II.D) Position, Momentum and Energy Representations

Where does Wave Mechanics fit in?

By expanding abstract vectors in the continuous orthonormal basis of position eigenvectors.

Recall position eigenfunctions

$$\psi_{\vec{r}_0}(\vec{r}) \equiv \delta^3(\vec{r}-\vec{r}_0)$$

The position eigenvalue equation is

$$\vec{r}\,\psi_{\vec{r}_0}(\vec{r}) = \vec{r}_0\,\psi_{\vec{r}_0}(\vec{r})$$

since $\vec{r}\,\delta^3(\vec{r}-\vec{r}_0) = \vec{r}_0\,\delta^3(\vec{r}-\vec{r}_0)$.

Also $\psi_{\vec{r}_0}(\vec{r})$ for all $\vec{r}_0$ formed a complete set of functions

$$\int d^3r_0\, \psi^*_{\vec{r}_0}(\vec{r}\,')\,\psi_{\vec{r}_0}(\vec{r}) = \delta^3(\vec{r}-\vec{r}\,')$$

That is

$$\psi(\vec{r}) = \int d^3r_0\, \psi(\vec{r}_0)\,\psi_{\vec{r}_0}(\vec{r})$$

$$= \int d^3r_0\, \psi(\vec{r}_0)\,\delta^3(\vec{r}-\vec{r}_0) = \psi(\vec{r}),$$

indeed,

and they obeyed the continuum normalization condition

$$\int d^3r\, \psi^*_{\vec{r}_0'}(\vec{r})\,\psi_{\vec{r}_0}(\vec{r}) = \delta^3(\vec{r}_0 - \vec{r}_0').$$

These wavefunctions formed a continuous basis for the extended space of square-integrable functions, $L^2(\mathbb{R}^3)$. Each position eigenfunction is in 1-1 correspondence with a (normalized) position eigenvector in an extended Hilbert space. We denote the eigenvector $|\vec{r}_0\rangle$, thus

$$\psi_{\vec{r}_0}(\vec{r}) \longleftrightarrow |\vec{r}_0\rangle .$$

$|\vec{r}_0\rangle$ is the abstract eigenvector of the abstract position operator $\vec{R}$

(notation convention: unless otherwise specified capital letters will be used to denote abstract operators like $\vec{R}$. Alternate conventions are placing subscripts "op" for operator on the same symbol as the eigenvalue like $\vec{r}_{op}$ for the position operator.)

Thus
$$\vec{R}\,|\vec{r}_0\rangle = \vec{r}_0\,|\vec{r}_0\rangle$$

eigenvector in $\mathcal{H}$

linear operator on $\mathcal{H}$

real number position eigenvalue

The correspondence between wavefunctions $\psi_{\vec{r}_0}(\vec{r})$ and eigenvectors $|\vec{r}_0\rangle$ is obtained by viewing $\psi_{\vec{r}_0}(\vec{r})$ as the components of $|\vec{r}_0\rangle$ in the $\{|\vec{r}\rangle\}$ basis. That is since the position eigenvalues are real $\vec{R}$ is a Hermitian operator, hence the $\{|\vec{r}\rangle\}$ is an orthonormal basis. Any vector in $\mathcal{H}$ can be expanded in terms of $\{|\vec{r}\rangle\}$

$$|\psi\rangle = \int d^3r\, \psi(\vec{r})\,|\vec{r}\rangle\,.$$

Since $\vec{R}=\vec{R}^{\dagger} \rightarrow \langle\vec{r}'|\vec{r}\rangle = 0$ for $\vec{r}\neq\vec{r}'$

recall:

$$\left.\begin{array}{l}\vec{R}\,|\vec{r}\rangle = \vec{r}\,|\vec{r}\rangle \\ \vec{R}\,|\vec{r}'\rangle = \vec{r}'\,|\vec{r}'\rangle\end{array}\right\} \Rightarrow \langle\vec{r}'|\vec{R}|\vec{r}\rangle = \vec{r}\,\langle\vec{r}'|\vec{r}\rangle$$

$$\langle\vec{r}'|\vec{R}|\vec{r}\rangle = \langle\vec{r}|\vec{R}^{\dagger}|\vec{r}'\rangle^{*} = \langle\vec{r}|\vec{R}|\vec{r}'\rangle^{*} = \vec{r}'\,\langle\vec{r}'|\vec{r}\rangle$$

So $\vec{r}\neq\vec{r}' \Rightarrow \langle\vec{r}'|\vec{r}\rangle = 0$

Thus $\langle\vec{r}'|\vec{r}\rangle$ only has values at $\vec{r}=\vec{r}'$; it is proportional to Dirac δ-functions and derivatives thereof. Derivatives can be viewed as differences so that the innerproduct for these is again zero. Thus only the local $\delta^3(\vec{r}-\vec{r}')$ occurs, $\langle\vec{r}'|\vec{r}\rangle = f(\vec{r})\delta^3(\vec{r}-\vec{r}')$. Without loss of generality we can choose $f(\vec{r})=1$, since by re-scaling $\vec{r}$ and $\vec{r}'$ by $f^{1/3}$ it disappears. So $\langle\vec{r}'|\vec{r}\rangle=\delta^3(\vec{r}-\vec{r}')$ the continuum normalization.

Hence

$$\langle\vec{r}|\psi\rangle = \int d^3r'\,\psi(\vec{r}')\underbrace{\langle\vec{r}|\vec{r}'\rangle}_{=\delta^3(\vec{r}-\vec{r}')}$$

$$= \psi(\vec{r})$$

In particular

$$\psi_{\vec{r}_0}(\vec{r}) = \langle\vec{r}|\vec{r}_0\rangle = \delta^3(\vec{r}-\vec{r}_0).$$

Now since the $\psi_{\vec{r}_0}(\vec{r})$ are complete we have

$$\int d^3r_0\,\psi^*_{r_0}(\vec{r})\psi_{r_0}(\vec{r}') = \delta^3(\vec{r}'-\vec{r})$$

which we write as

$$\int d^3r_0 \langle \vec{r}|\vec{r}_0\rangle^* \langle \vec{r}'|\vec{r}_0\rangle = \langle \vec{r}'|\vec{r}\rangle$$

$$= \int d^3r_0 \langle \vec{r}'|\vec{r}_0\rangle\langle \vec{r}_0|\vec{r}\rangle = \langle \vec{r}'|\vec{r}\rangle$$

$$\Rightarrow \int d^3r_0 |\vec{r}_0\rangle\langle \vec{r}_0| = \mathbb{1}$$

The completeness or closure identity for $\{|\vec{r}\rangle\}$

So we have that the position operator $\vec{R}$ is Hermitian with eigenvectors $|\vec{r}\rangle$ and real eigenvalues $\vec{r} \in \mathbb{R}^3$. The set $\{|\vec{r}\rangle\}$ are a continuous basis of orthonormal vectors for $\mathcal{H}$

$$\vec{R}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle \qquad \text{with}$$

1) Continuum normalization

$$\langle \vec{r}'|\vec{r}\rangle = \delta^3(\vec{r}-\vec{r}')$$

2) Completeness in $\mathcal{H}$

$$\mathbb{1} = \int d^3r\, |\vec{r}\rangle\langle\vec{r}| .$$

Note: For $|\psi\rangle = \int d^3r\, \psi(\vec r)\,|\vec r\rangle$

$$|\phi\rangle = \int d^3r\, \phi(\vec r)\,|\vec r\rangle$$

we have

$$\langle \psi| = \int d^3r\, \psi^*(\vec r)\,\langle \vec r|$$

$\Rightarrow$

$$\langle\psi|\phi\rangle = \left(\int d^3r\, \psi^*(\vec r)\langle\vec r|\right)\left(\int d^3r'\,\phi(\vec r')|\vec r'\rangle\right)$$

$$= \int d^3r \int d^3r'\, \psi^*(\vec r)\,\phi(\vec r')\,\underbrace{\langle\vec r|\vec r'\rangle}_{=\delta^3(\vec r'-\vec r)}$$

$$= \int d^3r\, \psi^*(\vec r)\,\phi(\vec r) \quad \text{as usual.}$$

This may also we viewed as inserting the identity operator $\mathbb{1} = \int d^3r\, |\vec r\rangle\langle\vec r|$

$$\langle\psi|\phi\rangle = \int d^3r\, \psi^*(\vec r)\,\phi(\vec r)$$

$$= \int d^3r\, \langle\vec r|\psi\rangle^* \langle\vec r|\phi\rangle$$

$$= \int d^3r\, \langle\psi|\vec r\rangle\langle\vec r|\phi\rangle$$

$$= \langle\psi|\underbrace{\left(\int d^3r\, |\vec r\rangle\langle\vec r|\right)}_{=\mathbb{1}}|\phi\rangle$$

$$= \langle\psi|\phi\rangle .$$

For any $|\psi\rangle \in \hat{\mathcal{H}}$, we can expand it in terms of position eigenvectors

$$|\psi\rangle = \int d^3r \, \psi(\vec{r}) |\vec{r}\rangle$$

where $\psi(\vec{r}) = \langle \vec{r} | \psi \rangle$, the components of the state vector $|\psi\rangle$ in the position eigenstate basis $\{|\vec{r}\rangle\}$ correspond to the functions $\psi(\vec{r})$ of the (extended) square-integrable function space $\mathcal{L}^2(\mathbb{R}^3)$.

Further we have that

$$\langle \psi | \phi \rangle = \int d^3r \langle \psi | \vec{r} \rangle \langle \vec{r} | \phi \rangle$$
$$= \int d^3r \, \psi^*(\vec{r}) \phi(\vec{r})$$

represents the inner product and

$$\langle \psi | \vec{R} | \phi \rangle = \int d^3r \langle \psi | \underbrace{\vec{R} | \vec{r} \rangle}_{= \vec{r} |\vec{r}\rangle} \langle \vec{r} | \phi \rangle$$
$$= \int d^3r \, \vec{r} \, \psi^*(\vec{r}) \phi(\vec{r}),$$

The matrix elements of the position operator $\vec{R}$ are given by the "wavefunction" integral. In particular the expectation value of any function of $\vec{R}$ is given by the familiar "wavefunction" expression for expectation values of the same function but now of $\vec{r}$

$$\langle \psi | F(\vec{R}) | \psi \rangle = \int d^3r \langle \psi | F(\vec{R}) | \vec{r} \rangle \langle \vec{r} | \psi \rangle$$

$$= \int d^3r \, \psi^*(\vec{r}) \, F(\vec{r}) \, \psi(\vec{r})$$

Since

$$F(\vec{R}) | \vec{r} \rangle = F(\vec{r}) | \vec{r} \rangle \, .$$

In order to make the correspondence between wavemechanics and the components of vectors in position space more concrete we will show that $\psi(\vec{r})$ obeys the Schrödinger wave equation when $|\psi\rangle$ obeys the operator Schrödinger equation of Postulate 4.

Towards this end we consider another Hermitian operator the momentum operator $\vec{P}$ and its eigenvectors $|\vec{p}\rangle$. Since, as with position $\vec{r}$, momentum is a real 3-vector $\vec{p}$ we have that $\vec{P}$ is Hermitian $\vec{P}=\vec{P}^{\dagger}$ and the

eigenvalue equation is

$$\vec{P}|\vec{p}\rangle=\vec{p}|\vec{p}\rangle\ ,\quad \vec{p}\in\mathbb{R}^3$$

As we argued in the position eigenstate case

$$\langle\vec{p}'|\vec{p}\rangle=0 \text{ if } \vec{p}\neq\vec{p}'$$

and so $\langle\vec{p}'|\vec{p}\rangle=f(\vec{p})\,\delta^3(\vec{p}-\vec{p}')$.
Again we can re-scale the momentum if desired, so we choose $f(\vec{p})$ a constant. By our previous convention, as we will see, we take the constant to be $(2\pi\hbar)^3$, thus

$$\langle\vec{p}'|\vec{p}\rangle=(2\pi\hbar)^3\delta^3(\vec{p}-\vec{p}'),$$ the

continuum normalization.

Now since $\{|\vec{p}\rangle\}$ are complete, we can expand any vector in terms of them $|\psi\rangle \in \hat{\mathcal{H}}$ then

$$|\psi\rangle = \int \frac{d^3p}{(2\pi\hbar)^3}\, \tilde{\psi}(\vec{p})\, |\vec{p}\rangle$$

and

$$\tilde{\psi}(\vec{p}) = \langle \vec{p}|\psi\rangle .$$

Substituting this above we have

$$|\psi\rangle = \int \frac{d^3p}{(2\pi\hbar)^3}\, |\vec{p}\rangle\langle\vec{p}|\psi\rangle$$

Since $|\psi\rangle$ is arbitrary we must have

$$\mathbb{1} = \int \frac{d^3p}{(2\pi\hbar)^3}\, |\vec{p}\rangle\langle\vec{p}| ,$$

The closure identity expressing in a succinct way the completeness of $\{|\vec{p}\rangle\}$.

As we shall see further, the component of $|\psi\rangle$ in the $\{|\vec{p}\rangle\}$ basis, $\tilde{\psi}(\vec{p})$, are just the momentum space wavefunctions.

In fact we have the inner product given by

$$\langle\psi|\phi\rangle = \langle\psi|\mathbb{1}|\phi\rangle$$

$$= \langle\psi|\left(\int\frac{d^3p}{(2\pi\hbar)^3}|\vec{p}\rangle\langle\vec{p}|\right)|\phi\rangle$$

$$= \int\frac{d^3p}{(2\pi\hbar)^3}\langle\psi|\vec{p}\rangle\langle\vec{p}|\phi\rangle$$

$$= \int\frac{d^3p}{(2\pi\hbar)^3}\tilde{\psi}^*(\vec{p})\tilde{\phi}(\vec{p})$$

and if $\langle\psi|\psi\rangle = 1$, the normalization is

$$1 = \langle\psi|\psi\rangle = \int\frac{d^3p}{(2\pi\hbar)^3}\tilde{\psi}^*(\vec{p})\tilde{\psi}(\vec{p})$$

$$= \int\frac{d^3p}{(2\pi\hbar)^3}|\tilde{\psi}(\vec{p})|^2 .$$

The matrix elements of the momentum operator $\vec{P}$ are, similarly,

$$\langle\psi|\vec{P}|\phi\rangle = \int\frac{d^3p}{(2\pi\hbar)^3}\langle\psi|\vec{P}|\vec{p}\rangle\langle\vec{p}|\phi\rangle$$

but $\vec{P}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle$, so

$$\langle\psi|\vec{P}|\phi\rangle = \int \frac{d^3p}{(2\pi\hbar)^3}\, \vec{p}\, \langle\psi|\vec{p}\rangle\langle\vec{p}|\phi\rangle$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3}\, \tilde{\psi}^*(\vec{p})\, \vec{p}\, \tilde{\phi}(\vec{p}) .$$

Hence the matrix elements of any function of $\vec{P}$ is just the usual momentum space wavefunction (expectation value like) case

$$\langle\psi|F(\vec{P})|\phi\rangle = \int \frac{d^3p}{(2\pi\hbar)^3}\, \tilde{\psi}^*(\vec{p})\, F(\vec{p})\, \tilde{\phi}(\vec{p})$$

Since

$$F(\vec{P})|\vec{p}\rangle = F(\vec{p})|\vec{p}\rangle .$$

Since the normalizable functions of position, $\psi(\vec{r})$, and the normalizable functions of momentum $\tilde{\psi}(\vec{p})$ are related by Fourier transform

$$\psi(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{+\frac{i\vec{p}\cdot\vec{r}}{\hbar}}\, \tilde{\psi}(\vec{p})$$

and

$$\tilde{\psi}(\vec{p}) = \int d^3r\, e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}}\, \psi(\vec{r})$$

we can find the components of the $\{|\vec{p}\rangle\}$ basis in the $\{|\vec{r}\rangle\}$ basis and vice-versa. That is

$$\langle\vec{r}|\psi\rangle = \psi(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} \langle\vec{r}|\vec{p}\rangle\langle\vec{p}|\psi\rangle$$

by completeness of $\{|\vec{p}\rangle\}$, but

$\langle\vec{p}|\psi\rangle = \tilde{\psi}(\vec{p})$ so

$$\langle\vec{r}|\psi\rangle = \psi(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} \langle\vec{r}|\vec{p}\rangle\, \tilde{\psi}(\vec{p}).$$

The Fourier expansion of $\psi(\vec{r})$ is

$$\psi(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{+i\frac{\vec{p}\cdot\vec{r}}{\hbar}}\, \tilde{\psi}(\vec{p})$$

thus we have

$$\boxed{\langle\vec{r}|\vec{p}\rangle = e^{+i\frac{\vec{p}\cdot\vec{r}}{\hbar}}}$$

As we expected the coordinate space wavefunction for the momentum eigenvector is just the plane wave.

Thus

$$|\vec{p}\rangle = \int d^3r \langle \vec{r}|\vec{p}\rangle |\vec{r}\rangle$$

$$= \int d^3r\, e^{i\frac{\vec{p}\cdot\vec{r}}{\hbar}} |\vec{r}\rangle$$

and since

$$\langle \vec{p}|\vec{r}\rangle = \langle \vec{r}|\vec{p}\rangle^*$$

$$= e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}}$$

we have

$$|\vec{r}\rangle = \int \frac{d^3p}{(2\pi\hbar)^3} \langle \vec{p}|\vec{r}\rangle |\vec{p}\rangle$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3} e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}} |\vec{p}\rangle$$

The coordinate space wavefunctions and the momentum space wavefunctions are just Fourier transforms of each other, as stated above.

For $|\psi\rangle \in \mathcal{H}$

$$|\psi\rangle = \int d^3r\, \psi(\vec{r})\, |\vec{r}\rangle$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3}\, \tilde{\psi}(\vec{p})\, |\vec{p}\rangle$$

with

$$\langle \vec{r}|\psi\rangle = \psi(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{+i\frac{\vec{p}\cdot\vec{r}}{\hbar}}\, \tilde{\psi}(\vec{p})$$

and $\langle \vec{p}|\psi\rangle = \tilde{\psi}(\vec{p}) = \int d^3r\, e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}}\, \psi(\vec{r})$

Finally we would like to determine the (infinite-dimensional) matrix representations for $\vec{R}$ and $\vec{P}$, that is the matrix elements of $\vec{R}$ and $\vec{P}$ in the $\{|\vec{r}\rangle\}$ basis and the $\{|\vec{p}\rangle\}$ basis.

We already know that

$$\langle \vec{r} \,|\vec{R}|\, \vec{r}\,'\rangle = \vec{r}\,\langle \vec{r}\,|\,\vec{r}\,'\rangle = \vec{r}\,\delta^3(\vec{r}-\vec{r}\,')$$

$$\langle \vec{p}\,|\vec{P}|\,\vec{p}\,'\rangle = \vec{p}\,\langle \vec{p}\,|\,\vec{p}\,'\rangle = \vec{p}\,(2\pi\hbar)^3\delta^3(\vec{p}-\vec{p}\,')$$

Since $\langle \vec{r}\,|\,\vec{p}\rangle$ is just a plane wave we can find the matrix elements

$$\langle \vec{r}\,|\vec{P}|\,\vec{r}\,'\rangle = \int \frac{d^3p}{(2\pi\hbar)^3}\langle \vec{r}\,|\vec{P}|\,\vec{p}\rangle\langle \vec{p}\,|\,\vec{r}\,'\rangle$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3}\,\vec{p}\,\underbrace{\langle \vec{r}\,|\,\vec{p}\rangle}_{=e^{\frac{i\vec{p}\cdot\vec{r}}{\hbar}}}\underbrace{\langle \vec{p}\,|\,\vec{r}\,'\rangle}_{=e^{-i\frac{\vec{p}\cdot\vec{r}\,'}{\hbar}}}$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3}\,\vec{p}\,e^{+i\vec{p}\cdot(\vec{r}-\vec{r}\,')/\hbar}$$

$$= \frac{\hbar}{i}\int \frac{d^3p}{(2\pi\hbar)^3}\,\vec{\nabla}_{\vec{r}}\,e^{\frac{i}{\hbar}\vec{p}\cdot(\vec{r}-\vec{r}\,')}$$

$$= \frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\,\delta^3(\vec{r}-\vec{r}\,')$$

note $\vec{r}$ is first argument

note this is gradient wrt $\vec{r}$

Thus in the $\{|\vec{r}\rangle\}$ basis the $\vec{P}$ operator has matrix elements

$$\langle\vec{r}|\vec{P}|\vec{r}'\rangle = \frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\,\delta^3(\vec{r}-\vec{r}') .$$

As well consider

$$\langle\vec{p}|\vec{R}|\vec{p}'\rangle = \int d^3r\, \langle\vec{p}|\vec{R}|\vec{r}\rangle\langle\vec{r}|\vec{p}'\rangle$$

$$= \int d^3r\, \vec{r}\, \underbrace{\langle\vec{p}|\vec{r}\rangle}_{=e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}}}\underbrace{\langle\vec{r}|\vec{p}'\rangle}_{=e^{+i\frac{\vec{p}'\cdot\vec{r}}{\hbar}}}$$

$$= \int d^3r\, \vec{r}\, e^{-\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{r}}$$

$$= -\frac{\hbar}{i}\vec{\nabla}_{\vec{p}}\int d^3r\, e^{-\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{r}}$$

$$= -\frac{\hbar}{i}\vec{\nabla}_{\vec{p}}\,(2\pi)^3\delta^3\left(\frac{1}{\hbar}(\vec{p}-\vec{p}')\right)$$

$$= -\frac{\hbar}{i}\vec{\nabla}_{\vec{p}}\,(2\pi\hbar)^3\delta^3(\vec{p}-\vec{p}')$$

note minus sign gradient wrt $\vec{p}$ $\vec{p}$ is first entry.

So in the $\{|\vec{p}\rangle\}$ basis $\vec{R}$ has the matrix elements

$$\langle\vec{p}|\vec{R}|\vec{p}'\rangle = -\frac{\hbar}{i}(2\pi\hbar)^3\vec{\nabla}_{\vec{p}}\,\delta^3(\vec{p}-\vec{p}')$$

So for arbitrary states $|\psi\rangle$, we find that

$$\langle\vec{r}|\vec{R}|\psi\rangle = \int d^3r'\,\langle\vec{r}|R|\vec{r}'\rangle\langle\vec{r}'|\psi\rangle$$

$$= \int d^3r'\,\vec{r}\,\delta^3(\vec{r}-\vec{r}')\langle\vec{r}'|\psi\rangle$$

$$= \vec{r}\langle\vec{r}|\psi\rangle$$

i.e. since $|\psi\rangle$ is arbitrary, $\langle\vec{r}|\vec{R} = \vec{r}\langle\vec{r}|$ so that

$$\langle\vec{r}|F(\vec{R}) = F(\vec{r})\langle\vec{r}| \; .$$

Also

$$\langle\vec{r}|\vec{P}|\psi\rangle = \int d^3r'\,\langle\vec{r}|\vec{P}|\vec{r}'\rangle\langle\vec{r}'|\psi\rangle$$

$$= \int d^3r'\,\frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\,\delta^3(\vec{r}-\vec{r}')\langle\vec{r}'|\psi\rangle$$

$$= \frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\int d^3r'\,\delta^3(\vec{r}-\vec{r}')\langle\vec{r}'|\psi\rangle$$

$$= \frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\langle\vec{r}|\psi\rangle \; .$$

i.e. since $|\psi\rangle$ is arbitrary,

$$\langle \vec{r}|\vec{P} = \frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\langle\vec{r}|,$$

so that

$$\langle\vec{r}|G(\vec{P}) = G\left(\frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\right)\langle\vec{r}|$$

$$\left(\langle\vec{r}|G(\vec{P})|\psi\rangle = G\left(\frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\right)\langle\vec{r}|\psi\rangle = G\left(\frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\right)\psi(\vec{r})\right).$$

Hence $\vec{r}$ represents the operator $\vec{R}$ and $\frac{\hbar}{i}\vec{\nabla}_{\vec{r}}$ represents the operator $\vec{P}$ in the coordinate (representation) basis $\{|\vec{r}\rangle\}$.

We can apply this to the product of $\vec{R}$ and $\vec{P}$ $\left(\vec{R} = X_1\underset{\hat{i}}{\hat{e}_1} + X_2\underset{\hat{j}}{\hat{e}_2} + X_3\underset{\hat{k}}{\hat{e}_3}\right)$

$$\langle\vec{r}|X_iP_j|\psi\rangle$$

$$= x_i\langle\vec{r}|P_j|\psi\rangle$$

$$= x_i\frac{\hbar}{i}\frac{\partial}{\partial x_j}\langle\vec{r}|\psi\rangle$$

On the other hand

$$\langle \vec{r} | P_j X_i | \psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial x_j} \left(\langle \vec{r} | X_i | \psi \rangle \right)$$

$$= \frac{\hbar}{i} \frac{\partial}{\partial x_j} \left(x_i \langle \vec{r} | \psi \rangle \right)$$

$$= \frac{\hbar}{i} \delta_{ij} \langle \vec{r} | \psi \rangle + x_i \frac{\hbar}{i} \frac{\partial}{\partial x_j} \langle \vec{r} | \psi \rangle$$

where $\vec{r} = x_1 \hat{e}_1 + x_2 \hat{e}_2 + x_3 \hat{e}_3$.

Hence

$$\langle \vec{r} | [X_i, P_j] | \psi \rangle = i\hbar \delta_{ij} \langle \vec{r} | \psi \rangle,$$

since $|\psi\rangle$ is arbitrary $\Rightarrow$

$$\langle \vec{r} | [X_i, P_j] = i\hbar \delta_{ij} \langle \vec{r} |,$$

and since $\{ |\vec{r}\rangle \}$ is a basis the operators are equal

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

This is an operator identity, no matter what representation we work in, $\{ |\vec{r}\rangle \}$, $\{ |\vec{p}\rangle \}$ etc., this is valid.

Similarly we find that

$$[X_i, X_j] = 0$$

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

along with $[X_i, P_j] = i\hbar\delta_{ij}$, these form the canonical commutation relations (CCR).

We are now able to recover Wave mechanics from our abstract formulation of quantum mechanics

Consider the Hamiltonian operator given by

$$H \equiv \frac{1}{2m}\vec{P}^2 + V(\vec{R})$$

where $\vec{P}$ and $V(\vec{R})$ are abstract operators in $\mathcal{H}$. But we have that

$$\langle \vec{r}|V(\vec{R}) = V(\vec{r})\langle \vec{r}|$$

while $\langle \vec{r}|\vec{P}^2 = \langle \vec{r}|P_iP_i = \frac{\hbar}{i}\frac{\partial}{\partial x_i}\langle \vec{r}|P_i$

$$= \left(\frac{\hbar}{i}\right)^2 \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_i}\langle\vec{r}|$$

$$= -\hbar^2 \nabla_{\vec{r}}^2 \langle\vec{r}| \quad .$$ Hence

the Hamiltonian operator H is represented in the coordinate basis by

$$\langle\vec{r}|H = \left[-\frac{\hbar^2}{2m}\nabla_{\vec{r}}^2 + V(\vec{r})\right]\langle\vec{r}| ,$$

that is H has matrix elements

$$\langle\vec{r}|H|\vec{r}\,'\rangle = \left[-\frac{\hbar^2}{2m}\nabla_{\vec{r}}^2 + V(\vec{r})\right]\delta^3(\vec{r}-\vec{r}\,').$$

Hence the Schrödinger equation for state $|\psi(t)\rangle$,

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H\,|\psi(t)\rangle ,$$

in the coordinate representation is

$$i\hbar\frac{\partial}{\partial t}\langle\vec{r}|\psi(t)\rangle = \langle\vec{r}|H|\psi(t)\rangle$$

$$= \left(-\frac{\hbar^2}{2m}\nabla_{\vec{r}}^2 + V(\vec{r})\right)\langle\vec{r}|\psi(t)\rangle$$

but the wavefunction $\psi(\vec{r},t) \equiv \langle\vec{r}|\psi(t)\rangle$ so that the

Schrödinger equation of wave mechanics results

$$\boxed{\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) &= \left[-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}} + V(\vec{r})\right]\psi(\vec{r},t) \\ &= H\left(\vec{r},\frac{\hbar}{i}\vec{\nabla}_{\vec{r}}\right)\psi(\vec{r},t). \end{aligned}}$$

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In a similar manner, we can repeat the above procedure in the momentum representation $\{|\vec{p}\rangle\}$. Recalling

$$\langle\vec{p}|\vec{P}|\vec{p}\,'\rangle = (2\pi\hbar)^3\,\vec{p}\,\delta^3(\vec{p}-\vec{p}\,')$$

$$\langle\vec{p}|\vec{R}|\vec{p}\,'\rangle = (2\pi\hbar)^3\left(-\frac{\hbar}{i}\right)\vec{\nabla}_{\vec{p}}\,\delta^3(\vec{p}-\vec{p}\,'),$$

or

$$\langle\vec{p}|G(\vec{P})|\psi\rangle = G(\vec{p})\,\langle\vec{p}|\psi\rangle$$

$$\langle\vec{p}|F(\vec{R})|\psi\rangle = F\left(-\frac{\hbar}{i}\vec{\nabla}_{\vec{p}}\right)\langle\vec{p}|\psi\rangle$$

we find as before

P, X Hermitian

Suppose $[~~X~~ P, X] = -i\hbar$

Consider $U(a) \equiv e^{-i/\hbar \, Pa} = 1 - \frac{i}{\hbar} Pa + \frac{1}{2}\left(\frac{-i}{\hbar}\right)^2 (Pa)^2 + \dots$

$a \in \mathbb{R}$

$$U^\dagger(a) = e^{+\frac{i}{\hbar} Pa} = U^{-1}(a) = U(-a)$$

$$U(a)\,U(b) = U(a+b)$$

Now $[U(a), X] = \left[1 - \frac{i}{\hbar} Pa + \frac{1}{2}\left(\frac{-i}{\hbar}\right)^2 PaPa + \dots, X\right]$

$$= -\frac{i}{\hbar}[Pa, X] + \frac{1}{2}\left(\frac{-i}{\hbar}\right)^2 [PaPa, X] + \dots$$

$$= -a + \frac{1}{2}\left(\frac{-i}{\hbar}\right)^2 \left(Pa[Pa, X] + [Pa, X]Pa\right) + \dots$$

$$= -a - a\left(\frac{-i}{\hbar}\right) Pa + \dots$$

$$= -a\left[1 - \frac{i}{\hbar} Pa + \frac{1}{2}\left(\frac{i}{\hbar}\right)^2 (Pa)^2 + \dots\right]$$

$$= -a\,U(a)$$

So $\boxed{X\,U(a) = U(a)[X + a]}$

1) Spectrum of $\underline{X}$:

$$\underline{X}|x\rangle = x|x\rangle \qquad |x\rangle \neq 0$$

$$\underline{X}\left(U(a)|x\rangle\right) = U(a)\left[(\underline{X}+a)|x\rangle\right]$$

$$= (x+a)\left(U(a)|x\rangle\right)$$

$U(a)|x\rangle \propto |x+a\rangle$. ~~So state~~

$\Rightarrow$ spectrum of $\underline{X}$ is all reals

(Note: If $\mathcal{H}$ is dim N, $\underline{X}$ has only N ev but from above ∞ ev $\Rightarrow [\underline{X},\underline{P}] = i\hbar$ cannot be for operators finite dimen. space)

2) degree of degeneracy

Assume x is not degenerate.

but $x+a$ is 2-fold deg. $|x+a;1\rangle, |x+a;2\rangle$
$\langle x+a;1|x+a;2\rangle = 0$

Note $U(-a)|x+a;1,2\rangle$ has ev $(x+a)-a = x$
~~is~~ & not colinear

$$\langle x+a;1|U^\dagger(-a)U(a)|x+a;2\rangle = \langle x+a;1|x+a;2\rangle = 0.$$

So x is 2-fold deg. — contradiction.
Thus all ev. of X have same degree of degeneracy. Assume non-degen.

3) Eigenvectors
define phase by

$$|x\rangle \equiv U(x)|0\rangle$$

$$U(a)|x\rangle = U(a)U(x)|0\rangle = U(x+a)|0\rangle$$
$$= |x+a\rangle.$$

→ So $\langle x|x'\rangle = \delta(x-x')$

4) $\{|x\rangle\}$ complete since $X = X^\dagger$.

$$|\psi\rangle = \int dx\, \psi(x)|x\rangle$$

$$\langle x'|\psi\rangle = \psi(x')$$

$$\langle x|U(a)|\psi\rangle = \langle x-a|\psi\rangle = \psi(x-a)$$

So $\langle x|U(-\epsilon)|\psi\rangle = \psi(x) + \frac{i}{\hbar}\epsilon\langle x|P|\psi\rangle + \cdots$

$$= \psi(x+\epsilon) = \psi(x) + \epsilon\frac{d}{dx}\psi(x)$$

$$\Rightarrow \langle x|P|\psi\rangle = \frac{\hbar}{i}\frac{d}{dx}\psi(x) = \frac{\hbar}{i}\frac{d}{dx}\langle x|\psi\rangle$$

$$\Rightarrow \boxed{\langle x|P = \frac{\hbar}{i}\frac{d}{dx}\langle x|}$$

c) P

$P|p\rangle = p|p\rangle$

$\langle x|P|p\rangle = p\langle x|p\rangle$

$\parallel$

$\frac{\hbar}{i}\frac{d}{dx}\langle x|p\rangle$

$\Rightarrow \quad \langle x|p\rangle = C\, e^{\frac{i}{\hbar}px}$

our convention $(2\pi\hbar)^{-\frac{1}{2}}$

$$\langle \vec{p} | [X_i, P_j] | \psi \rangle = \left[-\frac{\hbar}{i} \frac{\partial}{\partial p_i}, p_j \right] \langle \vec{p} | \psi \rangle$$
$$= i\hbar \, \delta_{ij} \langle \vec{p} | \psi \rangle$$

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

The Schrödinger equation in the momentum representation, the $\{|\vec{p}\rangle\}$ basis, becomes an integro-differential equation. Now

$$\langle \vec{p} | V(\vec{R}) = V\left(-\frac{\hbar}{i} \vec{\nabla}_{\vec{p}}\right) \langle \vec{p} |$$

$$\langle \vec{p} | \vec{P}^2 = \vec{p}^2 \langle \vec{p} | ,$$

hence the Hamiltonian operator is represented by

$$\langle \vec{p} | H = \left[\frac{\vec{p}^2}{2m} + V(i\hbar \vec{\nabla}_{\vec{p}}) \right] \langle \vec{p} | .$$

In particular its matrix elements are

$$\langle \vec{p} | H | \vec{p}' \rangle = \left[\frac{\vec{p}^2}{2m} + V(i\hbar \vec{\nabla}_{\vec{p}}) \right] \langle \vec{p} | \vec{p}' \rangle$$

$$= \left[\frac{\vec{p}^2}{2m} + V(i\hbar \vec{\nabla}_{\vec{p}}) \right] (2\pi\hbar)^3 \delta^3(\vec{p} - \vec{p}') .$$

As before the Schrödinger equation for state $|\psi(t)\rangle$,

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle,$$

in the momentum representation becomes

$$i\hbar \frac{\partial}{\partial t}\langle\vec{p}|\psi(t)\rangle = \langle\vec{p}|H|\psi(t)\rangle$$

$$= \left[\frac{\vec{p}^{\,2}}{2m} + V(i\hbar\vec{\nabla}_{\vec{p}})\right]\langle\vec{p}|\psi(t)\rangle.$$

It proves more useful to further analyze the potential term. Since $\langle\vec{p}|\psi(t)\rangle = \tilde{\psi}(\vec{p},t)$ is the Fourier transform of $\psi(\vec{r},t)$, we would like to re-express the above in terms of the Fourier transform of $V(\vec{r})$.

Defining the Fourier transform of the potential as

$$\tilde{V}(\vec{p}-\vec{p}\,') \equiv \int d^3r\, e^{-\frac{i}{\hbar}(\vec{p}-\vec{p}\,')\cdot\vec{r}}\, V(\vec{r})$$

(and likewise

$$V(\vec{r}-\vec{r}\,') \equiv \int \frac{d^3p}{(2\pi\hbar)^3}\, e^{+\frac{i}{\hbar}\vec{p}\cdot(\vec{r}-\vec{r}\,')}\, \tilde{V}(\vec{p})\Big)$$

we have that, for arbitrary $|\psi\rangle$,

$$V(i\hbar\vec{\nabla}_{\vec{p}})\langle\vec{p}|\psi\rangle = \langle\vec{p}|V(\vec{R})|\psi\rangle$$

$$= \int d^3r\, \underbrace{\langle\vec{p}|\vec{r}\rangle}_{=e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}}} \underbrace{\langle\vec{r}|V(\vec{R})|\psi\rangle}_{V(\vec{r})\langle\vec{r}|\psi\rangle}$$

$$= \int d^3r\, V(\vec{r})\, e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}}\langle\vec{r}|\psi\rangle$$

$$= \int \frac{d^3p'}{(2\pi\hbar)^3}\int d^3r\, V(\vec{r})\, e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}} \underbrace{\langle\vec{r}|\vec{p}\,'\rangle}_{=e^{+\frac{i}{\hbar}\vec{p}\,'\cdot\vec{r}}}\langle\vec{p}\,'|\psi\rangle$$

$$= \int \frac{d^3p'}{(2\pi\hbar)^3} \underbrace{\left[\int d^3r\, e^{-\frac{i}{\hbar}(\vec{p}-\vec{p}\,')\cdot\vec{r}}\, V(\vec{r})\right]}_{=\tilde{V}(\vec{p}-\vec{p}\,')} \langle\vec{p}\,'|\psi\rangle$$

$$= \int \frac{d^3p'}{(2\pi\hbar)^3}\, \tilde{V}(\vec{p}-\vec{p}\,')\,\langle\vec{p}\,'|\psi\rangle.$$

So

$$\boxed{\begin{aligned}\langle\vec{p}|V(\vec{R})|\psi\rangle &= V(i\hbar\vec{\nabla}_{\vec{p}})\langle\vec{p}|\psi\rangle \\ &= \int\frac{d^3p'}{(2\pi\hbar)^3}\tilde{V}(\vec{p}-\vec{p}\,')\langle\vec{p}\,'|\psi\rangle.\end{aligned}}$$

With $\langle\vec{p}|\psi(t)\rangle = \tilde{\psi}(\vec{p},t)$, the Schrödinger equation becomes an integro-differential equation in the momentum, $\{|\vec{p}\rangle\}$, eigenstate basis

$$\boxed{\begin{aligned}i\hbar\frac{\partial}{\partial t}\tilde{\psi}(\vec{p},t) &= \frac{\vec{p}^{\,2}}{2m}\tilde{\psi}(\vec{p},t) \\ &\quad + \int\frac{d^3p'}{(2\pi\hbar)^3}\tilde{V}(\vec{p}-\vec{p}\,')\tilde{\psi}(\vec{p}\,',t)\end{aligned}}$$

Finally, before studying the consequences of the postulates systematically let's just point out that for the above Hamiltonian operator

$$H = \frac{1}{2m}\vec{P}^2 + V(\vec{R}), \quad H\text{ is}$$

independent of time and we have that

$$|\psi(t)\rangle = e^{-iH(t-t_0)/\hbar}\,|\psi(t_0)\rangle ,$$

for finite time intervals.

More to the point, $H = H^\dagger$ and its set of eigenstates $\{|n\rangle\}$ forms a basis in $\mathcal{H}$

$$H|n\rangle = E_n|n\rangle$$

with $\{|n\rangle\}$ orthonormal

$$\langle m|n\rangle = \delta_{mn}$$

and complete

$$\sum_n{}' |n\rangle\langle n| = \mathbb{1} .$$

In this energy (representation) basis an arbitrary state $|\psi\rangle$ has the expansion

$$|\psi\rangle = \sum_n{}' \psi_n |n\rangle$$

with

$$\psi_n = \langle n|\psi\rangle$$

In particular

$$|\psi(t)\rangle = \sum_n \psi_n(t)|n\rangle ,$$

$$\psi_n(t) - \langle n|\psi(t)\rangle$$

and the Schrödinger equation becomes in the energy representation

$$i\hbar\frac{\partial}{\partial t}\psi_n(t) = E_n\,\psi_n(t)$$

thus

$$\psi_n(t) = e^{-\frac{i}{\hbar}E_n(t-t_0)}\,\psi_n(t_0).$$

That's

$\langle n|H = E_n\langle n|$ in the energy basis.

As we did for Wave Mechanics, we can investigate the consequences of the postulates and hence shed light on their physical content.

4.5) Consequences and Physical Interpretation of the Postulates