad \hat{V}(x,t)\bullet = V(\hat{x},t)\bullet = V(x,t)\bullet$$

are of prime importance in developing the forthcoming quantum equations and modeling the driven (or measurable or observable) events.

II. Klein-Gordon and Schrödinger Equations

Combining relativistic energy and momentum through velocity elimination:

$$E = mc^2 = \frac{m_0 c^2}{\sqrt{1-(v/c)^2}},$$

$$p = mv = \frac{m_0 v}{\sqrt{1-(v/c)^2}},$$

one gets the general momentum energy relationship:

$$E^2 = m_0^2 c^4 + p^2 c^2$$

from where the two possible energy solutions are obtained as

$$E = \pm\sqrt{m_0^2 c^4 + p^2 c^2}$$

with the Dirac celebrated energy solutions for the trapped particles ($\mathbf{p} = 0$)

$$E = \pm m_0 c^2$$

while fixing the intriguing Dirac seas of positive and negative energy limits within which the any given substantial particle ($m_0 \neq 0$) evolves, see Figure 2.X; eventually, it collapses into the referential zero level for the photonic case ($m_0 \to 0$).

However, the quantum correspondence principle applied upon the square of the above energy with energetic and momentum considered as operators and applied on the working wave-function $\psi_t(\mathbf{r})$,

$$\hat{E}^2 \psi_t(\mathbf{r}) = c^2 \hat{\mathbf{p}}^2 \psi_t(\mathbf{r}) + m_0^2 c^4 \hat{1} \psi_t(\mathbf{r})$$

leading with the so called Klein-Gordon equation:

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi_t(\mathbf{r}) = \left[\nabla^2 + \left(\frac{m_0 c}{\hbar}\right)^2\right]\psi_t(\mathbf{r})$$

or written in the (1+3)D form

$$\left[\square + \left(\frac{m_0 c}{\hbar}\right)^2\right]\psi_t(\mathbf{r}) = 0$$

where the D'Alambertian was defined in the ($x_0=ct$, $x_1=x$, $x_2=y$, $x_3=z$) ≈ (+, –, –, –) space-time relativistic metric

$$\square = \partial_\mu \partial^\mu = \partial_0^2 - \partial_i \partial^i \;,\; \partial^{\mu/i} = \partial / \partial x_{\mu/i} \;,\; \mu = 0,1,2,3 \;;\; i = \overline{1,3}\,.$$

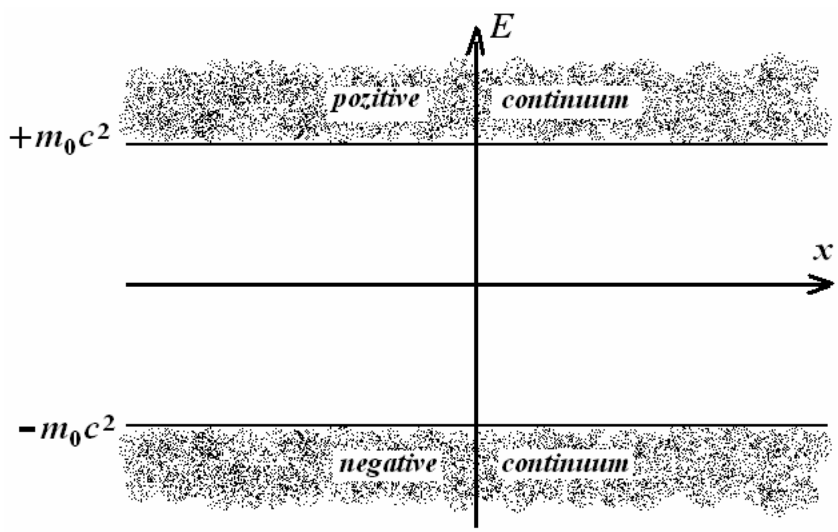

Figure 2.X. The separation ($2m_0c^2$) gap between the positive ($E>+\,m_0c^2$) and negative ($E<-m_0c^2$) continuum ("Dirac seas") for the energy of a relativistic particle.

Turning now to the non-relativistic motion, one expands the positive (or *electronic*) energy-momentum relativistic above solution in term of (v/c) yielding in the first order expansion,

$$\left(1+a\right)^{1/2}\Big|_{a\to 0} \cong 1 + a/2\,,$$

the actual relationship:

$$E \cong m_0 c^2 + \frac{p^2}{2m_0}$$

However, when the electronic motion is driven by a potential too, say $V(\mathbf{x})$, the last expression can be modified as such the energy spectrum be shifted with origin in the positive ($+\, m_0 c^2$) rest energy so that the working energy expression become

$$E \cong V(\mathbf{r}) + \frac{p^2}{2m_0};$$

Now, considering once more the operatorial version of this equation with energy and momentum operatorial rules applied on the wave-function, while noting the space operator as well as space dependent function(s) do not modify the space dependence, see above, the final result unfold as the famous Schrödinger temporal equation

$$i\hbar \frac{\partial}{\partial t}\psi_t(\mathbf{r}) = \left[-\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r})\right]\psi_t(\mathbf{r}),$$

in terms of Laplacian only this time:

$$\nabla^2 = \partial_i \partial^i,\ \partial^i = \partial / \partial x_i\ ,\ i = \overline{1,3}.$$