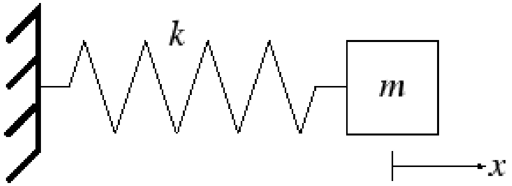
EE201/MSE207 Lecture 2

Schrödinger equation (1 dimensional, 1 particle)

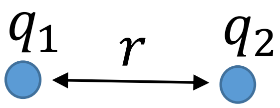
$$\boxed{i\hbar\frac{\partial\Psi(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x,t)\Psi(x,t)} \qquad \text{(SE)}$$

$V(x,t)$ is potential energy, usually just $V(x)$

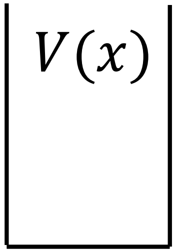
Examples

1) 

mass on spring, oscillator $V(x)=\dfrac{kx^2}{2}$

2) 

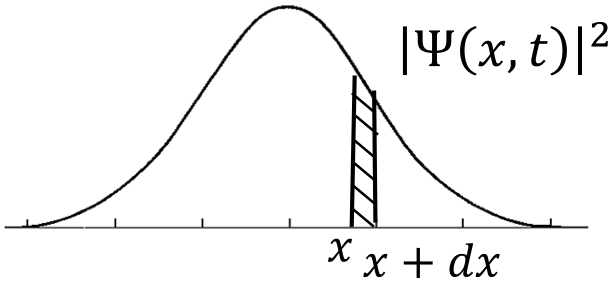
electrostatics $V(r)=\dfrac{q_1q_2}{4\pi\varepsilon\varepsilon_0 r}$

3) 

Electron in a box, “quantum well”

SE: $$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t)$$

$|\Psi(x,t)|^2 dx$ is the probability to find the particle between x and $x + dx$



Normalization

Total probability = 1 $\Rightarrow$ $$\boxed{\int_{-\infty}^{\infty}|\Psi(x,t)|^2 dx = 1}$$

Is this normalization consistent with SE?

Is it really $\frac{d}{dt}\int_{-\infty}^{\infty}|\Psi(x,t)|^2 dx = 0$?

Let us prove this.

Checking that normalization is consistent with SE

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\Psi(x,t)|^2dx=\int_{-\infty}^{\infty}\frac{\partial|\Psi(x,t)|^2}{\partial t}\,dx$$

SE $$\frac{\partial\Psi}{\partial t}=\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2}-\frac{i}{\hbar}V\Psi$$

conjugate
(V is real)

$$\frac{\partial\Psi^*}{\partial t}=\frac{-i\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2}+iV\Psi^*$$

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

$$=\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2}\Psi^*\underline{-\frac{i}{\hbar}V\Psi\Psi^*}-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\Psi\underline{+\frac{i}{\hbar}V\Psi^*\Psi}=$$

$$=\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2}-\frac{\partial^2\Psi^*}{\partial x^2}\Psi\right)=\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)$$

check
yourself!

So, $$\frac{d}{dt}\int_{-\infty}^{\infty}|\Psi(x,t)|^2dx=\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)dx$$

$$=\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{+\infty}=0$$

OK!
normalization
does not change

Notation:

$$f(x)\Big|_A^B\equiv f(B)-f(A)$$

Probability current

Theorem

Define $$P_{ab} = \int_a^b |\Psi(x,t)|^2 dx$$

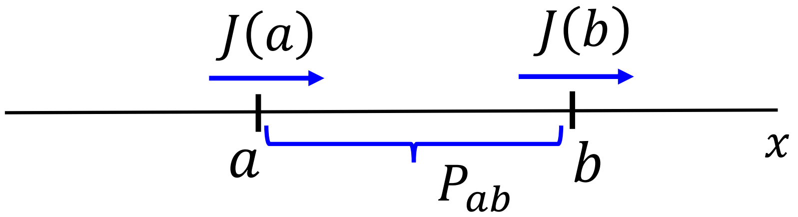
Probability of the particle being between a and b

Then $$\frac{d}{dt} P_{ab} = J(a,t) - J(b,t)$$

where $$\boxed{J(x,t) = \frac{i\hbar}{2m}\left(\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^* \frac{\partial \Psi}{\partial x}\right)}$$

Probability current

same combination as before, with minus sign



similar to charge and current

Proof

$$\frac{d}{dt}\int_a^b |\Psi(x,t)|^2 dx = \int_a^b \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right) dx =$$

$$= \frac{i\hbar}{2m}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\Bigg|_a^b = -J(b) + J(a)$$

proven

Momentum

Not easy to introduce because no velocity in QM. Try via averages.

Average position $$\langle x\rangle = \int_{-\infty}^{\infty} x\,|\Psi(x,t)|^2\,dx$$

(average over ensemble of identical particles, not over measurements repeated in time)

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty} x\,\frac{\partial|\Psi|^2}{\partial t}\,dx = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\,\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)dx =$$

$$= \left(\begin{matrix}\text{by parts,}\\ \text{nothing at} \pm\infty\end{matrix}\right) = -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)dx = -\frac{i\hbar}{m}\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx$$

integrals are equal (by parts)

Define average momentum $$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int_{-\infty}^{\infty}\Psi^*\frac{\partial\Psi}{\partial x}\,dx$$

So, $$\begin{cases}\langle x\rangle = \displaystyle\int_{-\infty}^{\infty}\Psi^* x\,\Psi\,dx \\ \langle p\rangle = \displaystyle\int_{-\infty}^{\infty}\Psi^*\underline{\left(-i\hbar\frac{\partial}{\partial x}\right)}\Psi\,dx\end{cases}$$

operator of momentum

Operator $\boxed{-i\hbar\frac{\partial}{\partial x}}$ represents momentum, similar to how x represents position

Recipe for average ("expectation") value for an "observable" $Q(x,p)$

The average ("expectation") value for any physical quantity ("observable") $Q(x,p)$ is equal

$$\boxed{\langle Q(x,p)\rangle = \int_{-\infty}^{\infty} \Psi^* \, Q\left(x, -i\hbar\frac{\partial}{\partial x}\right) \Psi \, dx}$$

Note that $\langle Q\rangle$ is always real for reasonable Q (agrees with common sense)

Example Kinetic energy $T = \dfrac{p^2}{2m} \rightarrow \dfrac{1}{2m}\left(-i\hbar\dfrac{\partial}{\partial x}\right)^2 = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}$

$$\langle T\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \Psi^*(x,t)\,\frac{\partial^2\Psi(x,t)}{\partial x^2}\,dx$$

Operator of total energy (Hamiltonian) $\hat{H} = \hat{T} + \hat{V} = \dfrac{\hat{p}^2}{2m} + \hat{V}$ (kinetic + potential)

$$\boxed{\hat{p} = -i\hbar\,\frac{\partial}{\partial x}}$$

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)}$$

SE: $$\boxed{i\hbar\,\frac{\partial\Psi}{\partial t} = \hat{H}\,\Psi}$$

Heisenberg uncertainty principle

For a wave there is a conflict between precise location and precise wavelength

Precise wavelength $\Rightarrow$ no location at all (everywhere)
Localization in space $\Rightarrow$ "wavepacket", spread in wavelength

Similar situation in QM, since momentum corresponds to wavelength $p = \dfrac{2\pi\hbar}{\lambda}$

Heisenberg uncertainty principle: $\boxed{\sigma_x \sigma_p \geq \hbar/2}$

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \int_{-\infty}^{\infty} x^2 |\Psi|^2 \, dx - \left(\int_{-\infty}^{\infty} x \, |\Psi|^2 \, dx \right)^2$$

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 = \int_{-\infty}^{\infty} \Psi^* \left(-\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} \right) dx - \left(\int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{\partial \Psi}{\partial x} \right) dx \right)^2$$

This is just a mathematical theorem: for any function $\Psi(x)$
we can prove this inequality

Very important physical implications: confined particle cannot be at rest
(confinement energy, electron "constantly moving" in an atom, etc.)

Idea of the proof (not really important)

Start with obvious inequality with an arbitrary real α

$$\int_{-\infty}^{\infty} |\alpha x\Psi + \partial\Psi/\partial x|^2 dx \geq 0$$

Therefore

$$\begin{aligned} 0 \leq \alpha^2\langle x^2\rangle + \alpha \overbrace{\int_{-\infty}^{\infty}(x\Psi\, \partial\Psi^*/\partial x + x\Psi^*\, \partial\Psi/\partial x)\, dx}^{-1 \text{ (via by parts)}} \\ + \underbrace{\int_{-\infty}^{\infty}(\partial\Psi^*/\partial x)(\partial\Psi/\partial x)\, dx}_{\text{(by parts)}} = \alpha^2\langle x^2\rangle - \alpha + \langle p^2\rangle/\hbar^2 \end{aligned}$$

Positive quadratic form in $\alpha \Rightarrow$ negative determinant

$$\langle x^2\rangle\langle p^2\rangle \geq (\hbar/2)^2$$

Then shifting x and p [$\Psi(x) \rightarrow \Psi(x)\, e^{-ip_0 x/\hbar}$], we obtain

$$\sigma_x\sigma_p \geq \hbar/2$$