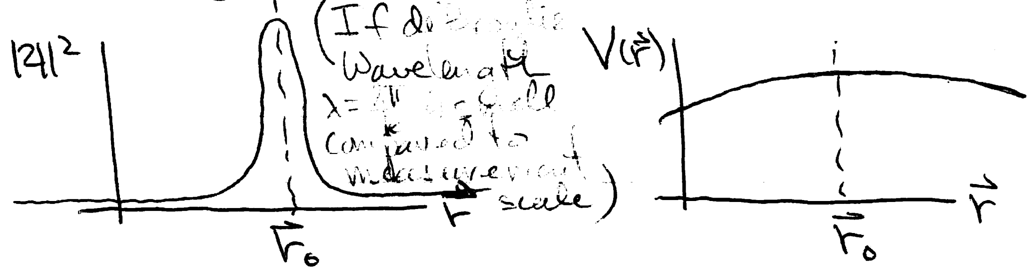
$$\langle \vec{r} \rangle = \int d^3r \, \vec{r} \, \psi^*(\vec{r},t)\psi(\vec{r},t) \approx \vec{r}_0$$

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

i.e.



Then $\langle \vec{p} \rangle \approx m\dot{\vec{r}}_0$; $\frac{d}{dt}\langle \vec{p} \rangle \approx m\ddot{\vec{r}}_0$

$$\frac{d}{dt}\langle \vec{p} \rangle \approx -\vec{\nabla} V(\vec{r}_0) \quad \text{and}$$

we obtain a local Newton's law $m\ddot{\vec{r}}_0 = -\vec{\nabla} V(\vec{r}_0)$.

1.3.6. The Heisenberg Uncertainty Principle

The expectation values of position and momentum can be used to define their root mean square deviations (consider 1-dimension for simplicity)

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

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

The Heisenberg uncertainty principle

states

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

<u>Proof</u>: (Weyl)

For real λ consider the function $F(\lambda)$ at some particular time t,

$$F(\lambda) \equiv \langle (x - \langle x \rangle - i\lambda(P - \langle P \rangle)) \times$$

$$\times (x - \langle x \rangle + i\lambda(P - \langle P \rangle)) \rangle$$

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

Integrating by parts in the numerator

$$= \frac{\int_{-\infty}^{+\infty} dx \, [(x - \langle x \rangle + i\lambda(-i\hbar \frac{\partial}{\partial x} - \langle p \rangle))\psi]^* \times [(x - \langle x \rangle + i\lambda(-i\hbar \frac{\partial}{\partial x} - \langle P \rangle))\psi]}{\int_{-\infty}^{+\infty} dx \, |\psi|^2}$$

$$F(\lambda) = \frac{\int_{-\infty}^{+\infty} dx \left|\left(x - \langle x\rangle + i\lambda\left(-i\hbar\frac{\partial}{\partial x} - \langle p\rangle\right)\right)\psi\right|^2}{\int_{-\infty}^{+\infty} dx\, |\psi|^2}$$

≥ 0 for all λ.

On the other hand we can expand terms in the definition of $F(\lambda)$ to give

$$F(\lambda) = \langle (x - \langle x\rangle)^2\rangle + \lambda^2\langle (P - \langle P\rangle)^2\rangle$$
$$+ i\lambda\langle [(X - \langle x\rangle), (P - \langle p\rangle)]\rangle$$

where we are careful about the ordering of the X and P operators. Since $\langle x\rangle$ and $\langle p\rangle$ are just numbers, the commutator just reduces to

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

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

$$= +i\hbar$$

So we find

$$F(\lambda) = (\Delta x)^2 + \lambda^2 (\Delta p)^2 - \hbar \lambda \geq 0 \text{ for all } \lambda.$$

$F(\lambda)$ is just a quadratic function of λ with a minimum value at some λ, call it λ_{min}. To find λ_{min} consider the first derivative

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

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

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

To check that it is indeed a minimum consider the second derivative

$$\frac{d^2F}{d\lambda^2} = 2(\Delta p)^2 > 0,$$ thus

it is a minimum. Since $F(\lambda) \geq 0$ for all λ we have

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

This implies

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

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

yields

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

or

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

and hence our desired result

$$\boxed{(\Delta x)(\Delta p) \geq \frac{\hbar}{2}}$$

We can have $\Delta x \Delta p = \frac{\hbar}{2}$ only if $F(\lambda_{min}) = 0$, this gives minimum uncertainty. $F(\lambda_{min}) = 0$ implies

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

Since the integrand is a modulus squared the integral vanishes only if

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

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

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