substituting $\lambda_{min} = \frac{\hbar}{2(\Delta p)^2}$, this becomes

$$\left(x - \langle x\rangle + \frac{i\hbar}{2(\Delta p)^2}\left(-i\hbar\frac{\partial}{\partial x} - \langle p\rangle\right)\right)\psi(x,t) = 0 .$$

This differential equation has the instantaneous solution

$$\psi(x,t) = A_t e^{\frac{i}{\hbar}\langle p\rangle x}\, e^{-\frac{(x-\langle x\rangle)^2}{\hbar^2/(\Delta p)^2}}$$

with A_t a constant in x. This is just a Gaussian wavefunction as in our earlier example. Hence the Gaussian wave packet has the least RMS deviation in position and momentum possible.

1.3.7. Stationary States

Consider the case of time independent potentials $V = V(\vec{r})$. The Schrödinger equation has the form

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

and we try a solution that separates the time and space variables of the form

$$\psi(\vec{r},t) = \psi(\vec{r})e^{-i\omega t} .$$

The Schrödinger equation becomes

$$\hbar\omega\,\psi(\vec{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}),$$

the time independent Schrödinger equation. By the Planck-Einstein relation $E=\hbar\omega$ is the energy of the particle. The wavefunction of $\psi(\vec{r},t) = \psi(\vec{r})e^{-iEt/\hbar}$ is called a stationary state solution to the Schrödinger equation since the probability density $|\psi(\vec{r},t)|^2 = |\psi(\vec{r})|^2$ is independent of time, that is stationary.

The time independent Schrödinger equation is written as

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

where $H \equiv -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$ is the Hamiltonian (energy) operator. This is nothing but an eigenvalue equation for the Hamiltonian operator. The eigenfunctions $\psi(\vec{r})$ of H give the stationary state with energy eigenvalue E, the allowed ~~energies~~ energies of the system. This spectrum of

H can be continuous, discrete (quantized) or both. Let n label the eigenvalues, E_n, and eigenfunctions, $\psi_n(\vec{r})$, of H (n may be continuous or discrete). The time independent Schrödinger equation becomes for each n

$$H\,\psi_n(\vec{r}) = E_n\,\psi_n(\vec{r}).$$

Since H is a Hermitian operator, by postulate 3 the eigenfunctions of $\{\psi_n(\vec{r})\}$ form a complete set. That is any wavefunction may be expanded in terms of them. Since

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

is a solution to the time dependent Schrödinger equation we have that any wavefunction $\psi(\vec{r},t)$ is given by

$$\psi(\vec{r},t) = \sum_n{}' C_n \psi_n(\vec{r})\, e^{-i\frac{E_n t}{\hbar}}$$

(That at any time

$$\psi(\vec{r},t) = \sum_n{}' C_n(t)\, \psi_n(\vec{r}).$$

Schrödinger's eq. $i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H\,\psi(\vec{r},t)$

implies ($t=0$, $c_n(0) \equiv c_n$)

$$c_n(t) = c_n e^{-i\frac{E_n t}{\hbar}}$$

since, as we will see the ψ_n are orthogonal.)

In order to invert this expansion we need some further properties of E_n and $\psi_n(\vec{r})$

Since $H\psi_n = E_n \psi_n$ we have

$$(H\psi_n)^* = E_n^* \psi_n^* \text{; thus we find}$$

$$\int d^3r \left[\psi_m^*(H\psi_n) - (H\psi_m)^*\psi_n\right]$$

$$= \left(E_n - E_m^*\right)\int d^3r\, \psi_m^* \psi_n .$$

But $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$ is a Hermitian operator, hence the LHS vanishes yielding

$$0 = \left(E_n - E_m^*\right)\int d^3r\, \psi_m^* \psi_n$$

If $m=n$, we find $E_n = E_n^*$ since $\int d^3r\, |\psi_n|^2 > 0$. Thus the energy eigenvalues are real.

If $m \neq n$, we find $\int d^3r\, \psi_m^* \psi_n = 0$, the stationary state eigenfunctions are orthogonal. Since we are free to normalize ψ_n as desired, we choose

$$\int d^3r\, |\psi_n|^2 = 1,$$

hence

$$\int d^3r\, \psi_m^* \psi_n = \delta_{mn},$$

the energy eigenfunctions are orthonormal.

Accordingly we can use the orthogonality of the eigenfunctions to invert the energy eigenfunction expansion of $\psi(\vec{r},t)$,

$$\psi(\vec{r},t) = \sum_n c_n \psi_n(\vec{r}) e^{-i\frac{E_n t}{\hbar}},$$

thus

$$\psi(\vec{r},0) = \sum_n c_n \psi_n(\vec{r}).$$

Multiplying by $\psi_m^*(\vec{r})$ and integrating of $\vec{r}$ yields

$$\int d^3r\, \psi_m^*(\vec{r})\psi(\vec{r},0) = \sum_n c_n \overbrace{\int d^3r\, \psi_m^*(\vec{r})\psi_n(\vec{r})}^{=\delta_{mn}}.$$

Thus $\boxed{C_m = \int d^3r\, \psi_m^*(\vec{r})\psi(\vec{r},0)}$.

By substituting this expression for the coefficient back into the expansion for $\psi(\vec{r},0)$ we obtain

$$\psi(\vec{r},0) = \sum_n{}' C_n \psi_n(\vec{r})$$

$$= \int d^3r' \Big(\sum_n{}' \psi_n^*(\vec{r}\,')\psi_n(\vec{r})\Big)\psi(\vec{r}\,',0)$$

This implies that

$$\boxed{\sum_n{}' \psi_n^*(\vec{r}\,')\psi_n(\vec{r}) = \delta^3(\vec{r}-\vec{r}\,')},$$

the completeness or closure relation.

Thus if the set of (energy) eigenfunctions are complete they obey the closure relation

$$\sum_n{}' \psi_n^*(\vec{r}\,')\psi_n(\vec{r}) = \delta^3(\vec{r}-\vec{r}\,'),$$

and visa versa.

By the Postulate 3, measuring the energy of the particle results in one of the eigenvalues E_n with the probability

$$P_n = |c_n e^{-i\frac{E_n t}{\hbar}}|^2 = |c_n|^2.$$

This probability is independent of time, another property of stationary states. Further for a wavefunction normalized to one we find

$$1 = \int d^3r\, \psi^*(\vec{r},t)\psi(\vec{r},t)$$

$$= \sum_{m,n}' c_m^* c_n e^{-i\frac{(E_n - E_m)t}{\hbar}} \underbrace{\int d^3r\, \psi_m^*(\vec{r})\psi_n(\vec{r})}_{=\delta_{mn}}$$

$$= \sum_n' c_n^* c_n .$$

Thus $\sum_n' |c_n|^2 = 1 = \sum_n' P_n$, consistent with $|c_n|^2$ being a probability. As well consider the expectation value of the energy in a state normalized to unity

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

but the Schrödinger equation implies $H\psi = i\hbar \frac{\partial}{\partial t}\psi$. Hence

$$\langle H \rangle = \int d^3r \sum_{m,n}' C_m^* \psi_m^*(\vec{r})\, e^{+i\frac{E_m t}{\hbar}} \times$$

$$\times\, i\hbar \frac{\partial}{\partial t}\left[C_n \psi_n(\vec{r})\, e^{-i\frac{E_n t}{\hbar}} \right]$$

$$= \sum_{m,n}' E_n C_m^* C_n\, e^{-i\frac{(E_n - E_m)t}{\hbar}} \times$$

$$\times \underbrace{\int d^3r\, \psi_m^*(\vec{r})\, \psi_n(\vec{r})}_{=\delta_{mn}}\,.$$

So

$$\boxed{\langle H \rangle = \sum_n' E_n |C_n|^2}\,,$$

again this leads to the interpretation that $|C_n|^2$ is the probability of measuring energy E_n in state $\psi(\vec{r},t)$. Thus E_n times its probability of being measured yields the average energy of the state.

Besides the eigenfunctions of the Hamiltonian we have considered the eigenfunctions of the Hermitian momentum operator $\vec{P}$. These were the plane waves

$$\varphi_{\vec{k}}(\vec{r}) = A\, e^{i\vec{k}\cdot\vec{r}}, \quad \text{where}$$

$$\vec{P}\,\varphi_{\vec{k}}(\vec{r}) = \hbar\vec{k}\,\varphi_{\vec{k}}(\vec{r}) \quad \text{and} \quad \vec{k}\in\mathbb{R}^3 .$$

These eigenfunctions are labelled by the continuum eigenvalues $\vec{k}$. Hence the Kronecker delta orthonormality relation will be replaced by the Dirac δ-function continuum normalization

$$\int d^3r\, \varphi^*_{\vec{k}'}(\vec{r})\,\varphi_{\vec{k}}(\vec{r})$$

$$= \int d^3r\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}\,|A|^2$$

$$= |A|^2 (2\pi)^3\,\delta^3(\vec{k}-\vec{k}') .$$

Conventionally we choose $A=1$

So $\varphi_{\vec{k}}(\vec{r}) \equiv e^{i\vec{k}\cdot\vec{r}}$ with normalization $\int d^3r\,\varphi^*_{\vec{k}'}(\vec{r})\,\varphi_{\vec{k}}(\vec{r}) = (2\pi)^3\delta^3(\vec{k}-\vec{k}')$

As well any wavefunction can be expanded in terms of the momentum eigenfunctions hence they obey the closure relation

$$\int \frac{d^3k}{(2\pi)^3} \varphi^*_{\vec{k}}(\vec{r}')\varphi_{\vec{k}}(\vec{r})$$

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

The $\{\varphi_{\vec{k}}(\vec{r})\}$ are complete, thus

$$\psi(\vec{r},t) = \int \frac{d^3k}{(2\pi)^3} g(\vec{k},t)\,\varphi_{\vec{k}}(\vec{r})$$

with

$$g(\vec{k},t) = \int d^3r\, \varphi^*_{\vec{k}}(\vec{r})\psi(\vec{r},t).$$

Besides energy and momentum eigenfunctions, position eigenfunctions are often a useful complete set of functions to use. The position operator is just multiplication by $\vec{r}$, clearly a Hermitian operator. The eigenfunctions are defined by

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

with their eigenvalue $\vec{r}_0$ labelling them. Since the Dirac delta function $\delta^3(\vec{r}-\vec{r}_0)$ sets $\vec{r}$ equal to $\vec{r}_0$ we have

$$\psi_{\vec{r}_0}(\vec{r}) = \delta^3(\vec{r}-\vec{r}_0), \quad \text{and}$$

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

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

These position eigenfunctions are orthonormal (in the continuum sense)

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

$$= \delta^3(\vec{r}_0-\vec{r}_0')$$

and are complete

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

$$= \delta^3(\vec{r}-\vec{r}').$$

Any wave function has the expansion

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

In general we see that it is not always possible to find normalizable (Kronecker) eigenfunctions of some Hermitian operator $A(\vec{r}, -i\hbar\vec{\nabla})$,

$$A\psi_a(\vec{r}) = a\psi_a(\vec{r}).$$ However, one can try to find a sequence of functions $\psi_N(\vec{r})$ that are normalizable such that for all N, $\int d^3r\, |\psi_N|^2 = 1$ and

$$\int d^3r \left| (A-a)\psi_N(\vec{r}) \right|^2 \to 0 \quad \text{as } N \to \infty .$$

Examples:

1) Consider one-dimensional position eigenstates, a sequence of normalizable functions approximating the Dirac delta function is

$$\psi^N_{x_0}(x) = \begin{cases} N & \text{if } |x-x_0| < \frac{1}{2N} \\ 0 & \text{if } |x-x_0| > \frac{1}{2N} \end{cases}.$$

We have that

$$\int_{-\infty}^{+\infty} dx \left| (x-x_0)\psi^N_{x_0}(x) \right|^2 = N^2 \int_{x_0-\frac{1}{2N}}^{x_0+\frac{1}{2N}} |x-x_0|^2 dx$$

$$= \frac{N^2}{3}(x-x_0)^3 \Big|_{x_0-\frac{1}{2N}}^{x_0+\frac{1}{2N}} = \frac{N^2}{3}\left(\frac{1}{8N^3} + \frac{1}{8N^3}\right) = \frac{1}{12N} \to 0 \quad \text{as } N \to \infty$$

At the same time $\int_{-\infty}^{+\infty} dx\, |\psi^N_{x_0}(x)|^2 = N$, for each N, $\psi^N_{x_0}(x)$ is normalizable. And as usual we see that in the distributional sense $\psi^N_{x_0}$ approaches a Dirac delta function as $N\to\infty$,

$$\lim_{N\to\infty} \int_{-\infty}^{+\infty} dx\, \psi^N_{x_0}(x)\,\psi(x) = \lim_{N\to\infty} N \int_{x_0-\frac{1}{2N}}^{x_0+\frac{1}{2N}} \psi(x)\,dx$$

$$= \lim_{N\to\infty} N \int_{-\frac{1}{2N}}^{+\frac{1}{2N}} \psi(y+x_0)\,dy \qquad (\text{let } x = y+x_0)$$

Now Taylor expand about x_0

$$= \lim_{N\to\infty} N \int_{-\frac{1}{2N}}^{+\frac{1}{2N}} \left[\psi(x_0) + y\,\psi'(x_0) + \cdots\right] dy$$

$$= \lim_{N\to\infty} N \left\{ \psi(x_0)\left(\frac{1}{2N}+\frac{1}{2N}\right) + \sum_{n=1}^{\infty} \psi^{(n)}(x_0) \left.\frac{y^{n+1}}{(n+1)!}\right|_{-\frac{1}{2N}}^{+\frac{1}{2N}} \right\}$$

$$= \psi(x_0) + \lim_{N\to\infty} \sum_{n=1}^{\infty} \psi^{(n)}(x_0) \frac{N\left(\frac{1}{2N}\right)^{n+1}\left(1+(-1)^n\right)}{(n+1)!}$$

$$= \psi(x_0).$$

Thus $\psi^N_{x_0}(x) \xrightarrow{N\to\infty} \psi_{x_0}(x) \doteq \delta(x-x_0)$

in the sense of distributions.

2) Similarly for momentum eigenstates, with momentum eigenvalue k_0

$$\psi_N^{k_0}(x) = \int_{-\infty}^{+\infty} g_N(k)\, e^{ikx}\, dk$$

$$g_N(k) = \begin{cases} N & \text{if } |k-k_0| < \frac{1}{2N} \\ 0 & \text{if } |k-k_0| > \frac{1}{2N} \end{cases}$$

$$\left[-i\hbar\frac{\partial}{\partial x} - \hbar k_0\right]\psi_N^{k_0}(x) = \int_{-\infty}^{+\infty} [\hbar k - \hbar k_0] \times$$
$$\times g_N(k)\, e^{+ikx}\, dk.$$

So $\displaystyle\int_{-\infty}^{+\infty} dx \left| \left(-i\hbar\frac{\partial}{\partial x} - \hbar k_0\right)\psi_N^{k_0}(x)\right|^2$

$$= 2\pi \int_{-\infty}^{+\infty} \left|(\hbar k - \hbar k_0)\, g_N(k)\right|^2 dk = \frac{\hbar^2 2\pi}{12N} \longrightarrow 0 \text{ as } N \to \infty.$$

Similarly $\quad g_N(k) \xrightarrow{N\to\infty} \delta(k-k_0)$

so that $\quad \psi_N^{k_0}(x) \xrightarrow{N\to\infty} e^{ik_0x}$

as desired.

Of course all this is as cumbersome

as wavepackets or using box normalization, since we understand the nature of these continuum normalized eigenfunctions we will, with appropriate care, use them directly.

1.3.8. Boundary Conditions on the Wavefunction

By Postulate 2, the probability density $\rho = |\psi(\vec{r},t)|^2$ is observable, hence it must be everywhere finite and continuous. $|\psi|^2$ is finite if and only if the wavefunction $\psi(\vec{r},t)$ is finite everywhere. Further it is a sufficient condition for $|\psi|^2$ to be continuous that $\psi(\vec{r},t)$ is continuous. Using the principle of superposition it can also be shown to be necessary. Assume ψ_1 is continuous and, by superposition, that $\psi = \psi_1 + \lambda\psi_2$ is a solution to the Schrödinger equation with ψ_1, ψ_2 solutions and $\lambda \in \mathbb{C}$. We can show that ψ_2 is continuous by considering

$|\psi_1|^2$, $|\psi_2|^2$ and $|\psi|^2 = |\psi_1 + \lambda\psi_2|^2$,

all of which are continuous. Since $|\psi|^2 = |\psi_1|^2 + |\lambda|^2|\psi_2|^2 + \lambda\psi_1^*\psi_2 + \lambda^*\psi_1\psi_2^*$ we have that

$$\lambda\psi_1^*\psi_2 + \lambda^*\psi_1\psi_2^* \text{ is continuous.}$$