More about Heisenberg's principle.

Heisenberg's uncertainty principle can be used to estimate the momentum (and kinetic energy) of a confined particle.

- If a particle is confined to a small region, the minimum uncertainty of its momentum ($\Delta p$) is approximately equal to the absolute value of its momentum ($|p|$).

Imagine a confined particle bouncing back and forth in the potential well, momentum swaps direction from time to time.


Heisenberg example revisited

- $e^-$ is confined to a space $5.00\, \text{nm}$ wide along the $x$ direction.
- Estimate (roughly) the magnitude of its momentum and hence kinetic energy.

Solution: $\Delta x \Delta p \geq \frac{\hbar}{2}$ and $\Delta \omega \geq |p|$ (if confined)

$e^-$ can be found anywhere within the $5\, \text{nm} \times \Delta x = 5\, \text{nm}$

$\Delta p \geq \frac{\hbar}{2\pi \Delta x} = 6.63 \times 10^{-34} (4\pi \times 5.00 \times 10^{-9}) = 1.06 \times 10^{-26} \, \text{kgms}^{-1}$

For a confined particle, $|p| \leq \Delta p = 1.1 \times 10^{-26} \, \text{kgms}^{-1}$ or more.

$K = p^2/2m = (1.06 \times 10^{-26})^2 (2 \times 9.11 \times 10^{-31}) = 6 \times 10^{-32} \, \text{J}$ or more

(Only 1 significant figure because this method is very rough)

$\psi$ & $\psi^2$ for Infinite Potential Well

- Simple. Don't need Schrödinger equation, de Broglie OK.
- Particle is confined $\therefore \psi$ similar to normal modes on a string.
- $U \to \infty$ at walls of I.P. well so particle can't go there; $\psi = \psi^2 = 0$ so node must occur at walls.
- Black down arrows $\downarrow$ where particle is most likely to be found.
- Red up arrows $\uparrow$ where particle is least likely to be found; $\psi = \psi^2 = 0$.

Energies for Infinite Potential Well

To find a formula for the energy levels:

- Use de Broglie equations:
  - $K = p^2/2m = h^2/2m\ell^2$.
  - Inside well $U=0 \therefore E_{\ell n} = K$ so;
  - $E_{\ell n} = h^2/2m\ell^2$ & $\ell_n = 2L/\ell$.

$E_n = \left( \frac{\hbar^2}{8mL^2} \right) \ell_n^2$.

Energy level diagram for I.P. Well

Suppose $e^-$ is confined to a 1-dimensional infinite potential well of width $1.00 \times 10^{-10} \, \text{m}$.

Draw an energy level diagram showing the first 4 levels.

$E_n = \left( \frac{\hbar^2}{8mL^2} \right) \ell_n^2$

"Ground state energy" is sometimes called "zero-point energy".
Text example HRW 40-2

- Electron is confined to a infinite potential well 100pm wide. It's in the n = 3 state, then absorbs a photon that raises it to n = 6 state. Find energy and wavelength of absorbed photon.

- Solution:
  \[ E_n = \frac{\hbar^2}{8mL^2} n^2 \]

  Photon (energy = h f) has increased energy of e^- by
  \[ E_n = (\hbar^2/8mL^2) (3^2 - 1^2) \]
  \[ = (6.63 \times 10^{-34})/(8 \times 9.11 \times 10^{-31} \times (100 \times 10^{-12})^2) \times (36 - 9) = 1.63 \times 10^{-16} \text{J} \]
  \[ = \hbar f = (6.63 \times 10^{-34} \times 3.00 \times 10^8)/(1.63 \times 10^{-16}) \]
  \[ = 1.22 \times 10^{-6} \text{m} \]

ψ & ψ² for Finite Potential Well

- If particle is trapped in a finite potential well, must solve Schrödinger's equation.
- ψ & ψ² for finite well similar to those in infinite well but weirder...
- Wavefunctions shown don't have same energy, but different shapes & orbital angular momentum.
- Need more quantum numbers to label all these orbitals.

REAL Finite Potential Well

- Circular wall formed from Fe atoms on Cu surface. "Quantum Corral". Diameter = 14nm

- Ripple inside is ψ² of a trapped electron seen from above

- Image made using a "Scanning Tunnelling Microscope" (STM)

Wavefunctions in Hydrogen

- Bohr model of hydrogen correctly predicts energy levels, but 2-D de Broglie wave picture of the wavefunctions is over-simplified. We need to solve Schrödinger equation in 3-D coulomb potential well

- Each Bohr orbit can be thought of as a spherically symmetric "electron shell" labelled with a quantum number n.
- Each shell divides into sub-shells which divide into orbitals with same energy, but different shapes & orbital angular momentum. Need more quantum numbers to label all these orbitals.

Quantum Numbers in Hydrogen

- n principal (shell) quantum number
  How much energy an e^- in that shell has (Bohr orbit number)
- l orbital angular momentum (sub-shell) q. number
  How much angular momentum an e^- in that sub-shell has
- m_l magnetic (orbital) q. number
  Which direction the e^- orbital angular momentum points in a magnetic field
- m_s e^- spin magnetic q. number
  Which direction the e^- spin points ("up" or "down") in mag. field

Don't worry too much about the precise definitions above, they are not examinable...
Orbitals in Hydrogen

• **n = 1 shell** (1 sub-shell, l=0 or s) (also called K shell)

  \[ m_l = 0 \]

  Each box is one orbital which fits two e\textsuperscript{-} states;
  spin up \( (m_s = +1/2) \) & spin down \( (m_s = -1/2) \)

• **n = 2 shell** (2 sub-shells, l=0,1 or s,p) (also called L shell)

  \[ m_l = 0, -1, 0, 1 \]

  m\textsubscript{l} values range from -1 to +1

• **n = 3 shell** (3 sub-shells, l=0,1,2 or s,p,d) (also called M shell)

  \[ m_l = 0, -1, 0, 1, -2, -1, 0, 1, 2 \]

  m\textsubscript{l} values range from -2 to +2

Chemist's orbitals

• Sub-shells can be sliced up into differently shaped orbitals.

• Chemists prefer a different set of orbitals because they illustrate chemical bonding more clearly e.g. \( p_x \), \( p_y \) & \( p_z \) orbitals