I. B) Consequences and Physical Interpretation:

1) Continuity Equation and Conservation of Probability:

$$\rho(\vec{r},t) \equiv |\psi(\vec{r},t)|^2 = \text{position probability density}$$

Observing particle somewhere in space must be constant in time (stable particle)

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

Then take complex conjugate of the equation

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V^*\psi^*$$

Hence

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t}|\psi|^2 = \psi^*\frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi$$

$$= \frac{1}{i\hbar}\Big[\psi^*\left(-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right) - \left(\frac{-\hbar^2}{2m}\nabla^2\psi^* + V^*\psi^*\right)\psi\Big]$$

$$= -\frac{\hbar}{2im}\vec{\nabla}\cdot\left(\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi\right) + \frac{1}{i\hbar}\psi^*\psi\,(V^* - V)$$

= B 1) $V = V^*$ since the potential energy V is real. ($\mathrm{Im}\, V \neq 0$ for unstable particles, since they decay, probability will change in time).

Define probability current density:

$$\vec{J}(\vec{r},t) \equiv \frac{\hbar}{2im}\left[\psi^* \vec{\nabla}\psi - (\vec{\nabla}\psi^*)\,\psi\right]$$

$$= \frac{1}{m}\,\mathrm{Re}\left[\psi^* \frac{\hbar}{i}\vec{\nabla}\psi\right]$$

Hence $\boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0}$ The Continuity Equation

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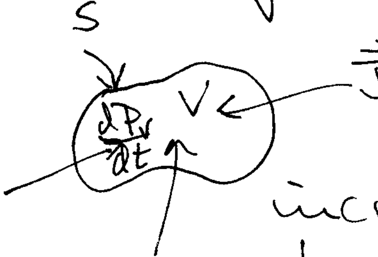
Integrate the continuity equation over volume V with boundary S

$$\int_V d^3r \,\frac{\partial}{\partial t}|\psi|^2 = -\int_V d^3r\, \vec{\nabla}\cdot\vec{J}$$

$$\overset{\text{by Gauss' Theorem}}{=} -\oint_S d\vec{S}\cdot\vec{J}$$

$\Rightarrow$ B) Thus

$$\frac{d}{dt}\overbrace{\int_V d^3r\,|\psi|^2}^{\text{Probability particle is in } V = P_V} = -\oint_S d\vec{S}\cdot\vec{J}$$



Thus if probability the particle is found in V increases $\Rightarrow$ probability must be flowing into the volume V

Hence $-\oint_S d\vec{S}\cdot\vec{J}$ is the rate of change of P_V. This means $\vec{J}$ is the probability current density.

This suggests the interpretation of $\frac{\hbar}{i}\vec{\nabla}$ as momentum since

$\rho = \psi^*\psi$ is the probability density then

the current density should be $\vec{J} =$ "$\rho\vec{v}$"
from our classical physics courses $=$ "$\rho\frac{\vec{P}}{m}$"

And we have

$$\vec{J} = \frac{\hbar}{2im}\left[\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi)^*\psi\right]$$

$$= \frac{1}{m}\,\mathrm{Re}\left[\psi^*\frac{\hbar}{i}\vec{\nabla}\psi\right]$$

which suggests that $\vec{P} = \frac{\hbar}{i}\vec{\nabla}$ and

$\frac{\vec{P}}{m} = \vec{V}$ is the velocity operator

∴B 1) Finally for $S \to \infty$ we have that $\psi \to 0$ sufficiently fast for the RHS above to vanish

$$\boxed{\frac{d}{dt}\int_{\substack{\text{all}\\\text{space}}} d^3r\, |\psi(\vec{r},t)|^2 = 0}$$

The probability of finding the particle somewhere in space is constant in time.

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2) Free Particle Wave Functions:

$V = 0$ (or constant)

(Suppose $V = v$ = constant; Let $\Psi(\vec{r},t) = e^{i\omega t}\psi(\vec{r},t)$

Schrödinger Eq:

$$i\hbar\frac{\partial \Psi}{\partial t} = \frac{\vec{p}^{\,2}}{2m}\Psi + v\Psi$$

but $\frac{\partial \Psi}{\partial t} = i\omega\Psi + e^{i\omega t}\frac{\partial}{\partial t}\psi(\vec{r},t)$

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

Let $\boxed{-\hbar\omega \equiv v}$ $\Rightarrow$

IB 2) $\Psi(\vec{r},t) = e^{\overbrace{-\frac{i}{\hbar}vt}^{\text{overall phase}}} \psi(\vec{r},t)$ and

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi(\vec{r},t)$$ V=0

Hence $V = v$ is equivalent to a free particle state. So $V=0$,

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2 \psi(\vec{r},t)$$

The plane wave solutions are

$$\psi_{\vec{k}}(\vec{r},t) = \frac{1}{N} e^{i(\vec{k}\cdot\vec{r} - \omega t)}$$

with N a normalization constant and plugging into Sch. eq.

$$i\hbar\frac{\partial}{\partial t}\psi = \hbar\omega\psi = -\frac{\hbar^2}{2m}\nabla^2\psi = \frac{\hbar^2 k^2}{2m}\psi$$

$$\Rightarrow \boxed{\hbar\omega = \frac{\hbar^2 k^2}{2m}}$$ and $\vec{k}$ is

Recall $\vec{k} = k\hat{n}$
k = wavenumber
$\hat{n}$ = direction of propagation of plane wave

unrestricted, it takes on a 3-fold continuum of values. Now Planck-Einstein relation told us the energy was $E = \hbar\omega$ for this monochromatic particle. While deBroglie gave us $\vec{p} = \hbar\vec{k}$. Thus

$$E = \frac{\vec{p}^{\,2}}{2m}$$ as required for a free particle of mass m!

I B 2) In addition we note that $\psi_{\vec{k}}(\vec{r},t)$ is the eigenfunction of momentum

$$\vec{p}\,\psi_{\vec{k}}(\vec{r},t) = \frac{\hbar}{i}\vec{\nabla}\,\psi_{\vec{k}}(\vec{r},t)$$

$$= \hbar\vec{k}\,\psi_{\vec{k}}(\vec{r},t)$$

with eigenvalue $\vec{p} = \hbar\vec{k}$.

Further ψ has probability amplitude

$$|\psi_{\vec{k}}|^2 = \frac{1}{|N|^2} = \text{constant, uniform}$$

position probability density everywhere in space! The particle is completely unlocalized — it has the same prob. to be anywhere. So the plane wave is <u>not</u> square-integrable (<u>not</u> normalizable)

$$\int_{\substack{\text{all}\\\text{space}}} d^3r\,|\psi_{\vec{k}}|^2 = \frac{1}{|N|^2}\int_{\substack{\text{all}\\\text{space}}} d^3r = \frac{1}{|N|^2}V_{\substack{\text{all}\\\text{space}}} = \infty$$

Therefore the plane wave <u>cannot</u> correspond to a physically realizable state of the particle. Insert p. -24'-

Of course if we are in a lab we don't expect to worry about our particles being on the moon — so we can think of space as cutoff at the walls of the

Although not of finite norm, the plane waves are orthogonal in the sense that

$$\int d^3r\, \psi^*_{\vec{k}'}(\vec{r},t)\, \psi_{\vec{k}}(\vec{r},t)$$

$$= \frac{1}{N^2} \underbrace{\int d^3r\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}}_{=(2\pi)^3\delta^3(\vec{k}-\vec{k}')} \underbrace{e^{-i\frac{\hbar}{2m}(\vec{k}^2-\vec{k}'^2)t}}_{=e^0=1}$$

when times a δ-function

$$= \frac{1}{N^2}(2\pi)^3\delta^3(\vec{k}-\vec{k}')$$

For convenience we may choose $N=1$ so that

$$\boxed{\int d^3r\, \psi^*_{\vec{k}'}(\vec{r},t)\, \psi_{\vec{k}}(\vec{r},t) = \delta^3(\vec{k}-\vec{k}')(2\pi)^3}$$

This is called "continuum normalization".

IB2) lab (∞'ly high potential) and the particle confined to the compact Volume of the lab — then all the integrals are finite ($\sim V_{lab} < \infty$) and the plane-waves are normalizable — more on this approach (BC at walls) when we do the example of the Infinite square well potential.

In practice we will continue to use plane wave wave functions since as eigenfunctions of the momentum operator they form a complete set (basis) of functions in terms of which we can expand arbitrary wavefunctions.

Indeed Schr. eq. was linear in ψ so it obeys the principle of linear superposition. Hence we can add plane wave solutions with different $\vec{k}$ to obtain a solution to the free Schr. equation

$$\left(\sum_{\vec{k}} N\phi(\vec{k})\psi_{\vec{k}}(\vec{r},t) = \right)\psi(\vec{r},t) = \int_{-\infty}^{+\infty} \frac{d^3k}{(2\pi)^3}\, \phi(\vec{k})\, e^{i(\vec{k}\cdot\vec{r} - \frac{\hbar \vec{k}^2}{2m}t)}$$

This solution is called a Wave Packet

–B2) This is nothing but Fourier's Theorem: Every square integrable function can be written as a superposition of plane waves.

Indeed at $t=0$ we have

$$\psi(\vec{r},0) = \int \frac{d^3k}{(2\pi)^3}\,\phi(\vec{k})\,e^{+i\vec{k}\cdot\vec{r}}$$

Multiplying by $e^{-i\vec{k}'\cdot\vec{r}}$ and integrating over space yields

$$\int d^3r\, e^{-i\vec{k}'\cdot\vec{r}}\,\psi(\vec{r},0)$$
$$= \int d^3r \int \frac{d^3k}{(2\pi)^3}\,\phi(\vec{k})\,e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}$$

But the Fourier expansion of the Dirac δ-function is

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

So

$$\boxed{\int d^3r\, e^{-i\vec{k}'\cdot\vec{r}}\,\psi(\vec{r},0) = \int d^3k\,\phi(\vec{k})\,\delta^3(\vec{k}-\vec{k}') = \phi(\vec{k}')}$$

$\phi(\vec{k})$ is the Fourier transform of $\psi(\vec{r},0)$

This is known as Plancherel's theorem.
$\psi(\vec{r},0)$ and $\phi(\vec{k})$ are F.T. of eachother.

Thus the wavefunction at $t=0$ determines $\phi(\vec{k})$, which by Schrödinger's equation, determines $\psi(\vec{r},t)$ at all times, i.e. the Sch. eq. is first order in $\frac{\partial}{\partial t}$.

Note: Even for $V \neq 0$, the Fourier expansion theorem applies, any square-integrable function can be written as a superposition of plane waves, however now the Fourier coefficients depend on time and must be determined by solving the Sch. eq. for them

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

$\phi(\vec{k},t)$ obeys Sch. eq. in momentum space, as we will see later

For free particle

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r},t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r},t)$$

$$\text{=B2)} \Rightarrow \quad i\hbar \frac{\partial}{\partial t}\phi(\vec{k},t) = \frac{\hbar^2 \vec{k}^2}{2m}\phi(\vec{k},t)$$

hence $\quad \phi(\vec{k},t) = \phi(\vec{k})\, e^{-i\omega_{\vec{k}} t}$

with $\quad \omega_{\vec{k}} = \dfrac{\hbar \vec{k}^2}{2m}$.

Example: Since a wave packet is a sum of different momentum plane waves, it is no longer a momentum eigenfunction. The wave packet contains a spread in momentum values. Consider a wave packet in one dimension that has a Gaussian distribution of momentum values about k_0

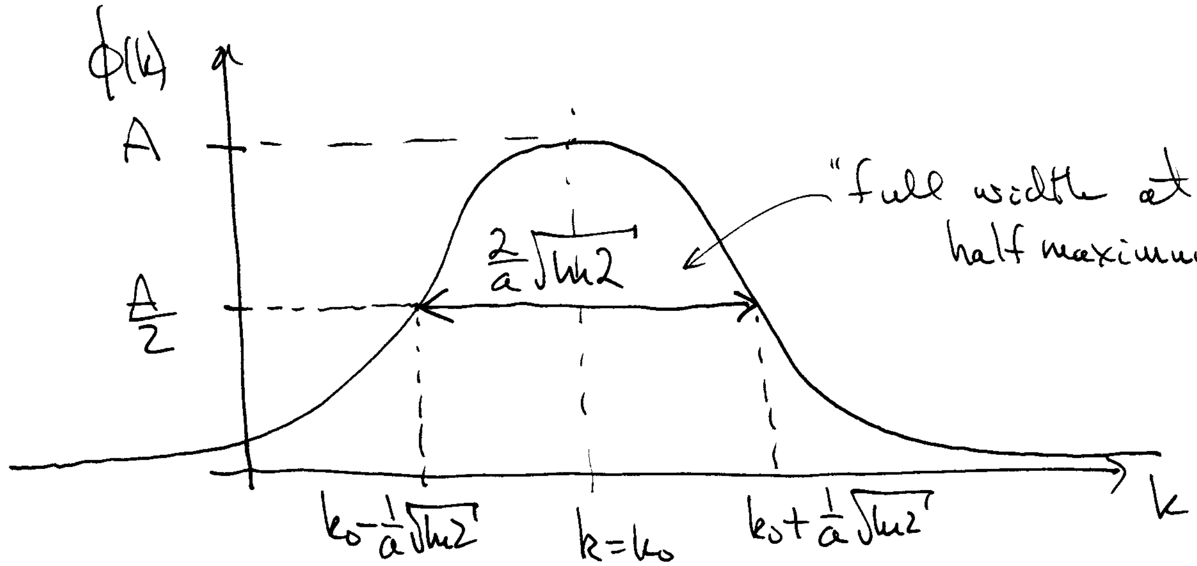
$$\psi(x,t) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, \phi(k)\, e^{i(kx-\omega_k t)}$$

with

$$\phi(k) \equiv A\, e^{-a^2(k-k_0)^2} \qquad \text{and}$$

recall $\omega_k = \dfrac{\hbar k^2}{2m}$ and A, a, k_0 are constants defining the form of the distribution

I $\sigma 2$)



1) Wave packet is peaked in momentum space ($\hbar k$) about $k = k_0$

2) As "a" increases the distribution sharpens about k_0. The particle is said to be "localized" in momentum space about $\hbar k_0$

3) The coordinate space wavefunction can be obtained by completing the square in the exponent and performing the integral

$$\psi(x,t) = A\int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, e^{-a^2(k-k_0)^2 + ikx - i\frac{\hbar k^2}{2m}t}$$

So the exponent is

$\rightarrow$ B2)

$$-a^2(k-k_0)^2 + ikx - i\frac{\hbar k^2}{2m}t$$

$$= -\left[a^2 + \frac{i\hbar t}{2m}\right]k^2 + (ix + 2a^2k_0)k - a^2k_0^2$$

Using the identity for "completing the square"

$$\alpha k^2 + 2\beta k + \gamma = \alpha\left(k + \frac{\beta}{\alpha}\right)^2 - \frac{\beta^2}{\alpha} + \gamma$$

we find $\alpha = -\left[a^2 + \frac{i\hbar t}{2m}\right]$; $\beta = \left(\frac{ix}{2} + a^2k_0\right)$; $\gamma = -a^2k_0^2$

$\Rightarrow$

$$-a^2(k-k_0)^2 + ikx - i\frac{\hbar k^2}{2m}t$$

$$= -\left[a^2 + \frac{i\hbar t}{2m}\right]\left[k - \frac{\left(\frac{ix}{2} + a^2k_0\right)}{\left(a^2 + \frac{i\hbar t}{2m}\right)}\right]^2 + \frac{\left(\frac{ix}{2} + a^2k_0\right)^2}{\left[a^2 + \frac{i\hbar t}{2m}\right]} - a^2k_0^2$$

$$= -\left[a^2 + \frac{i\hbar t}{2m}\right]\left[k - \hat{k}\right]^2$$

$$+ \frac{\left(-\frac{1}{4}x^2 + a^4k_0^2 + ia^2k_0x\right)}{\left[a^2 + \frac{i\hbar t}{2m}\right]} - \frac{a^2k_0^2\left[a^2 + \frac{i\hbar t}{2m}\right]}{\left[a^2 + \frac{i\hbar t}{2m}\right]}$$

iB2) where $\tilde{k} = \dfrac{\left(\frac{ix}{2} + a^2 k_0\right)}{\left(a^2 + \frac{i\hbar t}{2m}\right)}$

$$= -\left[a^2 + \frac{i\hbar t}{2m}\right]\left[k - \tilde{k}\right]^2$$

$$- \frac{1}{4\left(a^2 + \frac{i\hbar t}{2m}\right)}\Big[x^2 - \cancel{4a^4 k_0^2} - 4ik_0 x a^2$$
$$+ \cancel{4a^4 k_0^2} + 4ia^2 k_0^2 \frac{\hbar t}{2m}\Big]$$

$$= -\left[a^2 + \frac{i\hbar t}{2m}\right]\left[k - \tilde{k}\right]^2$$

add & subtract this term

$$- \frac{1}{4\left(a^2 + \frac{i\hbar t}{2m}\right)}\Big[x^2 - 4ik_0 x\left(a^2 + \frac{i\hbar t}{2m}\right)$$
$$+ 4ik_0 x\left(\frac{i\hbar t}{2m}\right) + 4ia^2 k_0^2 \frac{\hbar t}{2m}\Big]$$

$$= -\left[a^2 + \frac{i\hbar t}{2m}\right]\left[k - \tilde{k}\right]^2 + ik_0 x$$

$$- \frac{1}{4\left(a^2 + \frac{i\hbar t}{2m}\right)}\underbrace{\left[x^2 - 2x\frac{\hbar k_0}{m}t + 4i\frac{\hbar k_0^2}{2m}t a^2\right]}_{\text{now complete the square in } x}$$

$$= \left(x - \frac{\hbar k_0}{m}t\right)^2 - \frac{\hbar^2 k_0^2}{m^2}t^2$$
$$+ 4i\frac{\hbar k_0^2}{2m}t a^2$$

IB2)

$$= -\left[a^2 + \frac{i\hbar t}{2m}\right]\left[k - \bar{k}\right]^2 + ik_0 x - \frac{1}{4\left(a^2 + \frac{i\hbar t}{2m}\right)}\left[\left(x - \frac{\hbar k_0}{m}t\right)^2 + 4i\frac{\hbar k_0^2}{2m}t\left(a^2 + \frac{i\hbar t}{2m}\right)\right]$$

$$\boxed{\begin{aligned} &= -\left[a^2 + \frac{i\hbar t}{2m}\right]\left[k - \bar{k}\right]^2 + ik_0 x \\ &\quad - \frac{1}{4\left(a^2 + \frac{i\hbar t}{2m}\right)}\left(x - \frac{\hbar k_0}{m}t\right)^2 \\ &\quad - i\frac{\hbar k_0^2}{2m}t \\ \hline &= -a^2(k - k_0)^2 + ikx - i\frac{\hbar k^2}{2m}t \end{aligned}}$$

i=B2) So putting this into the Fourier Transform

$$\psi(x,t) = A e^{\left[ik_0x - \frac{i\hbar k_0^2}{2m}t - \frac{(x-\frac{\hbar k_0}{m}t)^2}{4(a^2+\frac{i\hbar t}{2m})}\right]} \times$$

$$\times \int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, e^{-(a^2+\frac{i\hbar t}{2m})(k-\tilde{k})^2}$$

(recall $\tilde{k}$ is indep of k)

But the Gaussian momentum integral is

$$\int_{-\infty}^{+\infty} dk\, e^{-\alpha(k-\tilde{k})^2} = \int_{-\infty}^{+\infty} dl\, e^{-\alpha l^2} = \sqrt{\frac{\pi}{\alpha}}$$

(let $l = k-\tilde{k}$) $\qquad$ ($\mathrm{Re}\,\alpha > 0$)

So we find

$$\boxed{\psi(x,t) = \frac{A}{2\sqrt{\pi}}\frac{1}{\sqrt{a^2+\frac{i\hbar t}{2m}}} \times e^{i\left[k_0x - \frac{\hbar k_0^2}{2m}t\right]} \times e^{-\frac{(x-\frac{\hbar k_0}{m}t)^2}{4[a^2+\frac{i\hbar t}{2m}]}}}$$

B2) The particle's position probability is

$$|\psi(x,t)|^2 = \frac{|A|^2}{4\pi} \frac{1}{\left(a^4 + \frac{\hbar^2 t^2}{4m^2}\right)^{1/2}} e^{-\frac{\left(x - \frac{\hbar k_0}{m} t\right)^2}{2a^2\left(1 + \frac{\hbar^2 t^2}{4m^2 a^4}\right)}}$$

Define $a(t) \equiv a \left(1 + \frac{\hbar^2 t^2}{4m^2 a^4}\right)^{1/2}$ with $a(0) = a$

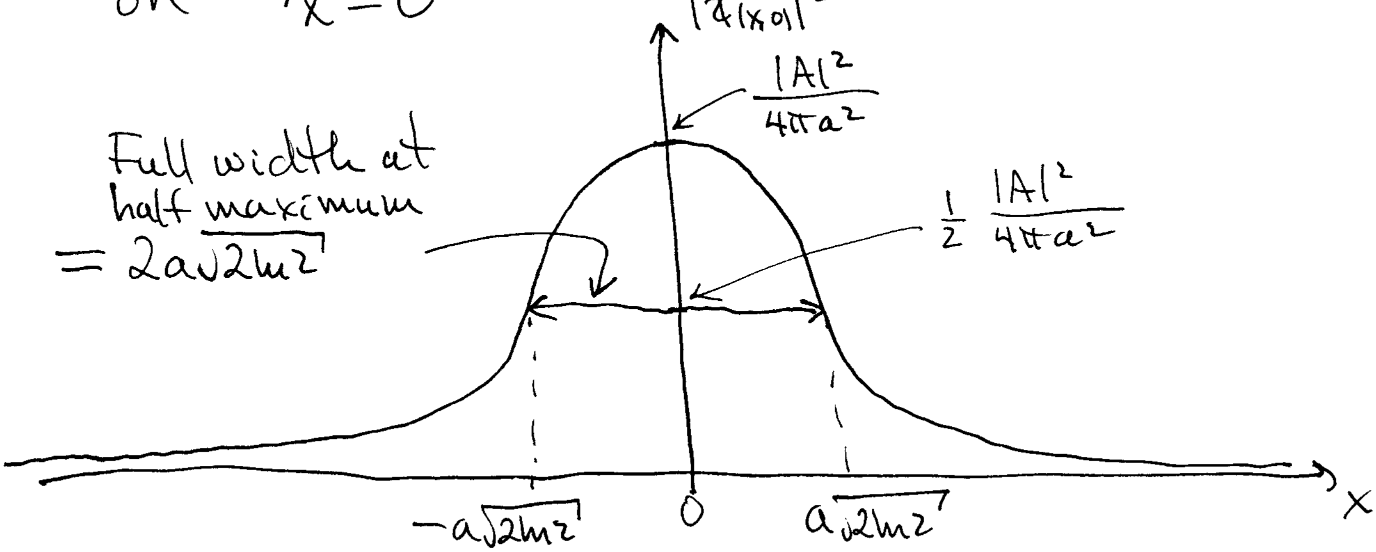
$\Rightarrow$

$$\boxed{|\psi(x,t)|^2 = \frac{|A|^2}{4\pi a\, a(t)} e^{-\frac{\left(x - \frac{\hbar k_0}{m} t\right)^2}{2a^2(t)}}}$$

For $t=0 \Rightarrow$

$$|\psi(x,0)|^2 = \frac{|A|^2}{4\pi a^2} e^{-\frac{x^2}{2a^2}}$$

This is a Gaussian distribution centered on $x = 0$

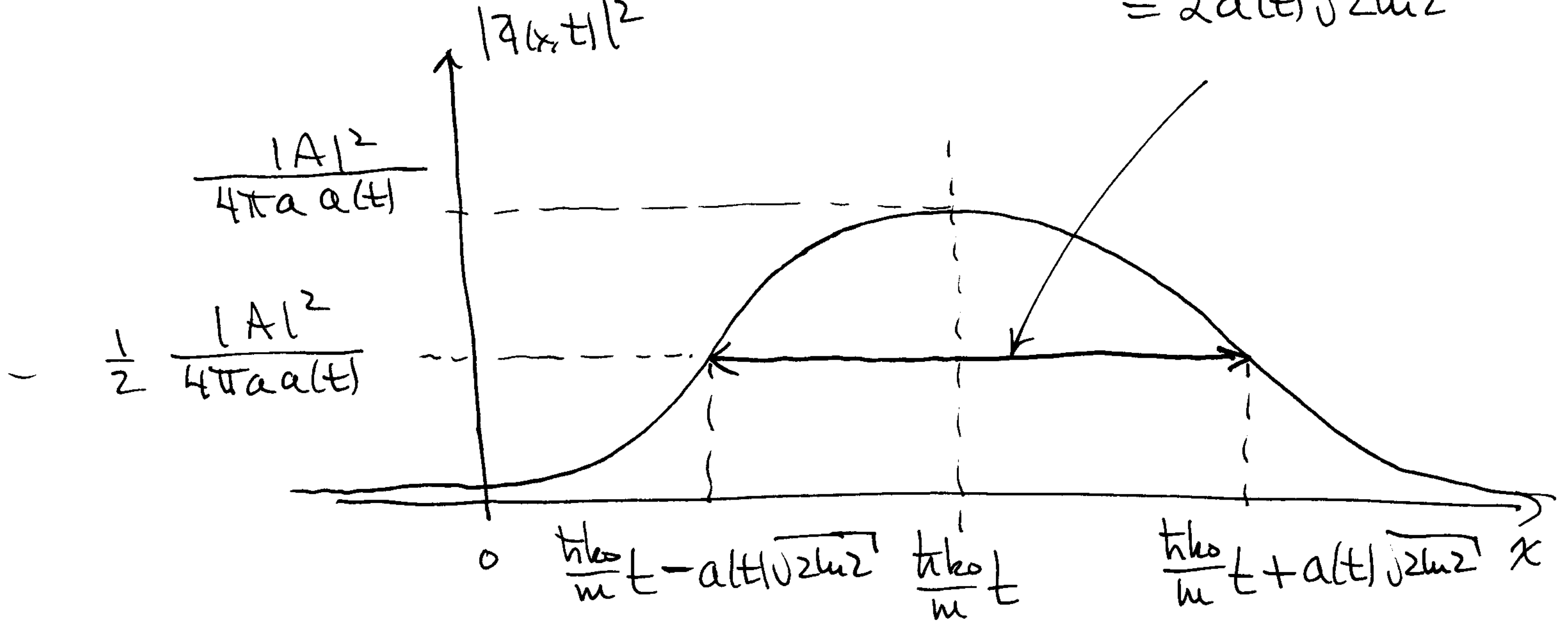


IB2) The smaller a - the more localized the particle becomes in x-space

For $t > 0$ the position probability density is still a Gaussian, now centered on

$$x = \frac{\hbar k_0}{m} t$$

Full width at $\frac{1}{2}$ max. $= 2a(t)\sqrt{2\ln 2}$



Remarks:

1) A Gaussian distribution of momenta, $\phi(k)$, leads to a Gaussian spatial distribution for $|\psi|^2$

I-B 2) 2) $|\psi|^2$ is the position probability density. So the average or Mean position is

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} dx\, x\, |\psi(x,t)|^2}{\int_{-\infty}^{+\infty} dx\, |\psi(x,t)|^2}$$

$$= \frac{\int_{-\infty}^{+\infty} dx\, x\, e^{-\frac{(x-\frac{\hbar k_0}{m}t)^2}{2a^2(t)}}}{\int_{-\infty}^{+\infty} dx\, e^{-\frac{(x-\frac{\hbar k_0}{m}t)^2}{2a^2(t)}}}$$

let $y = x - \frac{\hbar k_0}{m} t$ so that

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} dy\, (y + \frac{\hbar k_0}{m} t)\, e^{-y^2/2a^2(t)}}{\int_{-\infty}^{+\infty} dy\, e^{-y^2/2a^2(t)}}$$

But $\int_{-\infty}^{+\infty} dy\, y\, e^{-y^2/2a^2(t)} = 0$ since the integrand is odd in y.

Hence $$\boxed{\langle x \rangle = \frac{\hbar k_0}{m} t}$$

The mean value of the particle's position is just the peak's position and it moves like a classical free particle with

$$v = \frac{\hbar k_0}{m} = \frac{p_0}{m}.$$

$\Rightarrow$ B 2) 3) The RMS deviation in the particle's position is defined by

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$$

Thus

$$
\begin{aligned}
(\Delta x)^2 &= \langle (x - \langle x \rangle)^2 \rangle \\
&= \langle x^2 - 2\langle x \rangle x + \langle x \rangle^2 \rangle \\
&= \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2 \\
&= \langle x^2 \rangle - \langle x \rangle^2
\end{aligned}
$$

As previously

$$
\begin{aligned}
\langle x^2 \rangle &= \frac{\int_{-\infty}^{+\infty} dx\, x^2 \, |\psi(x,t)|^2}{\int_{-\infty}^{+\infty} dx\, |\psi(x,t)|^2} \\
&= \frac{\int_{-\infty}^{+\infty} dy \left[y^2 + \left(\frac{\hbar k_0 t}{m} \right)^2 \right] e^{-\frac{y^2}{2a^2(t)}}}{\int_{-\infty}^{+\infty} dy \; e^{-y^2/2a^2(t)}}
\end{aligned}
$$

where again we used $\int_{-\infty}^{+\infty} dy\, y e^{-y^2/2a^2(t)} = 0$ for the cross-term.

B2) 3) Trick:
$$\int_{-\infty}^{+\infty} dy\, y^2 e^{-\beta y^2} = -\frac{d}{d\beta}\underbrace{\int_{-\infty}^{+\infty} dy\, e^{-\beta y^2}}_{=\sqrt{\pi/\beta}}$$

$$= -\frac{d}{d\beta}\sqrt{\frac{\pi}{\beta}} = \frac{\sqrt{\pi}}{2\beta^{3/2}},$$

$$\Rightarrow \quad \int_{-\infty}^{+\infty} dy\, y^2 e^{-y^2/2a^2(t)} = \sqrt{2\pi}\, a^3(t)$$

$$\left(\int_{-\infty}^{+\infty} dy\, e^{-y^2/2a^2(t)} = \sqrt{2\pi}\, a(t)\right)$$

Hence
$$\langle x^2\rangle = a^2(t) + \left(\frac{\hbar k_0 t}{m}\right)^2$$

and so
$$\boxed{(\Delta x)^2 = a^2(t) = a^2\left(1 + \frac{\hbar^2 t^2}{4m^2 a^4}\right)}$$

As time increases the deviation in position increases; the wavepacket is said to 'spread'.

This is clear from graph of $|\psi|^2$, the full width at half maximum was $2a(t)\sqrt{2\ln 2}$, it increases as time increases.

Likewise we can calculate the standard deviation in the momentum and the mean momentum

If k- is distributed as prob. amplitude $\phi(k) = Ae^{-a^2(k-k_0)^2}$

then
$$\langle p \rangle = \langle \hbar k \rangle = \frac{\int_{-\infty}^{+\infty} \frac{dk}{2\pi} \hbar k \, |\phi(k)|^2}{\int_{-\infty}^{+\infty} \frac{dk}{2\pi} |\phi(k)|^2}$$

$$= \hbar k_0$$

and
$$\langle p^2 \rangle = \hbar^2 \langle k^2 \rangle = \frac{\hbar^2 \int_{-\infty}^{+\infty} \frac{dk}{2\pi} k^2 |\phi(k)|^2}{\int_{-\infty}^{+\infty} \frac{dk}{(2\pi)} |\phi(k)|^2}$$

$$= \frac{\hbar^2}{4a^2} + \hbar^2 k_0^2$$

$$\Rightarrow (\Delta p)^2 = \frac{\hbar^2}{4a^2} \quad ; \quad \Delta p = \frac{\hbar}{2a}$$

Hence at $t=0$ $\boxed{\Delta x \Delta p = \frac{1}{2}\hbar}$ The Gaussian wave packet has the minimum uncertainty in position and momentum, consistent with the Heisenberg uncertainty principle.

Note: we get the same result by calculating

$$\langle p\rangle = \frac{\int_{-\infty}^{+\infty} dx\, \psi^*(x,t)\,\frac{\hbar}{i}\frac{d}{dx}\psi(x,t)}{\int_{-\infty}^{+\infty} dx\, |\psi|^2} \quad (=\hbar k_0)$$

$$\langle p^2\rangle = \frac{\int_{-\infty}^{+\infty} dx\, \psi^*(x,t)\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2\psi(x,t)}{\int_{-\infty}^{+\infty} dx\, |\psi|^2} = \left(\frac{\hbar^2}{4a^2}+\hbar^2 k_0^2\right)$$

quite tedious, but

This is true in general.

2) $t>0$

$$\Delta x\,\Delta p = \frac{1}{2}\hbar\sqrt{1+\frac{\hbar^2 t^2}{4m^2 a^4}} > \frac{1}{2}\hbar$$

The uncertainty in position increases while that in momentum is fixed.

I-B2) 4.) As the wave packet spreads the height of the peak decreases so that the area under $|\psi|^2$ is constant.
That is the wave packet is indeed square-integrable

$$\int_{-\infty}^{+\infty} dx\, |\psi(x,t)|^2 = \frac{|A|^2}{4\pi a\, a(t)} \int_{-\infty}^{+\infty} dx\, e^{-\frac{(x-\frac{\hbar k_0}{m}t)^2}{2a^2(t)}}$$

$$= \frac{|A|^2}{4\pi a\, a(t)} \sqrt{\pi \cdot 2}\; a(t)$$

$$= \frac{|A|^2}{\sqrt{8\pi}\, a}$$

Normalize wave function for convenience:

$$\int_{-\infty}^{+\infty} dx\, |\psi|^2 = 1 = \frac{|A|^2}{\sqrt{8\pi}\, a}$$

$$\Rightarrow \quad A = (8\pi)^{1/4} a^{1/2} e^{i\varphi}$$

arb. $\varphi \in \mathbb{R}$
choose it to be $\varphi = 0$

$$\boxed{A = (8\pi)^{1/4} a^{1/2}}$$

I B2) Normalizable wave packet has spread in position and momentum. $\Delta x \Delta p \geq \frac{1}{2}\hbar$

1) localized in momentum $\Rightarrow$ spread in position ("a" increases)

2) localized in position $\Rightarrow$ spread in momentum ("a" decreases to include more plane waves in sum)

In the limit $a \to \infty$ the wave packet has only 1-momentum, it is a plane wave

Recall $$2\pi\delta(k-k_0) = \lim_{a\to\infty} \sqrt{4\pi}\, a\, e^{-a^2(k-k_0)^2}$$

(limit in the sense of distributions)

So choose $A = \sqrt{4\pi}\, a \frac{1}{N}$ and

$$\lim_{a\to\infty} \phi(k) = \frac{1}{N} 2\pi \delta(k-k_0) \quad \text{hence}$$

$$\psi(x,t) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, \phi(k)\, e^{i(kx-\omega_k t)}$$

$$\xrightarrow[a\to\infty]{} \frac{1}{N} e^{i(k_0 x - \omega_{k_0} t)}, \text{ the}$$

single plane wave with momentum $\hbar k_0$ and energy $\hbar\omega_{k_0} = \frac{\hbar^2 k_0^2}{2m}$.

I B 2) Of course the wave function is no longer square-integrable

$$\int_{-\infty}^{+\infty} dx\, |\psi(x,t)|^2 = \frac{|A|^2}{\sqrt{8\pi}\, a} = a\sqrt{2\pi} \xrightarrow[a\to\infty]{} \infty$$

as expected.

I B 3) Expectation Values: (For simplicity let ψ be normalized: $\int d^3r\, |\psi(\vec{r},t)|^2 = 1$)

Since $|\psi(\vec{r},t)|^2$ is the position probability density the expectation value of any function, $f(\vec{r})$, of position is

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

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

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

- IB3) Since

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

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

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

$$=\int\frac{d^3k}{(2\pi)^3}\,\phi^*(\vec{k},t)\,\phi(\vec{k},t)=\int\frac{d^3k}{(2\pi)^3}\,|\phi(\vec{k},t)|^2$$

- This is known as Parseval's Theorem

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

Thus we interpret $\phi(\vec{k},t)$ as a momentum probability density with $\phi(\vec{k},t)$ the momentum space wave function.

The momentum probabity - that is the probability the particle has momentum differentially close to $\hbar\vec{k}$ at time t is

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

IB3) This just follows from Postulate 3: The eigenfunctions of momentum (plane waves) are complete so expand any $\psi(\vec{r},t)$ in terms of them:

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

$$\vec{P}\,\varphi_{\vec{k}}(\vec{r}) = \frac{\hbar}{i}\vec{\nabla}\varphi_{\vec{k}}(\vec{r})$$

$$= (\hbar\vec{k})\,\varphi_{\vec{k}}(\vec{r})$$

So

$$\psi(\vec{r},t) = \int \frac{d^3k}{(2\pi)^3}\,\phi(\vec{k},t)\,\frac{1}{A}\,\varphi_{\vec{k}}(\vec{r})$$

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

Further, the coefficients in the expansion are interpreted as probability amplitudes

$$\Rightarrow \qquad dP(\vec{k},t) = |\phi(\vec{k},t)|^2\,\frac{d^3k}{(2\pi)^3}.$$

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

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

- IB3) For example : $\langle \vec{p} \rangle = \int \frac{d^3k}{(2\pi)^3} \hbar \vec{k} \, |\phi(\vec{k},t)|^2$

The Fourier Transform of ψ can be inverted

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

So

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

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

$$\times \int d^3r' \, e^{-i\vec{k}\cdot\vec{r}\,'} \psi(\vec{r}\,',t)$$

$$= \int d^3r \, d^3r' \, \psi^*(\vec{r},t) \cdot \int \frac{d^3k}{(2\pi)^3} \left[\underbrace{g\left(\frac{\hbar}{i}\vec{\nabla}\right)}_{=g(\hbar\vec{k})} e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')} \right] \times$$

$$\times \psi(\vec{r}\,',t)$$

$$= \int d^3r \, d^3r' \, \psi^*(\vec{r},t) \, g\left(\frac{\hbar}{i}\vec{\nabla}\right) \underbrace{\int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}}_{=\delta^3(\vec{r}-\vec{r}\,')} \psi(\vec{r}\,',t)$$

$$= \int d^3r \, \psi^*(\vec{r},t) \, g\left(\frac{\hbar}{i}\vec{\nabla}\right) \int d^3r' \, \delta^3(\vec{r}-\vec{r}\,') \, \psi(\vec{r}\,',t)$$

$$= \boxed{\int d^3r \, \psi^*(\vec{r},t) \, g\left(\frac{\hbar}{i}\vec{\nabla}\right) \psi(\vec{r},t) = \langle g \rangle}$$

I.B3) As expected, in coordinate space the momentum is represented by the differential operator $\vec{P} = \frac{\hbar}{i}\vec{\nabla}$.

Combining results, we have the expectation value of a general function of $\vec{r}, \vec{p}$, $f(\vec{r},\vec{p})$ for the particle in state $\psi(\vec{r},t)$ is

$$\boxed{\begin{aligned}\langle f(\vec{r},\vec{p})\rangle &= \int d^3r\, \psi^*(\vec{r},t)\, f(\vec{r},\vec{P})\,\psi(\vec{r},t)\\ &= \int d^3r\, \psi^*(\vec{r},t)\, f\left(\vec{r}, \frac{\hbar}{i}\vec{\nabla}\right)\psi(\vec{r},t)\end{aligned}}$$

I.B4) Canonical Commutation Relations: Arb. ψ

$[A,B] \equiv AB-BA$

$$[x_i, P_j]\psi(\vec{r},t) = [x_i, -i\hbar\frac{\partial}{\partial x_j}]\psi(\vec{r},t)$$

$$\equiv x_i \frac{\hbar}{i}\frac{\partial}{\partial x_j}\psi(\vec{r},t) - \frac{\hbar}{i}\frac{\partial}{\partial x_j} x_i \psi(\vec{r},t)$$

$$= \cancel{\frac{\hbar}{i} x_i \frac{\partial \psi}{\partial x_j}} - \frac{\hbar}{i}\frac{\partial x_i}{\partial x_j}\psi(\vec{r},t) - \cancel{\frac{\hbar}{i} x_i \frac{\partial \psi}{\partial x_j}}$$

$$= -\frac{\hbar}{i}\delta_{ij}\,\psi(\vec{r},t)$$

- IB4) As an operator relation (identity) then

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

(As if operators act on all functions to the right $[x_i, P_j]\psi(\vec{r},t)$)

Similarly $[x_i, x_j] = 0$

$$[P_i, P_j] = 0$$

The 3 sets of equations constitute the canonical commutation relations

IB5) Ehrenfest's Theorem and Classical Mechanics

Continuity Eq.:

$$\frac{\partial}{\partial t}(\psi^*\psi) + \vec{\nabla}\cdot\frac{\hbar}{2im}(\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi) = 0$$

Multiply by $\vec{r}$ and integrate over all space

$$\frac{d}{dt}\int d^3r \ \psi^*\vec{r}\psi$$

$$= \frac{i\hbar}{2m}\int d^3r \ \vec{r}\,\vec{\nabla}\cdot(\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi)$$

I-5) Integrate RHS by parts:

$$\int d^3r\, \vec{\nabla}\cdot(x_i \vec{J}) = \int d^3r\, J_i + \int d^3r\, x_i \vec{\nabla}\cdot\vec{J}$$

$\parallel$ G.T.

$$\oint_{S\to\infty} d\vec{S}\cdot(x_i\vec{J}) \to 0$$

but as $S\to\infty$, $\psi\to 0$ sufficiently rapidly so that we may neglect these surface terms

$\Rightarrow$

$$\frac{d}{dt}\int d^3r\, \psi^* \vec{r}\,\psi = \frac{-i\hbar}{2m}\int d^3r \left[\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi\right]$$

Again, integrate second term on RHS by parts

$$\int d^3r\, (\vec{\nabla}\psi^*)\psi = -\int d^3r\, \psi^*\vec{\nabla}\psi + \cancel{\int_{S\to\infty} d\vec{S}\, \psi^*\psi} \to 0$$

So

$$\frac{d}{dt}\int d^3r\, \psi^*\vec{r}\,\psi = \int d^3r\, \psi^*\left(\frac{\hbar}{im}\vec{\nabla}\psi\right)$$

But $\langle \vec{r}\rangle = \int d^3r\, \psi^*\vec{r}\,\psi$

I-85) And

$$\langle \vec{P} \rangle = \int d^3r\, \psi^* \frac{\hbar}{i} \vec{\nabla} \psi$$

Hence $\boxed{\frac{d}{dt}\langle \vec{r} \rangle = \frac{1}{m}\langle \vec{P} \rangle}$

As in classical mechanics.

Similarly

$$\frac{d}{dt}\langle \vec{P} \rangle = \int d^3r \frac{\hbar}{i}\left[\frac{\partial}{\partial t}\psi^* \vec{\nabla}\psi + \psi^* \vec{\nabla}\frac{\partial}{\partial t}\psi\right]$$

Use Schrödinger's eq.

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

and its c.c.

$$-i\hbar \frac{\partial}{\partial t}\psi^* = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*$$

And the integrand becomes:

$$\left(-i\hbar \frac{\partial}{\partial t}\psi^* \vec{\nabla}\psi - \psi^* \vec{\nabla}\, i\hbar \frac{\partial}{\partial t}\psi\right)$$

$$= -\frac{\hbar^2}{2m}\nabla^2\psi^* \vec{\nabla}\psi + V\psi^* \vec{\nabla}\psi$$

$$+ \frac{\hbar^2}{2m}\psi^* \vec{\nabla}\nabla^2\psi - \psi^* \vec{\nabla}(V\psi)$$

(B 5)

$$= -\frac{\hbar^2}{2m}\frac{\partial}{\partial x_i}\left[\left(\frac{\partial}{\partial x_i}\psi^*\right)\vec{\nabla}\psi - \psi^*\frac{\partial}{\partial x_i}\vec{\nabla}\psi\right]$$

$$- \psi^*\psi\vec{\nabla}V$$

$\Rightarrow$

$$\frac{d}{dt}\langle\vec{P}\rangle = \int d^3r\,(-\vec{\nabla}V)|\psi|^2$$

$$-\frac{\hbar^2}{2m}\int d^3r\,\frac{\partial}{\partial x_i}\left[\frac{\partial\psi^*}{\partial x_i}\vec{\nabla}\psi - \psi^*\frac{\partial}{\partial x_i}\vec{\nabla}\psi\right]$$

As usual the 2nd term on the RHS vanishes as $S\to\infty$, $\psi\to 0$ sufficiently rapidly.

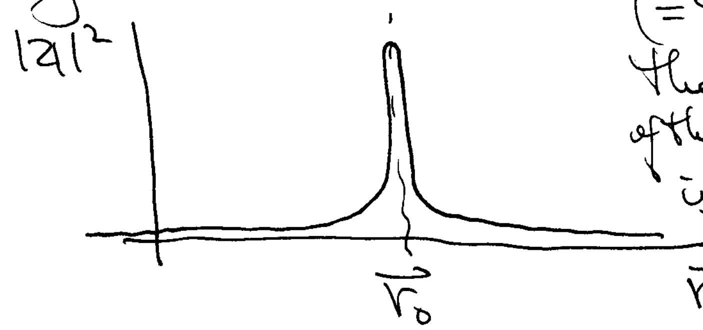
Hence

$$\boxed{\frac{d}{dt}\langle\vec{P}\rangle = -\langle\vec{\nabla}V\rangle}$$

For a sufficiently localized state (so we can drop the surface terms) Newton's 2nd law is valid for expectation values.

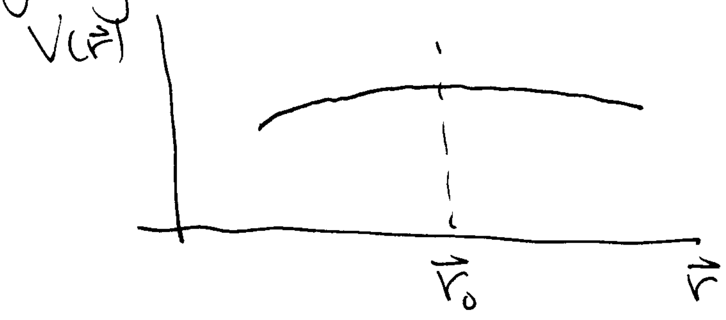
I B5) Further for a "classical limit"

1) The wavefunction of the particle is "very" localized "sufficiently localized" (= This is true is the de Broglie wavelength of the particle $\lambda = \frac{2\pi\hbar}{p}$ is small compared to the measurement scale)



So that $\langle \vec{r} \rangle = \int d^3r\, \psi^* \psi\, \vec{r} \approx \vec{r}_0$

2) All potentials are sufficiently slowly varying about $\vec{r}_0$



Then not only $\langle \vec{F} \rangle$ ~~can~~ but also $\langle \vec{\nabla} V \rangle$ can be expanded about $\vec{r}_0$

$$\langle \vec{\nabla} V \rangle = \int d^3r\, \vec{\nabla} V(\vec{r})\, |\psi(\vec{r},t)|^2 \approx \vec{\nabla} V(\vec{r}_0)$$

Then $\langle \vec{P} \rangle = m \frac{d}{dt} \langle \vec{r} \rangle = m \dot{\vec{r}}_0$

$$\frac{d}{dt} \langle \vec{P} \rangle \approx m \ddot{\vec{r}}_0$$

(IB5) and so
$$\frac{d}{dt}\langle \vec{P}\rangle = -\langle \vec{\nabla} V\rangle \approx -\vec{\nabla} V(\vec{r}_0)$$
$$\Rightarrow \boxed{m\ddot{\vec{r}}_0 = -\vec{\nabla} V(\vec{r}_0)}$$

Thus we obtain a <u>local</u> Newton's 2nd law.

We can generalize the time variation of expectation values to yield

Ehrenfest's Theorem: $F = F(\vec{X}, \vec{P}, t)$
$$\boxed{\frac{d}{dt}\langle F\rangle = \frac{i}{\hbar}\langle [H,F]\rangle + \left\langle \frac{\partial F}{\partial t}\right\rangle}$$

$$\langle F\rangle = \int d^3r\, \psi^*(\vec{r},t)\, F(\vec{r}, \tfrac{\hbar}{i}\vec{\nabla}, t)\, \psi(\vec{r},t)$$

with ψ normalized to 1.

$$\frac{d}{dt}\langle F\rangle = \int d^3r \left[\frac{\partial \psi^*}{\partial t} F\psi + \psi^* F \frac{\partial \psi}{\partial t} + \psi^* \frac{\partial F}{\partial t}\psi\right]$$

As before apply the Schröding eq.
$$i\hbar \frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi \equiv H\psi$$

and its complex conjugate $-i\hbar\frac{\partial}{\partial t}\psi^* = (H\psi)^*$

last term above

I.35) So $\frac{d}{dt}\langle F\rangle = \langle \frac{\partial F}{\partial t}\rangle$

$$+ \frac{i}{\hbar}\int d^3r \left[(H\psi)^* F\psi - \psi^* F (H\psi) \right]$$

But H is a Hermitian operator $\Rightarrow$

$$\frac{d}{dt}\langle F\rangle = \langle \frac{\partial F}{\partial t}\rangle + \frac{i}{\hbar}\int d^3r\, \psi^* \underbrace{(HF - FH)}_{=[H,F]}\psi$$

Thus we find

$$\boxed{\frac{d}{dt}\langle F\rangle = \frac{i}{\hbar}\langle [H,F]\rangle + \langle \frac{\partial F}{\partial t}\rangle}$$

Ehrenfest's Thm.

IB6) The Heisenberg Uncertainty Principle

Consider 1-dimension for simplicity:

If $\Delta x \equiv \sqrt{\langle (X - \langle X\rangle)^2\rangle}$

$\Delta p \equiv \sqrt{\langle (P - \langle P\rangle)^2\rangle}$,

Then $\Delta x \Delta p \geq \frac{\hbar}{2}$.

i-36) Proof: (Weyl) $\left(\text{let} \int_{-\infty}^{+\infty} dx\, \psi^* \psi = 1\right)$

For real λ consider the function $F(\lambda)$ at time t:

$$F(\lambda) \equiv \Big\langle \big(X - \langle X\rangle - i\lambda(P - \langle P\rangle)\big) \times$$
$$\times \big(X - \langle X\rangle + i\lambda(P - \langle P\rangle)\big)\Big\rangle$$

$$= \int_{-\infty}^{+\infty} dx\, \psi^* \left(x - \langle X\rangle - i\lambda\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle P\rangle\right)\right) \times$$
$$\times \left(x - \langle X\rangle + i\lambda\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle P\rangle\right)\right)\psi$$

Integrate by parts; ignore endpoint terms:

$$= \int_{-\infty}^{+\infty} dx \left[\left(x - \langle X\rangle + i\lambda\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle P\rangle\right)\right)\psi\right]^* \times$$
$$\times \left[\left(x - \langle X\rangle + i\lambda\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle P\rangle\right)\right)\psi\right]$$

$$\boxed{\begin{array}{l} F(\lambda) = \displaystyle\int_{-\infty}^{+\infty} dx \left| \left(x - \langle X\rangle + i\lambda\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle P\rangle\right)\right)\psi\right|^2 \\ F(\lambda) \geq 0 \text{ for all } \lambda. \end{array}}$$

Now expand terms in definition of $F(\lambda)$

I B 6)

$$F(\lambda) = \underbrace{\langle (X - \langle X\rangle)^2 \rangle}_{=(\Delta x)^2} + \lambda^2 \underbrace{\langle (P - \langle P\rangle)^2 \rangle}_{=(\Delta p)^2}$$

$$+ i\lambda \langle [(X - \langle X\rangle), (P - \langle P\rangle)] \rangle$$

Now $\langle X\rangle, \langle P\rangle$ are just numbers (c-numbers) but X, P are operators (q-numbers), so the commutator reduces to

$$\langle [X - \langle X\rangle, P - \langle P\rangle] \rangle = \langle [X, P] \rangle$$

$$= \int_{-\infty}^{+\infty} dx\, \psi^* [x, \tfrac{\hbar}{i}\tfrac{\partial}{\partial x}] \psi = i\hbar \int_{-\infty}^{+\infty} dx\, |\psi|^2$$

$$= +i\hbar$$

$\Rightarrow$

$$\boxed{F(\lambda) = (\Delta x)^2 + \lambda^2 (\Delta p)^2 - \hbar\lambda \geq 0, \ \forall \lambda}$$

Now $F(\lambda)$ is just a quadratic function of λ with a minimum at $\lambda = \lambda_{min}$,

$$\frac{dF}{d\lambda} = -\hbar + 2(\Delta p)^2 \lambda$$

$$\left.\frac{dF}{d\lambda}\right|_{\lambda=\lambda_{min}} = 0 = -\hbar + 2(\Delta p)^2 \lambda_{min}$$

$$\Rightarrow \boxed{\lambda_{min} = \frac{\hbar}{2(\Delta p)^2}}$$

B(6) Check it is a minimum

$$\frac{d^2F}{d\lambda^2} = 2(\Delta p)^2 > 0 \quad \checkmark.$$

Since $F(\lambda) \geq 0$ for all λ $\Rightarrow$

$$F(\lambda_{min}) \geq 0$$

$$\Rightarrow F(\lambda_{min}) = (\Delta x)^2 + \lambda_{min}^2 (\Delta p)^2 - \hbar \lambda_{min} \geq 0$$

Substitute $\lambda_{min} = \frac{\hbar}{2(\Delta p)^2}$ $\Rightarrow$

$$F(\lambda_{min}) = (\Delta x)^2 + \frac{\hbar^2}{4(\Delta p)^2} - \frac{\hbar^2}{2(\Delta p)^2} \geq 0$$

$$\Rightarrow \quad (\Delta x)^2 \geq \frac{\hbar^2}{4(\Delta p)^2}$$

Hence $\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}}$.

We have $\Delta x \Delta p = \frac{1}{2}\hbar$ only if

$F(\lambda_{min}) = 0$, $\Rightarrow$

$$\int_{-\infty}^{+\infty} dx \left| \left(x - \langle X \rangle + i\lambda_{min} \left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle P \rangle \right) \right) \psi \right|^2 = 0$$

-B6) This is true only if

$$\left(x - \langle X\rangle + i\lambda_{min}\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle P\rangle\right)\right)\psi(x,t) = 0$$

Substituting $\lambda_{min} = \frac{\hbar}{2(\Delta p)^2}$ $\Rightarrow$

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

At time t, This is a differential equation for ψ — the instantaneous solution is

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

A_t a constant in x. This is just a

Gaussian Wave Packet — it has the least RMS deviation in position and momentum possible.

I B7) Stationary States:

Consider time independent potentials $V = V(\vec{r})$

Schrödinger's Equation is

$$\underbrace{i\hbar\frac{\partial}{\partial t}}_{\substack{\text{only time} \\ \text{derivatives} \\ \text{no space}}}\psi(\vec{r},t) = \underbrace{\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]}_{\substack{\text{only space } (\vec{r}) \text{ derivatives} \\ \text{and potential} \\ \text{no time}}}\psi(\vec{r},t)$$

The space and time dependence separates: Solution by separation of variables

$$\boxed{\text{Ansatz: } \psi(\vec{r},t) \equiv \psi(\vec{r})\, e^{-i\omega t}}$$

with ω = constant. Sch. eq. becomes

$$i\hbar\frac{\partial}{\partial t}\left(\psi(\vec{r})e^{-i\omega t}\right) = \hbar\omega\left(\psi(\vec{r})e^{-i\omega t}\right)$$

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

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

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

(-37) $\Rightarrow$

$$\boxed{\begin{array}{c} \hbar\omega\,\psi(\vec{r}) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) \\ \quad\| \qquad\qquad\qquad \| \\ E\,\psi(\vec{r}) = H\,\psi(\vec{r}) \end{array}}$$

The time independent Schrödinger Equation

The energy of the particle $E = \hbar\omega$ according to the Planck-Einstein relation. The wavefunction

$$\psi(\vec{r},t) = \psi(\vec{r})\,e^{-iEt/\hbar}$$

is called the stationary state solution to the Sch. eq. since

$$|\psi(\vec{r},t)|^2 = |\psi(\vec{r})|^2$$

is independent of the time - hence stationary.

The time independent Schrödinger Eq.

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

where $H \equiv -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$ is the Hamiltonian (Energy) operator.

I B7) This is an eigenvalue equation for the Hamiltonian. The eigenfunction $\psi(\vec{r})$ of H gives the stationary state with energy eigenvalue E, these will be the allowed energies of the system. The spectrum of energy eigenvalues can be continuous, discrete (quantized) or both.

Let n label the eigenvalues E_n and eigenfunctions $\psi_n(\vec{r})$ of H. For now let the eigenvalues be discrete — we will let the sums become integrals etc., in the continuous case as needed. Hence, the time independent Schrödinger equation for each n becomes

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

Since H is Hermitian, by postulate 3 the eigenfunctions $\psi_n(\vec{r})$ form a complete set — hence any solution 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 Sch. eq., then

I-B 7) Any solution $\psi(\vec{r},t)$ can be written as a superposition

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

[That is

$$\psi(\vec{r},t) = \sum_n c_n(t)\psi_n(\vec{r}),$$ substitute

into Sch. eq.

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \sum_n i\hbar \frac{d c_n(t)}{dt} \psi_n(\vec{r})$$

$$= H\psi(\vec{r},t) = \sum_n c_n(t) \underbrace{H\psi_n(\vec{r})}_{=E_n\psi_n(r)} = \sum_n E_n c_n(t)\psi_n(\vec{r})$$

Since the $\psi_n(\vec{r})$ are independent $\Rightarrow$

$$i\hbar \frac{d c_n(t)}{dt} = E_n c_n(t) \text{ for each } n$$

let $c_n(0) = c_n$ = constants at $t=0$ $\Rightarrow$

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

Now we can invert the above expansion by using orthogonality properties of eigenfunctions:

I-B 7) Recall $H \equiv -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$ is a Hermitian operator, $H^\dagger = H$

Now $H\psi_n = E_n \psi_n \Rightarrow (H\psi_n)^* = E_n^* \psi_n^*$

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

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

But recall $\int d^3r \, (H\psi_m)^* \psi_n \underset{H=H^\dagger}{=} \int d^3r \, (H^\dagger \psi_m)^* \psi_n$

$\underset{\text{definition of hermitian conjugate}}{=} \int d^3r \, \psi_m^* (H\psi_n)$

definition of hermitian conjugate.

Hence LHS above is 0:

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

1) $m = n$, $0 = (E_n - E_n^*) \underbrace{\int d^3r \, |\psi_n|^2}_{\neq 0}$

$$\Rightarrow \boxed{E_n = E_n^* = \text{real } \#}$$

The energy eigenvalues are real.

2) $m \neq n$, $0 = \underbrace{(E_n - E_m)}_{\neq 0} \int d^3r \, \psi_m^* \psi_n$

$$\Rightarrow \boxed{\int d^3r \, \psi_m^* \psi_n = 0}$$

IB7) 2) The stationary state eigenfunctions are orthogonal. Since we are free to normalize ψ_n as desired (we have assumed E_n is discrete), choose

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

Hence $\boxed{\int d^3r\, \psi_m^* \psi_n = \delta_{mn}}$ the energy eigenfunctions are orthonormal

Use this orthogonality of the eigenfunctions to invert the energy eigenfunction expansion of $\psi(\vec{r},t)$

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

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

Multiply by $\psi_m^*(\vec{r})$ and integrate over $\vec{r}$

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

$$= \sum_n' c_n \delta_{mn}$$

$$= c_m$$

IB7) The coefficients c_n are determined by the initial value of the wavefunction $\psi(\vec{r},0)$

$$\boxed{c_n = \int d^3r\, \psi_n^*(\vec{r})\, \psi(\vec{r},0)}$$

Suppose we substitute this back into the energy eigenfunction expansion for $\psi(\vec{r},0)$

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

This implies that

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

This is called the completeness or closure relation.

Thus if the set of (energy, in this case,) 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 visaversa.

I37) By postulate 3, measuring the energy of the particle results in one of the eigenvalues E_n with the probability

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

This probability is independent of time.

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

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

$$= \sum_n{}' c_n^* c_n$$

$$= \sum_n{}' |c_n|^2$$

Hence $\sum_n{}' P_n = \sum_n{}' |c_n|^2 = 1$, as required of a probability interpretation for $|c_n|^2$.

Since P_n is the probability of measuring energy E_n of the particle, the expectation value of the energy operator H is given by

I B7) $\langle H \rangle = \sum_n' E_n |C_n|^2.$

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

Now expand each ψ :

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

but $H\psi_n = E_n \psi_n$

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

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

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

Hence $|C_n|^2$ is the prob. of measuring energy E_n in state $\psi(\vec{r},t)$. Hence E_n times the prob. of being measured, summed over all possibilities yields the average energy of the state.

I B 7) Besides energy eigenfunctions we also considered momentum eigenfunctions — plane waves

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

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

These eigenfunctions are labelled by a continuum of eigenvalues $\vec{k}$ — hence the Kronecker delta orthonormality relation must be replaced by the Dirac δ-function <u>continuum normalization</u>

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

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

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

We choose the convention $A = 1 \Rightarrow$

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

continuum normalization

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

IB7) Further, any wavefunction may be expanded in terms of plane waves (Fourier expansion) hence they obey the closure relation

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

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

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

with $\phi(\vec{k},t) = \int d^3r\, \varphi_{\vec{k}}^*(\vec{r})\, \psi(\vec{r},t)$.

Besides energy and momentum (operators) observables, we may also observe the position of the particle. The position operator is just multiplication by $\vec{r}$. Hence position eigenfunctions $\psi_{\vec{r}_0}(\vec{r})$ obey the eigenvalue equation

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

with the eigenvalue $\vec{r}_0 \in \mathbb{R}^3$ labelling them.

1B7) Since the Dirac delta function $\delta^3(\vec{r}-\vec{r}_0)$ sets $\vec{r}$ to $\vec{r}_0$ we have the eigenfunction

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

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

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

These position eigenfunctions are not ~~even~~ functions, but are distributions and are not square-integrable.

Once again they are continuum normalized

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

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

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

and they are complete

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

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

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

IB7) Any wavefunction has the expansion

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

IB8) <u>Boundary Conditions on the Wavefunction</u>

According to postulate 2, the probability density $\rho = |\psi(\vec{r},t)|^2$ is observable. Hence it must be everywhere <u>finite</u> and <u>continuous</u>. $|\psi|^2$ is finite if and only if <u>$\psi(\vec{r},t)$</u> is <u>finite</u> <u>everywhere</u>.

It is sufficient 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, by superposition $\psi = \psi_1 + \lambda\psi_2$ is a solution to the Sch. eq. if ψ_1 & ψ_2 are solutions and $\lambda \in \mathbb{C}$. We can show the ψ_2 is continuous. $|\psi_1|^2$, $|\psi_2|^2$ and $|\psi_1 + \lambda\psi_2|^2 = |\psi|^2$ are all 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

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

I B8) Let $\lambda = \lambda^* \Rightarrow \psi_1^* \psi_2 + \psi_1 \psi_2^*$ is continuous
Let $\lambda = -\lambda^* \Rightarrow \psi_1^* \psi_2 - \psi_1 \psi_2^*$ is continuous

Hence $\psi_1^* \psi_2$ must be continuous, and since ψ_1 is continuous, this implies ψ_2 must be continuous, i.e.

$$\lim_{\epsilon \to 0} \left[\psi_1^*(x+\epsilon)\psi_2(x+\epsilon) - \psi_1^*(x)\psi_2(x) \right] = 0$$

$$= \lim_{\epsilon \to 0} \psi_1^*(x) \left[\psi_2(x+\epsilon) - \psi_2(x) \right]$$

$$\Rightarrow \lim_{\epsilon \to 0} \left[\psi_2(x+\epsilon) - \psi_2(x) \right] = 0$$

where we have excluded pathological ψ_1's with zeros at x by assumption.

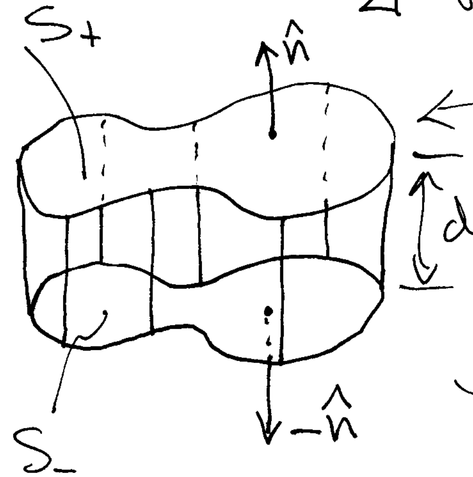
Hence continuity of $|\psi|^2$ and the principle of superposition $\Rightarrow$ $\underline{\psi \text{ is continuous}}$

Next, consider integrating the Schrödinger equation $\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \psi = E\psi$ over volume Ω

$$\int_\Omega d^3r\, \nabla^2 \psi = \frac{2m}{\hbar^2} \int_\Omega d^3r\, V\psi - \frac{2mE}{\hbar^2} \int_\Omega d^3r\, \psi$$

B9) Using Gauss' Theorem on the LHS $\Rightarrow$

$$\int_{\Omega} d^3r\, \nabla^2\psi = \oint_{\Sigma_t' = \partial\Omega} d\vec{S}\cdot\vec{\nabla}\psi = \frac{2m}{\hbar^2}\int_{\Omega} d^3r\, V\psi - \frac{2mE}{\hbar^2}\int_{\Omega} d^3r\,\psi$$



Surface Σ_t' bounding infinitesimal volume Ω with infinitesimal height dh.

The surface integral over the sides is infinitesimal and hence negligible, so

$$\oint_{\Sigma_t'} d\vec{S}\cdot\vec{\nabla}\psi = \int_{S_+} d\vec{S}\cdot\vec{\nabla}\psi + \int_{S_-} d\vec{S}\cdot\vec{\nabla}\psi$$

$$= \int_{S_+} da\, \hat{n}\cdot\vec{\nabla}\psi - \int_{S_-} da\, \hat{n}\cdot\vec{\nabla}\psi$$

since S_+, S_- have oppositely directed normals, $d\vec{S} = \hat{n}\, da$ of S_+ and $d\vec{S} = -\hat{n}\, da$ on S_-.

Since ψ is continuous and the volume Ω is infinitesimal we may neglect $\int_{\Omega} d^3r\,\psi$ also.

→B8) <u>If V is non-singular in Ω</u>, then $\int_\Omega d^3r\, V\psi$ is negligible.

hence
$$\int_{S_+} da\, \hat{n}\cdot\vec{\nabla}\psi = \int_{S_-} da\, \hat{n}\cdot\vec{\nabla}\psi$$

$$\Rightarrow \hat{n}\cdot\vec{\nabla}\psi\Big|_{S_+} = \hat{n}\cdot\vec{\nabla}\psi\Big|_{S_-}$$
, that is the gradient is continuous across the volume. Since the volume is arbitrary ⇒

$\boxed{\vec{\nabla}\psi \text{ is continuous wherever the potential } V \text{ is non-singular}}$

<u>If V is singular</u> (ex. Dirac δ-function), then the BC for $\vec{\nabla}\psi$

can be obtained by integrating the Sch. eq. as above. Or represent the singular potential as sequence of regular potentials for which $\vec{\nabla}\psi$ is continuous, then take the limit at the end to obtain the correct wavefunction.

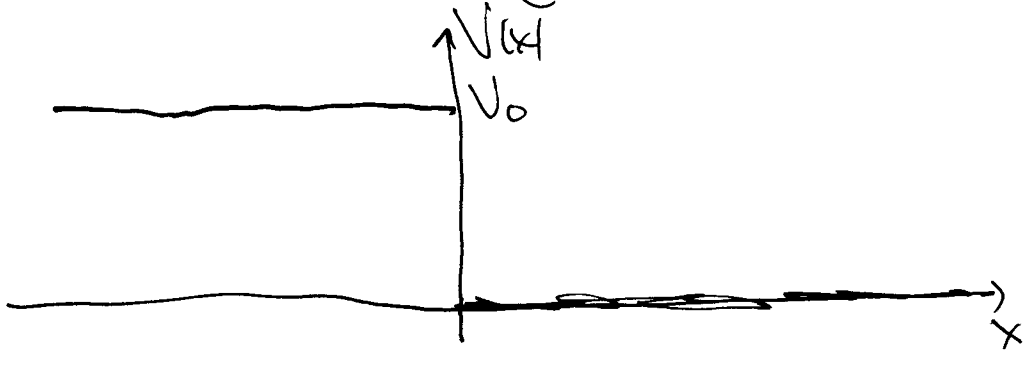
-38) Summary: Boundary Conditions on the Wavefunction

1) ψ is everywhere finite
2) ψ is everywhere continuous
3) For non-singular potentials, $\vec{\nabla}\psi$ is continuous.

4) For singular potentials, either integrate Sch. eq or take limit of 3) to determine BC for $\vec{\nabla}\psi$.

Example: Consider a particle of mass m and energy $E>0$ in one dimension moving in the potential

$$V(x) = \begin{cases} V_0 > 0 & \text{if } x<0 \\ 0 & \text{if } x>0 \end{cases}$$



B8) The Sch. equation in the 2-regions is given by

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V_0\psi(x) = E\psi(x) \quad ; x<0$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \quad ; x>0$$

Define $k \equiv \sqrt{\frac{2mE}{\hbar^2}} > 0$ since $E>0$.

and $\nu_0 = \frac{2mV_0}{\hbar^2} = \text{constant} > 0$.

So the Sch. eq becomes

$$\frac{d^2\psi}{dx^2} + (k^2 - \nu_0)\psi = 0 \quad , x<0$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad , x>0.$$

Consider the case when $0<E<V_0$, that is $0<k^2<\nu_0$.

Let $\kappa \equiv \sqrt{\nu_0 - k^2} > 0$ the equations become

$$\frac{d^2}{dx^2}\psi - \kappa^2\psi = 0 \quad x<0$$

$$\frac{d^2}{dx^2}\psi + k^2\psi = 0 \quad x>0.$$

-B8) The solution is

$$\psi(x) = \begin{cases} A_- e^{\chi x} + B_- e^{-\chi x} & , x<0 \\ A_+ \cos kx + B_+ \sin kx & , x>0. \end{cases}$$

Next we must match solutions and apply our BC on $\psi(x)$

1) ψ is finite everywhere:

$\psi(-\infty)$ is finite $\Rightarrow$ $\boxed{B_- = 0}$

2) ψ is continuous everywhere

$$\lim_{\epsilon \to 0} \left[\psi(-\epsilon) = \psi(+\epsilon) \right]$$

$$\Rightarrow \boxed{A_- = A_+}$$

3) V is non-singular $\Rightarrow$ $\frac{d\psi}{dx}$ is continuous everywhere $\Rightarrow$

$$\lim_{x \to 0^-} \frac{d}{dx}\psi(x) = \lim_{x \to 0^+} \frac{d}{dx}\psi(x)$$

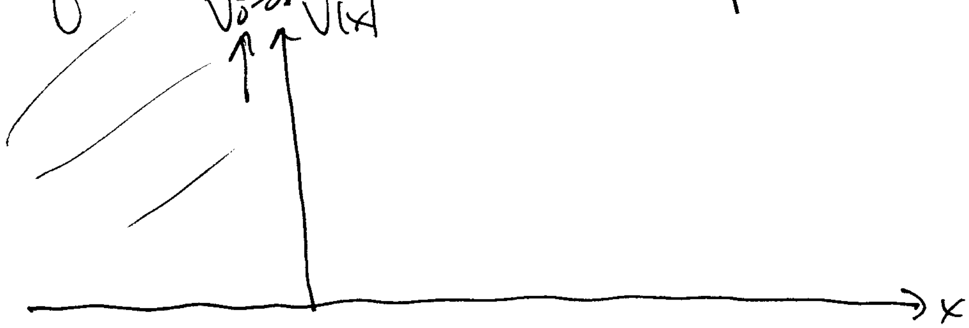
$$\Rightarrow \boxed{\chi A_- = k B_+}$$

B8) Hence let $B_+ \equiv N \Rightarrow$

$$\psi(x) = \begin{cases} N \frac{k}{\chi} e^{\chi x} , & x<0 \\ N(\sin kx + \frac{k}{\chi}\cos kx) , & x>0 . \end{cases}$$

This satisfies the Schrödinger eq. and is everywhere continuous and finite with its derivative continuous everywhere.

Suppose we let $V_0 \to \infty$ this will determine the correct BC for the infinite potential barrier



For $V_0 \to \infty \Rightarrow \quad N_0 = \frac{2mV_0}{\hbar} \to 0$

$\left(k = \sqrt{\frac{2mE}{\hbar^2}} < \infty\right) \qquad \chi = \sqrt{N_0 - k^2} \to \infty$

Hence

$$\psi(x) = \begin{cases} 0 & \text{if } x<0 \\ N \sin kx & \text{if } x>0 . \end{cases}$$

I-B8) Hence in the region where $V(x) \to \infty$ the wavefunction $\psi(x) \to 0$. $\psi(x)$ is still finite and continuous everywhere. But now the derivative of ψ is no longer continuous where the potential has the infinite discontinuity, i.e. at $x=0$,

$$\lim_{x \to 0^-} \frac{d}{dx}\psi(x) = 0 \ , \quad \text{but}$$

$$\lim_{x \to 0^+} \frac{d}{dx}\psi(x) = kN \neq 0 \ .$$