

Of course the wave-function is no longer normalizable $\int_{-\infty}^{+\infty} dx |\psi(x,t)|^2 = \frac{|A|^2}{\sqrt{8\pi}a} = a\sqrt{2\pi} \xrightarrow{a \rightarrow \infty} \infty$

as expected. However the ^{relevant} observables will be finite in this limit since this normalization factor is cancelled from numerator and denominator, as in the calculation of energy, say, before the limit $a \rightarrow \infty$ is taken.

1.3.3. Expectation Values

Since $|\psi(\vec{r},t)|^2$ is the position probability density (let $\int d^3r |\psi(\vec{r},t)|^2 = 1$ for simplicity) the expectation value of any function, $f(\vec{r})$, of position is given by

$$\langle f \rangle \equiv \int d^3r f(\vec{r}) |\psi(\vec{r},t)|^2.$$

Further, any square-integrable wave function (even for $V \neq 0$) can be Fourier expanded

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

Since $\psi(\vec{r}, t)$ is normalized to one, we have

$$1 = \int d^3r |\psi(\vec{r}, t)|^2 = \int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} g^*(\vec{k}', t) g(\vec{k}, t) \int d^3r e^{i(\vec{k}-\vec{k}') \cdot \vec{r}}$$

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

hence

$$1 = \frac{1}{(2\pi)^3} \int d^3k \int d^3k' g^*(\vec{k}', t) g(\vec{k}, t) \delta^3(\vec{k}-\vec{k}')$$

\Rightarrow

$$\boxed{1 = \int \frac{d^3k}{(2\pi)^3} |g(\vec{k}, t)|^2}$$

This is known as Parseval's Theorem

$$\int d^3r |\psi(\vec{r}, t)|^2 = \int \frac{d^3k}{(2\pi)^3} |g(\vec{k}, t)|^2 = 1.$$

Since $|g(\vec{k}, t)|^2$ integrates to 1, like a probability density, we interpret $g(\vec{k}, t)$ to be the momentum space wavefunction of the particle and that the momentum probability density is

$$dP(\vec{k}, t) = |g(\vec{k}, t)|^2 \frac{d^3k}{(2\pi)^3}$$

That is, $dP(\vec{k}, t)$ is the probability that a particle at time t has momentum differentially close to $\hbar\vec{k}$.

This interpretation also follows from Postulate 3: the principle of spectral decomposition applied to the momentum operator

$$\vec{P} = -i\hbar\vec{\nabla}.$$

Recall the postulate states that we can expand any wavefunction in terms of the eigenfunctions of a Hermitian operator. Indeed \vec{P} is Hermitian, for ψ_1, ψ_2 normalizable wavefunctions

$$\begin{aligned} & \int d^3r [\vec{P}\psi_1(\vec{r}, t)]^* \psi_2(\vec{r}, t) \\ &= \int d^3r [-i\hbar\vec{\nabla}\psi_1]^* \psi_2 \\ &= \int d^3r (+i\hbar) (\vec{\nabla}(\psi_1^* \psi_2) - \psi_1^* \vec{\nabla}\psi_2) \\ &= i\hbar \int d^3r \vec{\nabla}(\psi_1^* \psi_2) \\ &\quad + \int d^3r \psi_1^* (-i\hbar\vec{\nabla}\psi_2) \end{aligned}$$

but $\psi_1, \psi_2 \rightarrow 0$ as $r \rightarrow \infty$ sufficiently fast

so that

$$\int d^3r \vec{\nabla} (\psi_1^* \psi_2) = \int_{S \rightarrow \infty} d\vec{S} (\psi_1^* \psi_2) = 0$$

hence \vec{P} is Hermitian

$$\begin{aligned} \int d^3r [\vec{P} \psi_1(\vec{r}, t)]^* \psi_2(\vec{r}, t) \\ = \int d^3r \psi_1^*(\vec{r}, t) [\vec{P} \psi_2(\vec{r}, t)] \end{aligned}$$

As we have shown, the eigenfunctions of momentum are plane waves

$$\psi_{\vec{k}}(\vec{r}) = A e^{i\vec{k} \cdot \vec{r}}$$

with A a constant and $\vec{k} \in \mathbb{R}^3$, so that

$$\begin{aligned} \vec{P} \psi_{\vec{k}}(\vec{r}) &= -i\hbar \vec{\nabla} \psi_{\vec{k}}(\vec{r}) \\ &= (\hbar \vec{k}) \psi_{\vec{k}}(\vec{r}) \end{aligned}$$

According to Postulate 3, any wavefunction can be expanded in terms of $\psi_{\vec{k}}(\vec{r})$

$$\begin{aligned} \psi(\vec{r}, t) &= \int \frac{d^3k}{(2\pi)^3} g(\vec{k}, t) \psi_{\vec{k}}(\vec{r}) \\ &= \int \frac{d^3k}{(2\pi)^3} g(\vec{k}, t) e^{i\vec{k} \cdot \vec{r}} \quad (\text{let } Ag \rightarrow g) \end{aligned}$$

Further the postulate interprets the coefficients in the expansion as probability amplitudes. That is the probability for observing the momentum of the particle at time t to be in the interval $\hbar^3 d^3k$ about $\hbar\vec{k}$ is

$$dP(\vec{k}, t) = |g(\vec{k}, t)|^2 \frac{d^3k}{(2\pi)^3}$$

Hence the expectation value of any function of momentum $\vec{p} = \hbar\vec{k}$, $f(\vec{p})$, is

$$\langle f \rangle = \int \frac{d^3k}{(2\pi)^3} f(\hbar\vec{k}) |g(\vec{k}, t)|^2$$

For example $\langle \vec{p} \rangle = \int \frac{d^3k}{(2\pi)^3} \hbar\vec{k} |g(\vec{k}, t)|^2$.

The Fourier transform of ψ can be inverted to obtain

$$g(\vec{k}, t) = \int d^3r e^{-i\vec{k}\cdot\vec{r}} \psi(\vec{r}, t)$$

This can be used to re-express expectation values of the momentum,

-47-

$$\begin{aligned}\langle f \rangle &= \int \frac{d^3k}{(2\pi)^3} f(\hbar\vec{k}) |g(\vec{k}, t)|^2 \\ &= \int \frac{d^3k}{(2\pi)^3} f(\hbar\vec{k}) \underbrace{\int d^3r e^{+i\vec{k}\cdot\vec{r}} \psi^*(\vec{r}, t) \times \int d^3r' e^{-i\vec{k}\cdot\vec{r}'} \psi(\vec{r}', t)}_{= g(\vec{k}, t)}\end{aligned}$$

$$= \int d^3r d^3r' \psi^*(\vec{r}, t) \times$$

$$\times \underbrace{\int \frac{d^3k}{(2\pi)^3} f(\hbar\vec{\nabla}) e^{+i\vec{k}\cdot(\vec{r}-\vec{r}')} \psi(\vec{r}', t)}_{= f(\hbar\vec{k})}$$

$$= \int d^3r d^3r' \psi^*(\vec{r}, t) f(\hbar\vec{\nabla}) \delta^3(\vec{r}-\vec{r}') \psi(\vec{r}', t)$$

$$\begin{aligned}\langle f \rangle &= \int d^3r \psi^*(\vec{r}, t) f(\hbar\vec{\nabla}) \psi(\vec{r}, t) \\ &= \int \frac{d^3k}{(2\pi)^3} f(\hbar\vec{k}) |g(\vec{k}, t)|^2\end{aligned}$$

As expected in coordinate space the momentum is represented by the gradient operator $\vec{p} = -i\hbar\vec{\nabla}$.

-48-

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

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

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 \vec{p} 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

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