Quantum Transport: Atom to Transistor

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Lecture 6: Schrödinger Equation: Basic Concepts

Ref. Chapter 2.1

Network for Computational Nanotechnology

nanoHUB
online simulations and more

Retouch on Concepts

00:00

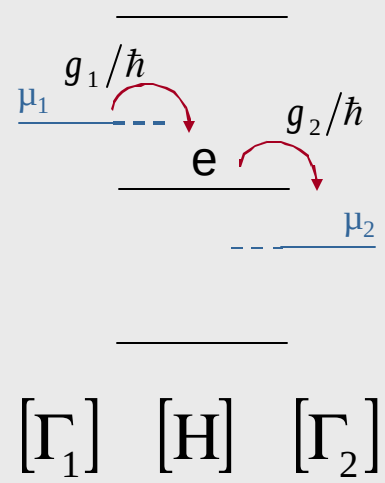
- Recall: In order for current to flow, states must lie between the two electro-chemical potentials

- And, in a multi-level conductor with ‘n’ energy levels we need nXn matrices to describe the single level analogues

e, ?$_{1,2}$, $D_e(E)$, U_{scf}, N:

$e \rightarrow [\mathrm{H}]$	Hamiltonian Matrix
$g_{1,2} \rightarrow [\Gamma_{1,2}(E)]$	Broadening Matrix
$2pD_e(E) \rightarrow [\mathrm{A}(E)]$	Spectral Function
$U_{\mathrm{scf}} \rightarrow [U_{\mathrm{scf}}]$	Self-Consistent Potential Matrix
$N \rightarrow [r]$	Density Matrix

General Picture



Next Few Lectures

02:30

- We will concentrate on how to write the Hamiltonian for various systems

- Start from simplest case and move up: Hydrogen atom (H) to Silicon atom (Si), to simple molecules (H_2), to solids

- Often to get the Hamiltonian for a given system we must use numerical methods (e.g. finite difference method)

- For anything more complicated than the Hydrogen atom we cannot use analytic methods

- Many practical problems requiring numerical methods can be solved quickly on a PC

- So, where does Hamiltonian come from? *Answer: The Schrödinger Equation*

- This lecture: The Schrödinger Equation
- Next lecture: Finite Difference Method
- Subsequent lecture: examples

The Schrödinger Equation

08:35

- The Schrödinger Equation:

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

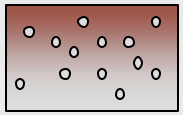
- Original motivation for creating the Schrödinger Equation comes from discrete photon emission energy bands that were observed when Hydrogen-like atoms were heated. These energy levels could not be explained using classical physics

- The photon emission bands did, however, follow a pattern: $h\nu = E_0(1/n^2 - 1/m^2)$.

such that each higher internal atomic energy level related to a ground state energy with the integer ratio $E_n = E_o/n^2$

Discrete Energy Spectrum

Heat up a Hydrogen-like gas…



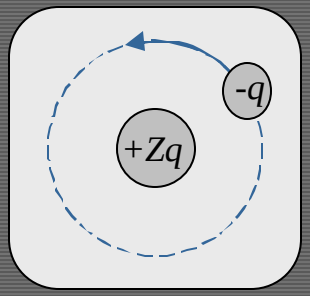
Discrete Energy Spectrum observed

$h\nu$

Classical Model for Atom

14:02

- First step was to use classical physics. Picture a single electron orbiting a nucleus of charge +Zq (this is the Hydrogen-like atom)



- Equate electrostatic and centripetal forces:

$$\frac{Zq^2}{4\pi\varepsilon_0 r^2} = \frac{m\mathrm{v}^2}{r} \quad \text{Thus,} \quad \mathrm{v}^2 = \frac{Zq^2}{4\pi\varepsilon_0 mr}$$

- And electron energy is given as:
  E = Potential + Kinetic

$$= \frac{-Zq^2}{4\pi\varepsilon_0 r} + \frac{1}{2}m\mathrm{v}^2 = \frac{-Zq^2}{4\pi\varepsilon_0 r} + \frac{1}{2}m\left(\frac{Zq^2}{4\pi\varepsilon_0 mr}\right)$$

$$= \frac{-Zq^2}{8\pi\varepsilon_0 r}$$

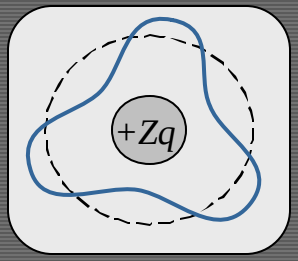
- But this is wrong!
  - Energy is not discrete (r is continuous)!
  - The electron is under continual centripetal acceleration and so must radiate EM waves, eventually collapsing into the nucleus.

Bohr Model

17:32

- How do we get around this problem?
- de Broglie suggested that we endow the electron with wave like properties to get discrete energies.
- A wavelength ? would be associated to the electron.
  $? = h/(mv)$
- Using this concept, circumference of a Hydrogen-like atom, must be an integer multiple of ? such that:
  - $2pr = n? = n(h/mv)$

Electron wave harmonic orbital about a Hydrogen-like atom



- So, with a wave like character, only certain radii are allowed
- Surprisingly, for a Hydrogen-like atom this gives the correct energy levels, substituting back into the classical equations we get:

- $$r_n = \left(\frac{n^2}{Z}\right)a_0, \text{ where } \quad a_0 = \frac{4pe_0\hbar^2}{mq^2}$$
- $$E_n = -\left(\frac{Z^2}{n^2}\right)E_0, \text{ where } \quad E_0 = \frac{q^2}{8pe_0a_0}$$

Vibrating String

22:34

•This heuristic insight was put on a solid basis by the Schrödinger Equation:

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

• How does the Schrödinger Equation lead to discrete energy levels?

• Consider a vibrating string

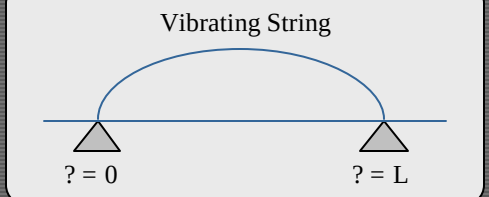
• The general one-dimensional wave equation is:

$$\frac{\partial^2 u}{\partial t^2} = \mathrm{v}^2 \frac{\partial^2 u}{\partial u^2}$$

where $u = Ae^{ikx}e^{-i?t}$ v: speed

and $?^2 = \mathrm{v}^2 k^2$

• If we tie down the two ends …



Infinite Square Well

27:08

• … then the wave equation of the string becomes: $u = A\,sin(kx)\,e^{-i?t}$, where:
• $k = np/L$, and $? = vk$
hence certain discrete frequencies:

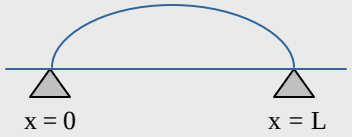
$$? = npv/L$$

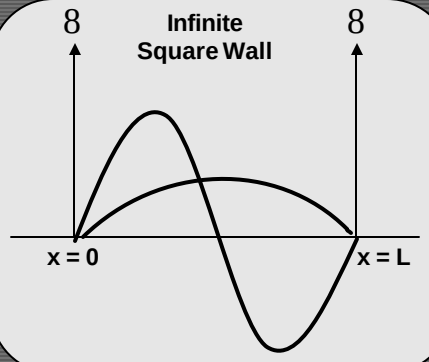
• The quantum analogue of a 1-dimensional vibrating string is the particle in a box (or infinite square well)

• The 1-dimensional Schrödinger Equation is:

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

Harmonically oscillating string





Solution to the Infinite Square Well

32:09

• In free space, solution to the 1-dimensional Schrödinger Equation gives:

$$\Psi(x,t) = e^{\pm ikx} e^{-iEt/\hbar} \qquad \therefore E = \frac{\hbar^2 k^2}{2m}$$

• In the infinite square well, boundary conditions are such that ? = 0 at x= 0 and x = L

• Thus, inside the infinite square well we get

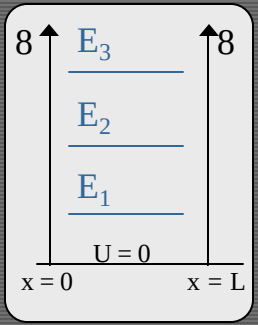
$?(x,t) = \sin(kx) e^{-iEt/h}$, where $k=(np)/L$

and

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 p^2 n^2}{2mL^2} (n = 1,2,3...)$$

Just like the vibrating string!

Infinite Square Well with Discrete Energy Levels

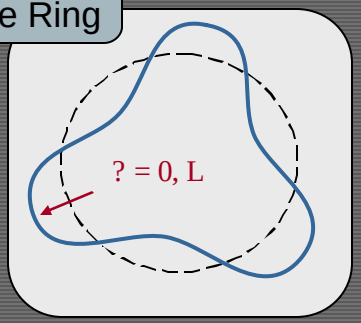


• Therefore, as seen here, we get discrete energy levels

• To solve the Schrödinger Equation for the Hydrogen atom requires more algebra, but qualitatively the result is the same

The Ring, another kind of box

The Ring



- Why do we sometimes use a ring instead? *Answer: Mathematically it is a whole lot easier to manage (i.e. with solids)*

- *Makes use of periodic boundary conditions*

- Often when boundary conditions don't really matter we use a ring

- The ring structure has eigenfunctions :

$? = \sin(kx)e^{-iEt/h}$ and

$? = \cos(kx)\, e^{-iEt/h}$

or otherwise formulated as …

$? = Ae^{+ikx}e^{-iEt/h}$ and

$? = Ae^{-ikx}e^{-iEt/h}$

In each case the corresponding Eigenvatues are: $k=(2pn)/L$, where n = 1,2,3…

- Carbon nanotubes are probably the only real example where the periodic boundary condition is real and not just a mathematical convenience.

Meaning of ?

46:36

- What does ? really represent?

- It is believed that ? *? gives a probability distribution.

- Add the probability distribution of all electrons to get the electron density.

- So, for lots of levels, electron density is given by:

$$n = \sum_i (\Psi_i^*)\Psi_i$$

- Next: Method of finite differences