

Quantum Transport:

Atom to Transistor

Prof. Supriyo Datta
ECE 659
Purdue University

01.31.2003

Lecture 8: Schrödinger Equation: Examples

Ref. Chapter 2.3



Network for Computational Nanotechnology



Retouch on Concepts

00:00

- Recall, the analytical form of the Schrödinger Equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = H_{op} \Psi(\vec{r}, t)$$

where $H_{op} = \frac{-\hbar^2}{2m} \nabla^2 + U(\vec{r})$

- In numerical form: $i\hbar \frac{\partial}{\partial t} \{ \Psi \} = [H] \{ \Psi \}$

With the eigenvalue equation $[H] \{ a \} = E_a \{ a \}$

Last time we looked at the Schrödinger Equation in one dimension. Along 'x' a discrete set of lattice points were placed.

With the discrete set of lattice points shown on the right, the Schrödinger Equation was converted into a difference equation.

Summary:

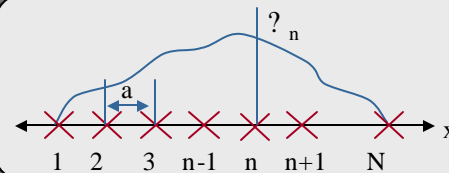
Ψ - became a column vector

U - became a diagonal NxN matrix

$\frac{-\hbar^2}{2m} \nabla^2$ - became a tri-diagonal NxN matrix

- And the corresponding eigenvectors and eigenvalues form a set by which wave functions may be represented as a linear combination of eigen vectors.

$$\{ \Psi \} = \sum_a C_a \{ a \} e^{-iE_a t / \hbar}$$



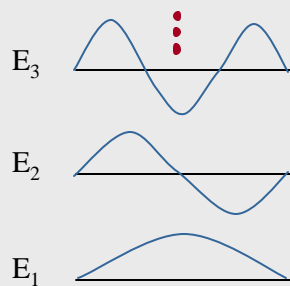
Retouch on Concepts

05:21

Finally, it is important to emphasize that eigenvalues correspond to energies and eigenvectors to wavefunctions.

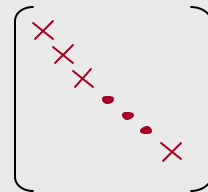
Computationally it is rather easy to find matrix eigenvectors and eigenvalues. For example in Matlab we simply call "[V,D]=eig(H)".

Wave Functions and Energies

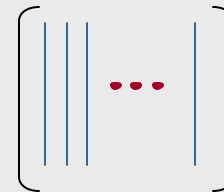


Matrix D provides the eigenvalues in a diagonal matrix and Matrix V provides the corresponding eigenvectors as columns of a square matrix.

D=



V=



Separating Variables

08:39

- The main advantage of the numerical method is that once it is solved for a particular dimensional structure, that same method may then be applied with little difficulty to other scenarios of the same nature.

Example: The slanted well has a complicated analytical solution (involving Airy Functions) but numerically the solution is the same as that implemented for the infinite square well.

Slanted Well



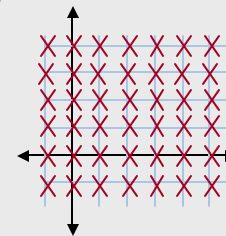
- So, how do we go beyond the one dimensional numerical solution seen thus far?
- In two dimensions the Hamiltonian operator looks like:

$$Hop = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + U(x, y)$$

The lattice for this operator is shown below .

It is straight forward to extend the finite difference method to two dimensions, the main problem is size. i.e

100x100 pts=10,000 pts



Reducing the Lattice

14:32

- One solution is to separate the 2-D problem into two 1-D. However, this is only possible if the potential is separable:

$$U(x, y) = U_x(x) + U_y(y)$$

- Analytically this is done by separation of variables.

Let, $\Psi(x, y) = X(x) \times Y(y)$

Thus, $E_x X(x) = \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U_x(x) \right] X(x)$

$$E_y Y(y) = \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + U_y(y) \right] Y(y)$$

Where $E = E_x + E_y$

From,

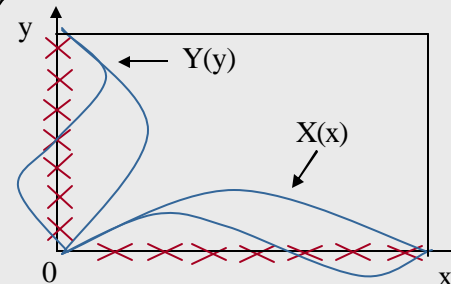
$$E\Psi(x, y) = \left[\frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + U(x, y) \right] \Psi(x, y)$$

time independent form

- Numerically this translates into two 1-D lattices (one for the x-axis and one for the y-axis).

- For example, take a two dimensional infinite square well:

2-D Infinite Square Well

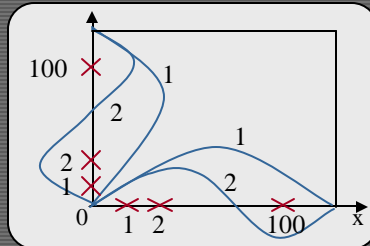


2-D Infinite Square Well

22:00

- Numerically if we split the x and y lattices by 100 points. How many eigenvectors will result?

Infinite Square Well



- Ans: Total=100x100=10000 eigenvectors. We combine $X(x)$ and $Y(y)$ functions such that $\psi_{nm}(x,y) = X_n(x) Y_m(y)$

- Notice that two eigenvectors with the same $m+n$ value do not necessarily have the same energy:
- Take eigenvectors $\{\psi_{22}\}$ and $\{\psi_{13}\}$, which has more energy?

$$\text{Recall: } E_n = \frac{\hbar^2 p^2 n^2}{2mL^2}$$

$$\therefore (E_{13} = E_1 + E_3) > (E_{22} = E_2 + E_2)$$

- Now what about a 3-D infinite square well or a 3-D box? The same thing, separation of variables gives eigenfunctions of $\psi_{111}, \psi_{112}, \dots$ etc.

Hydrogen Atom

27:16

- Consider the Hydrogen Atom, can it be handled by separation of variables?
- The Hydrogen atom cannot be separated in Cartesian coordinates

$$H_{op} = \frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - \frac{q^2}{4\pi\epsilon_0 \sqrt{x^2 + y^2 + z^2}}$$

But it can be separated in spherical coordinates such that U becomes

$$\frac{-q^2}{4\pi\epsilon_0 r}$$

- Note: A similar approach can be taken with all atoms but not with molecules because you don't have this spherical symmetry.
- So separation of variables in spherical coordinates gives the radial Hamiltonian as:

$$\frac{-\hbar^2}{2m} \left[\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{L(?, f)}{r^2} \right] - \frac{q^2}{4\pi\epsilon_0 r}$$

- In general ? becomes

$$\Psi(r, ?, f) = R(r)\Theta(?)\Phi(f)$$

Hydrogen Atom

Time = 34:40

- Note: The radial equation

$$ER(r) = \frac{-\hbar^2}{2m} \left[\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) \right] R(r) + \left(\frac{-\hbar^2 l(l+1)}{2m r^2} - \frac{q^2}{4\pi\epsilon_0 r} \right) R(r)$$

can be simplified by letting $R(r) = f(r)/r$

Thus,
$$\frac{dR(r)}{dr} = \frac{f'(r)}{r} - \frac{f(r)}{r^2}$$

$$\frac{d^2 R(r)}{dr^2} = \frac{f''(r)}{r} - \frac{f'(r)}{r^2} - \frac{f'(r)}{r^2} + \frac{2f(r)}{r^3}$$

$$\therefore \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) R(r) = \frac{f''(r)}{r}$$

- Hence, the entire radial equation simplifies to:

$$Ef(r) = \frac{-\hbar^2}{2m} \frac{d^2 f(r)}{dr^2} - \frac{q^2}{4\pi\epsilon_0 r} f(r) + \frac{\hbar^2 l(l+1)}{2m r^2} f(r)$$

- Furthermore, the radial equation gives the s,p,d levels of the hydrogen atom for different values of "l":

s: l=0

p: l=1

D: l=2, etc

Hydrogen Atom

40:54

- How do we get a numerical solution to the hydrogen atom?
- Ans: We set up a discrete axis along a radial axis and solve the appropriate radial Hamiltonian matrix for $l=0, 1, 2, \dots$



- Back to the hydrogen Hamiltonian, where does $l(l+1)$ come from?
- Ans: $l(l+1)$ forms the eigenvalues of the spherical harmonics or angular part of

$$\Psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

- Where,

$$L(\theta, \phi) = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2},$$

and $Y_l^m = \Theta_l(\theta)\Phi_m(\phi)$

$$L(\mathbf{q}, \mathbf{f}) Y_l^m = -l(l+1) Y_l^m$$

- Note: The angular term, Y_l^m , is the same for all atoms which results in isotropic behavior. It is only the radial term that changes.



Summary

49:01

- Closing Notes:

- For higher dimensions use separation of variables whenever possible.
- Separable solutions are of the form $\Psi(r, \theta, \phi) = R(r)Y_l^m(\theta, \phi)$
- The angular term is the same for all separable spherical solutions.
- For hydrogen-like atoms the radial term can be treated as a 1-D numerical problem with coulomb potential
$$\frac{-Zq^2}{4\pi\epsilon_0 r}$$

and angular “potential”
$$+ \frac{\hbar^2 l(l+1)}{2mr^2}$$