10. The Mathematical Foundations of Quantum Mechanics II

10.1 Representation Theory

The state of a particle is completely described by the normalized wave function \( \psi(r, t) \), which we have used until now. In the Schrödinger equation,

\[
\left( \frac{p^2}{2m} + V(r) \right) \psi(r, t) = i\hbar \frac{\partial}{\partial t} \psi(r, t)
\]

(10.1)

which gives us the evolution in time of the state, we expressed the momentum operator by the differential operator, i.e.

\[
p = -i\hbar \nabla.
\]

(10.2)

This representation \( \psi(r, t) \) of a particle state is called the coordinate representation. Because of Heisenberg's uncertainty principle, the momentum \( p \) of a particle is not exactly known if its position \( r \) is fixed. According to (3.50), the average momentum is

\[
\langle p \rangle = \int \psi^*(r, t)(-i\nabla)\psi(r, t) dV.
\]

(10.3)

We can extract information about the momentum of a particle from the wave function \( \psi(r, t) \) if we expand it in terms of eigenfunctions of the momentum operator; this is simply a Fourier transformation. The Fourier integral reads

\[
\psi(r, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int a(p, t) \exp \left( \frac{i}{\hbar} p \cdot r \right) d^3p = \int a(p, t) \psi_p(r) d^3p.
\]

(10.4)

The integration is extended over all of momentum space; the function \( a(p, t) \) is the Fourier transform of \( \psi(r, t) \) at time \( t \). The plane waves \( \psi_p(r) \) are eigenfunctions of the momentum (see Example 4.4). Indeed, we have

\[
\psi_p = \frac{1}{(2\pi\hbar)^{3/2}} \exp \left( \frac{i}{\hbar} p \cdot r \right), \quad \text{with} \quad \hat{p} \psi_p = \frac{\hbar}{i} \nabla \exp \left( \frac{i}{\hbar} p \cdot r \right) = p \psi_p.
\]

(10.5)

Now, by inspection of (10.4) it becomes evident that the function \( a(p, t) \) describes the particle state as completely as the function \( \psi(r, t) \). We call \( a(p, t) \) the momentum representation of the state of the particle. With the reciprocity of the Fourier transformation, it follows from (10.4) that

\[
a(p, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int \psi(r, t) \exp \left( \frac{i}{\hbar} p \cdot r \right) d^3r = \int \psi(r, t) \psi_p^*(r) d^3r.
\]

(10.6)
Hence, if \( \psi(\mathbf{r}, t) \) is known, we can construct \( a(p, t) \) according to (10.6); and, vice versa, if \( a(p, t) \) is known, we are able to construct \( \psi(\mathbf{r}, t) \) through (10.4). Analogously, the equivalence of the normalization can easily be shown:

\[
\int |\psi(\mathbf{r}, t)|^2 \, d^3 r = \int |a(p, t)|^2 \, d^3 p ,
\]

(10.7)

Indeed, (3.41) expresses this fact for particles within a box. The relation corresponding to (10.3) for the average of the position operator reads

\[
\langle \hat{r} \rangle = \int a^*(p, t) (i\hbar \nabla_p) a(p, t) \, d^3 p ,
\]

(10.8)

where \( \nabla_p = (\partial/\partial p_x, \partial/\partial p_y, \partial/\partial p_z) \) is the nabla or del operator in momentum space. Indeed, we can easily calculate with (10.4)

\[
\langle r \rangle = \int \psi^*(\mathbf{r}, t) r \psi(\mathbf{r}, t) \, d^3 r
\]

\[
= \int d^3 r \, d^3 p \, d^3 p' \, a^*(p, t) \psi_p^*(\mathbf{r}) a(p', t) \psi_p(\mathbf{r})
\]

\[
= \int d^3 p \, d^3 p' \, a^*(p, t) a(p', t) \int d^3 r' \psi_p^*(\mathbf{r}) r \psi_p(\mathbf{r}) .
\]

(10.9)

Now, by use of the first equation in (10.5), we can replace the vector \( \mathbf{r} \) in the space integral by

\[
\int d^3 r \, \psi_p^*(\mathbf{r}) r \psi_p(\mathbf{r}) = \int \psi_p^*(\mathbf{r})(-i\hbar \nabla_p') \psi_p(\mathbf{r}) d^3 r
\]

\[
= -i\hbar \nabla_p' \int \psi_p^*(\mathbf{r}) \psi_p(\mathbf{r}) d^3 r = -i\hbar \nabla_p' \delta^3(\mathbf{p} - \mathbf{p}') ,
\]

(10.10)

so that (10.9) becomes

\[
\langle r \rangle = \int d^3 p \, d^3 p' \, a^*(p, t) a(p', t)(-i\hbar \nabla_p') \delta^3(\mathbf{p} - \mathbf{p}')
\]

\[
= \int d^3 p \, a^*(p, t) \left[ a(p', t)(-i\hbar) \delta^3(\mathbf{p} - \mathbf{p}') \right]_{\mathcal{C} \to \infty} - \int d^3 p' \, (-i\hbar \nabla_p) a(p', t) \delta^3(\mathbf{p} - \mathbf{p}')
\]

\[
= \int d^3 p \, a^*(p, t) (i\hbar \nabla_p) a(p, t) .
\]

The function \( a(p, t) \) represents the momentum distribution of the particle state \( \psi(\mathbf{r}, t) \). The absolute square \( |a(p, t)|^2 \) gives the probability of finding the particle with definite momentum \( p \), i.e. with the wave function

\[
\psi_p(\mathbf{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \exp \left( \frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r} \right)
\]

in the state \( \psi(\mathbf{r}, t) \). Hence, \( |a(p, t)|^2 \) is the probability density in momentum space.

Up to now we have based our considerations on the physical point of view that the coordinate wave function \( \psi(\mathbf{r}, t) \) of a particle is determined by measuring its spatial distribution. The momentum distribution follows by Fourier transformation. But often in physics we must adopt a reverse approach; for example, in electron scattering experiments, momentum distributions (form factors) are measured. Then the (spatial) charge distribution of a nucleus follows from a Fourier analysis (see, e.g., Example 11.8).