Combining this with the previous result for expectation values of $\vec{r}$, we have the expectation value for a general function of $\vec{r}$ and $\vec{p}$, $f(\vec{r},\vec{p})$, as

$$\langle f(\vec{r},\vec{p})\rangle = \int d^3r\, \psi^*(\vec{r},t)\, f(\vec{r},-i\hbar\vec{\nabla})\, \psi(\vec{r},t).$$

1.3.4. Canonical Commutation Relations

As seen above, care must be taken in the ordering of the $\vec{r}$ and $\vec{p}$ arguments in the function f since in the coordinate space expectation value the momentum is replaced with the gradient $\vec{p} = -i\hbar\vec{\nabla}$. Clearly factors of $\vec{r}$ and $\vec{p}$ cannot be simply interchanged since their commutator does not vanish

$$\begin{aligned}
[x_i, p_j] &= [x_i, -i\hbar\tfrac{\partial}{\partial x_j}] \\
&= x_i(-i\hbar)\frac{\partial}{\partial x_j} - (-i\hbar)\frac{\partial}{\partial x_j} x_i \\
&= -i\hbar x_i\frac{\partial}{\partial x_j} + i\hbar\delta_{ij} + i\hbar x_i\frac{\partial}{\partial x_j} \\
&= i\hbar\delta_{ij},
\end{aligned}$$

where it is understood that the derivatives act on everything to their right. That is as if an arbitrary function $\psi(\vec{r},t)$ was present

$$[x_i, P_j]\,\psi(\vec{r},t) = i\hbar\delta_{ij}\,\psi(\vec{r},t),$$

since ψ is arbitrary, this is an operator identity.

Further we can simply check that

$$[x_i, x_j] = 0$$

$$[P_i, P_j] = 0 \quad .$$

These three sets of equations constitute the <u>canonical commutation relations</u>. Of the 6 operators $\vec{r}, \vec{P}$ only the x_i and P_i (that is x with P_x, y with P_y, z with P_z) operators do not commute.

As we shall see later, we can define (abstract) position $\bar{X}$ and momentum $\bar{P}$ operators which obey the CCR

$$[X_i, P_j] = i\hbar\delta_{ij}$$

We can represent this operator algebra on functions of $\vec{r}$, that is the coordinate space wavefunctions $\psi(\vec{r},t)$, by multiplication by $\vec{r}$ and action of the gradient $-i\hbar\vec{\nabla}$,

$$\vec{X} \longrightarrow \vec{r}$$
$$\vec{P} \longrightarrow -i\hbar\vec{\nabla} .$$

Or, if we consider momentum space wavefunctions $\varphi(\vec{k},t)$, the operators and their algebra can be represented by action of the gradient $i\vec{\nabla}_k$ and multiplication by $\hbar\vec{k}$,

$$\vec{X} \longrightarrow i\vec{\nabla}_k$$

$$\vec{P} \longrightarrow \hbar\vec{k}$$

as we can see from our discussion of expectation values.

(Thus care must always be taken when considering the ordering of factors of $\vec{X}$ and $\vec{P}$.)