Quantum Mechanics: a short introduction

Gert Aarts

Swansea University
Prifysgol Abertawe

Quantum mechanics

- quantum mechanics is the basic theory underlying all of physics
- developed in the first part of the 20th century to address some fundamental questions
  - why are atoms stable?
  - what is light?
  - why do spectra from e.g. stars have discrete lines?
  - ...
- it has led to a revolution in physics, replacing classical (Newtonian) mechanics

Quantum mechanics

perhaps surprisingly, QM had immediate impact on the understanding of materials

- conductors
- insulators
- *superconductors*
- *semi-conductors*

and hence led to the development of

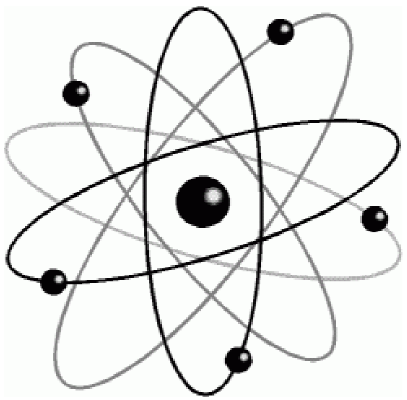
- transistors
- computer chips
- nanotechnology
- cell phones, tablets ...

Quantum mechanics

therefore, all the technology you are currently using builds on quantum mechanics

in this lecture, I want to highlight one feature of QM

- energy quantisation
- responsible for the stability of matter
- and ultimately material properties



Classical energy

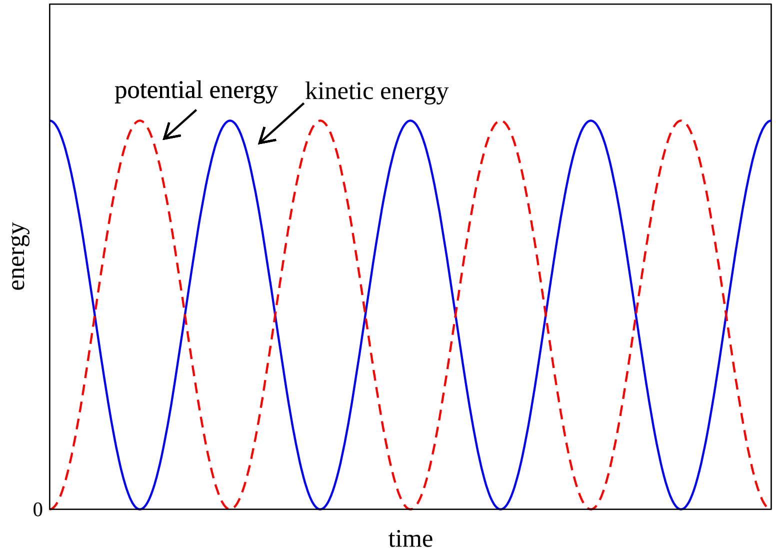
in Newtonian mechanics, the energy of a particle can take any value (modulo constraints)
example:

- particle in harmonic potential: $V(x) = \frac{1}{2}kx^2$
- total conserved energy:

$$E = K + V = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 \geq 0$$

- determined by initial conditions: here

$$x(t = 0) = 0$$
$$v(t = 0) = v_0$$



Quantum harmonic oscillator

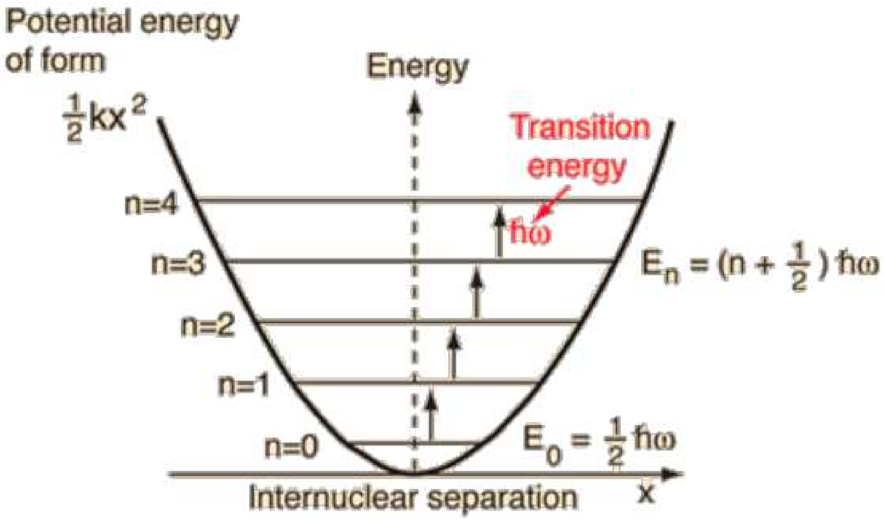
in quantum mechanics, energy is quantised: not all energy values are allowed

- harmonic oscillator, with spring constant $k = m\omega^2$:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad\qquad n = 0, 1, 2...$$

groundstate, state with lowest energy:

- classical: $E_0 = 0$, particle at rest in minimum of potential
- quantum: $E_0 = \frac{1}{2}\hbar\omega$, due to 'quantum fluctuations'
- $\hbar$ is Planck's constant



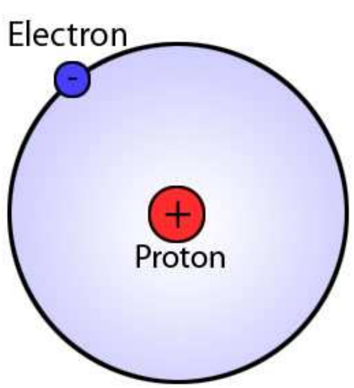
Quantum transitions

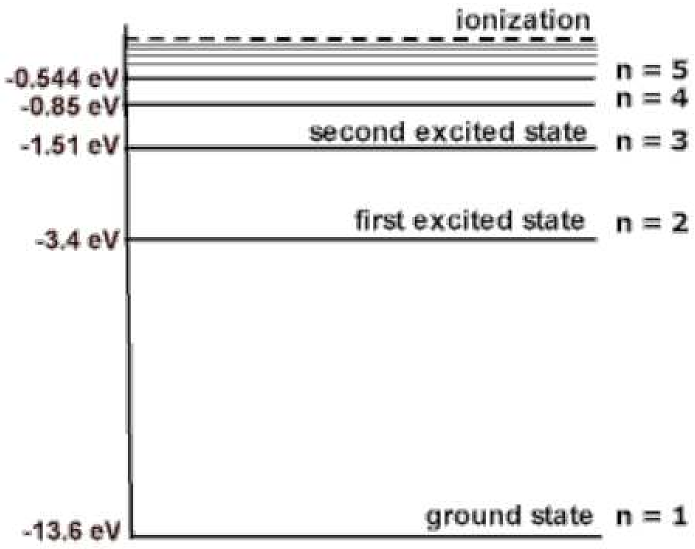
- energy changes discontinuously: $\Delta E = E_m - E_n$
- other transitions not allowed

also true in other systems, such as hydrogen atom

$$E_n = -\frac{13.6}{n^2}\,\text{eV} \qquad\qquad n = 1, 2, 3...$$

leads to stability of matter





Schrödinger equation

- these features follow from the Schrödinger equation
- postulated by Erwin Schrödinger in 1925
- describes dynamics of the wave function $\psi(t,x)$
- in one space dimension:

$$i\hbar\frac{\partial}{\partial t}\psi(t,x) = H\psi(t,x)$$

with the Hamiltonian (energy function)

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

of the form ‘kinetic $+$ potential energy’

Schrödinger equation

- this equation was devised, not derived
- spectrum of hydrogen and other systems is computable and agrees with observations
- meaning of wave function not immediately clear
- standard interpretation (Bohr, Born)

$$P(t,x) = |\psi(t,x)|^2$$

  probability density to find particle at position x at time t
- normalisation

$$\int_{-\infty}^{\infty} dx\, |\psi(t,x)|^2 = 1$$

  hence $\psi(t,x) \to 0$ as $x \to \pm\infty$

Solving the Schrödinger equation

partial differential equation

$$i\hbar\frac{\partial}{\partial t}\psi(t,x) = H\psi(t,x)$$

- elaborate solutions in general
- time-independent problem

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

- ordinary differential equation (in one dimension)

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$$

- analytically solvable for selected potentials

Solving the Schrödinger equation

harmonic oscillator: $V(x) = \frac{1}{2}m\omega^2 x^2$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right]\psi(x) = E\psi(x)$$

in this lecture: consider the groundstate only, $E = E_0$

ansatz: $\psi_0(x) = A_0 e^{-ax^2}$ normalisable, $a > 0$

compute:

$$\frac{d}{dx}\psi_0(x) = -2axA_0e^{-ax^2} = -2ax\psi_0(x)$$

$$\frac{d^2}{dx^2}\psi_0(x) = -2a\psi_0(x) - 2ax\frac{d}{dx}\psi_0(x) = \left(-2a + 4a^2x^2\right)\psi_0(x)$$

Solving the Schrödinger equation

- substitute in Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\left(-2a+4a^2x^2\right)+\frac{1}{2}m\omega^2x^2\right]\psi_0(x)=E_0\psi_0(x)$$

$$\left[\frac{\hbar^2 a}{m}-E_0+\left(-\frac{2\hbar^2a^2}{m}+\frac{1}{2}m\omega^2\right)x^2\right]\psi_0(x)=0$$

- nontrivial solution:

$$\frac{2\hbar^2a^2}{m}=\frac{1}{2}m\omega^2 \qquad E_0=\frac{\hbar^2 a}{m}$$

or

$$a=\frac{m\omega}{2\hbar} \qquad E_0=\frac{1}{2}\hbar\omega$$

Groundstate

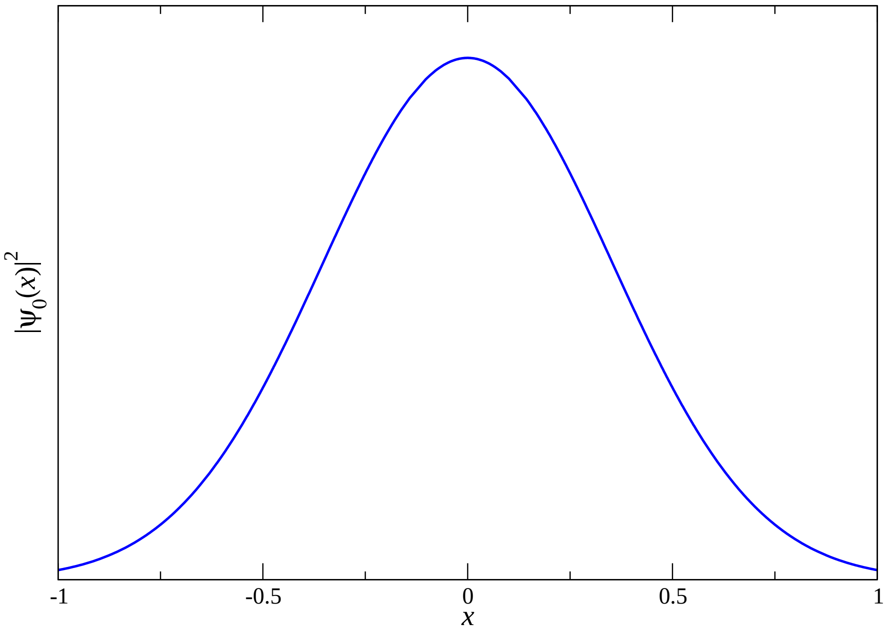
- wave function of the groundstate

$$\psi_0(x) = A_0 e^{-ax^2} \qquad a = \frac{m\omega}{2\hbar} \qquad E_0 = \frac{1}{2}\hbar\omega$$

- normalisation

$$\int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = 1$$

$$A_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

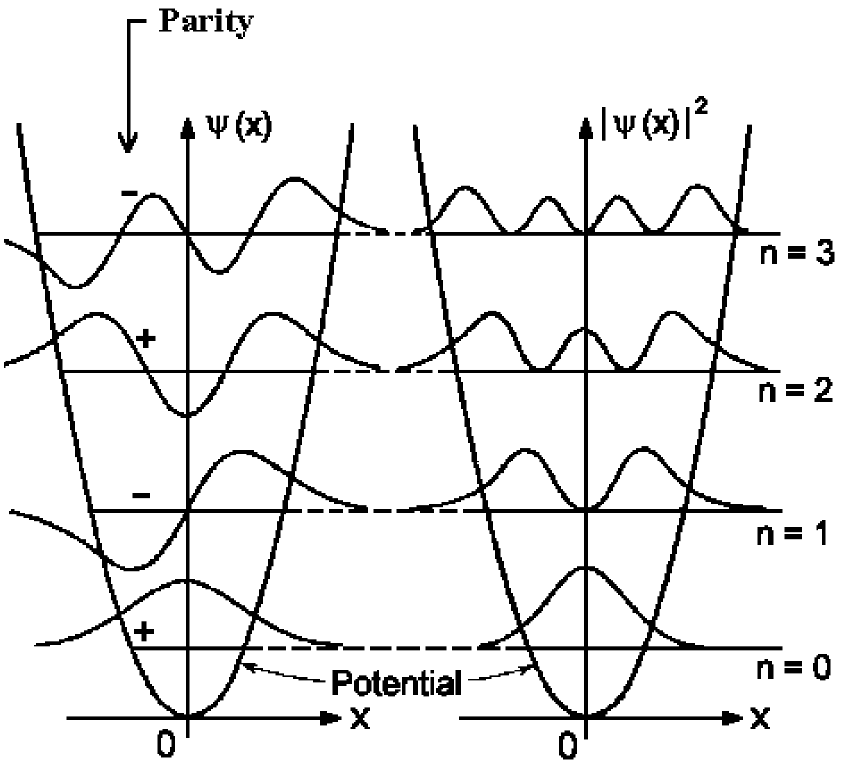


- classical dynamics:
groundstate $x = 0$

- quantum dynamics:
nonzero probability to detect particle anywhere!

Excited states

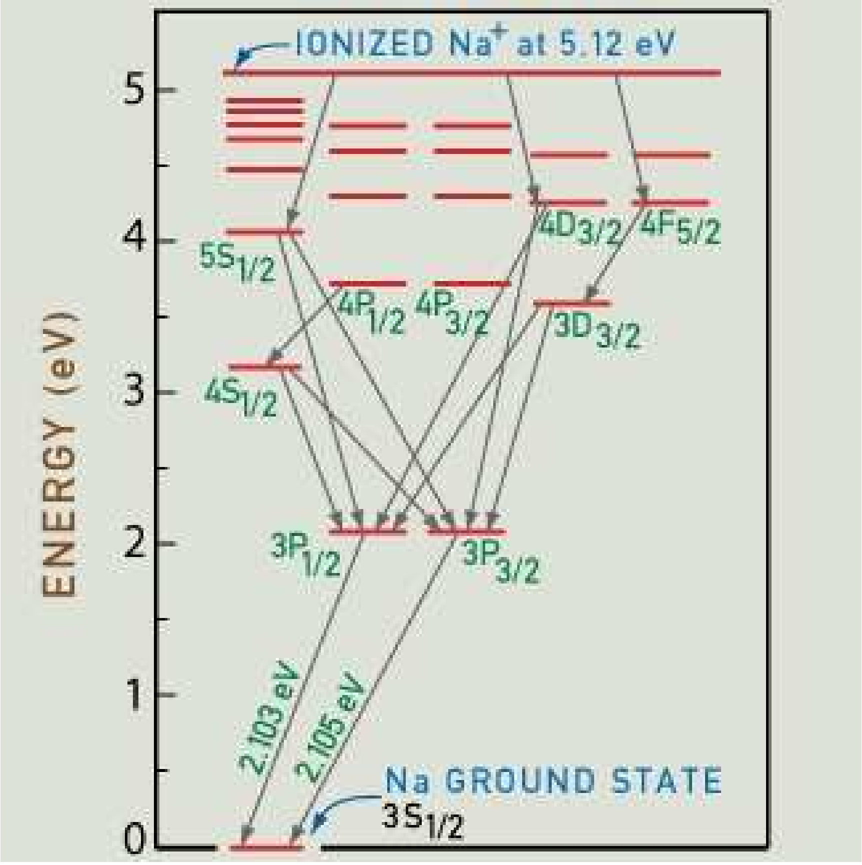
- extend calculation to states with higher energy



- every next wave function has additional zero
- alternate even and odd wave functions

More complicated spectra

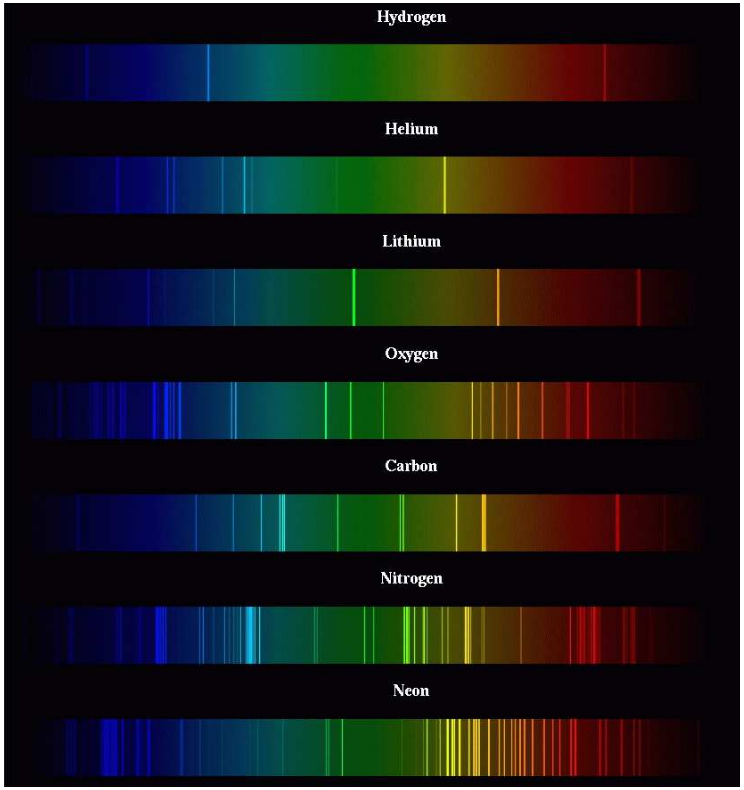
- extend to atoms and molecules
- example:



- spectrum of sodium

Application: Composition of stars

- light emitted by stars arises from transitions between energy levels in elements
- every element has a unique finger print



- observation of spectral lines determines composition

Quantum mechanics

- rich topic, taught at undergraduate and postgraduate level
- fundamental to our understanding of Nature
- ... the Universe
- ... applied science
- ... and of technology!