Quantum Transport: Atom to Transistor

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Lecture 6: Schrödinger Equation: Basic Concepts
Ref. Chapter 2.1

Network for Computational Nanotechnology
General Picture

• 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

\[ e, \gamma_{1,2}, D_{\alpha}(E), U_{scf}, N: \]

\[ \varepsilon \rightarrow [H] \quad \text{Hamiltonian Matrix} \]

\[ \gamma_{1,2} \rightarrow [\Gamma_{1,2}(E)] \quad \text{Broadening Matrix} \]

\[ 2\pi D_{\varepsilon}(E) \rightarrow [A(E)] \quad \text{Spectral Function} \]

\[ U_{scf} \rightarrow [U_{scf}] \quad \text{Self-Consistent Potential Matrix} \]

\[ N \rightarrow [\rho] \quad \text{Density Matrix} \]

Retouch on Concepts
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 (H₂), 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:
\[ i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) + U(\vec{r})\Psi(\vec{r}, t) \]

• 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: 
\[ \hbar \nu = E_0 \left( \frac{1}{n^2} - \frac{1}{m^2} \right) \]

such that each higher internal atomic energy level related to a ground state energy with the integer ratio 
\[ E_n = E_0 / n^2 \]

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

\[
\frac{Zq^2}{4\pi\varepsilon_0 r^2} = \frac{mv^2}{r} \quad \text{Thus,} \quad v^2 = \frac{Zq^2}{4\pi\varepsilon_0 mr}
\]

• Equate electrostatic and centripetal forces:

\[
E = \text{Potential} + \text{Kinetic}
\]

\[
= -\frac{Zq^2}{4\pi\varepsilon_0 r} + \frac{1}{2} mv^2 = -\frac{Zq^2}{4\pi\varepsilon_0 r} + \frac{1}{2} m \left( \frac{Zq^2}{4\pi\varepsilon_0 mr} \right)
\]

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

• And electron energy is given as:

• 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.
• 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 $\lambda$ would be associated to the electron. $\lambda = h / (mv)$
  • Using this concept, circumference of a Hydrogen-like atom, must be an integer multiple of $\lambda$ such that:
    • $2pr = n\lambda = n(h / mv)$

• 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:

$$r_n = \left(\frac{n^2}{Z}\right) a_0,$$
where $a_0 = \frac{4\pi\varepsilon_0 h^2}{mq^2}$

$$E_n = -\left(\frac{Z^2}{n^2}\right)E_0,$$
where $E_0 = \frac{q^2}{8\pi\varepsilon_0 a_0}$
• 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

\[ \frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \]

where \( u = Ae^{ikx}e^{-i\omega t} \)

and \( \omega^2 = v^2k^2 \)

• If we tie down the two ends …

Vibrating String

\( ? = 0 \quad ? = L \)
... then the wave equation of the string becomes: \( u = A \sin(kx) \ e^{-i\omega t} \), where:
- \( k = np/L \), and \( \omega = v_k \)
hence certain discrete frequencies:
\( \omega = npv/L \)

- 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:

\[
\frac{i\hbar}{\partial t} \frac{\partial \Psi}{\partial x} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}
\]
• In free space, solution to the 1-dimensional Schrödinger Equation gives:

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

• In the infinite square well, boundary conditions are such that \( \Psi = 0 \) at \( x = 0 \) and \( x = L \)

• Thus, inside the infinite square well we get

\[ \Psi(x,t) = \sin(kx)e^{-iEt/\hbar}, \text{ where } k = (np)/L \]

and

\[ E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \quad (n = 1, 2, 3, ...) \]

Just like the vibrating string!

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

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

  \[ \psi = \sin(kx)e^{-iEt/h} \]
  \[ \psi = \cos(kx)e^{-iEt/h} \]

  or otherwise formulated as ...

  \[ \psi = Ae^{ikx}e^{-iEt/h} \] and
  \[ \psi = Ae^{-ikx}e^{-iEt/h} \]

  In each case the corresponding eigenvalues are: \( k = (2\pi n)/L \), 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.
• What does $\Psi$ really represent?
• It is believed that $\Psi^*$ 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:
  \[ n = \sum_i (\Psi_i^*) \Psi_i \]