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Schrodinger Equation

The important part of a transport equation is the Hamiltonian. So, as a first step is understanding the transport properties of a system, one has to learn how to write down the Hamiltonian matrix for a given device structure.

2.1 Hydrogen Atom

Important equations:

Bohr radius:

$$r_n = \frac{n^2}{Z} a_0 \tag{1}$$

where $a_0 = 4\pi\epsilon_0 \hbar^2 / mq^2 = 0.0529nm$

Orbital energy:

$$E_n = -\frac{Z^2}{n^2} E_0 \tag{2}$$

where $E_0 = q^2 / 8\pi\epsilon_0 a_0 = 13.6eV(1Rydberg)$

2.2 Method of Finite Differences

So given a partial differential equation, we convert it into a matrix equation.

$$\begin{gathered} \text{wavefunction } \Psi(\vec{r}, t) \to \text{column vector } \{\Psi(t)\} \\ \text{differential operator } H_{op} \to \text{matrix } [H] \end{gathered} \tag{3}$$

The Schrodinger equation then becomes:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = H_{op} \Psi(\vec{r}, t) \to i\hbar \frac{\partial}{\partial t} \{\Psi(\vec{r}, t)\} = [H_{op}]\{\Psi(\vec{r}, t)\} \tag{4}$$

An essential step in solving the Schrodinger equation using numerical method is to obtain the matrix representing the Hamiltonian operator.

$$H_{op} = -\frac{\hbar}{2m}\frac{d^2}{dt^2} + U(x) \tag{5}$$

> Basically, what we are doing is to turn a differential equation into a difference equation.

Using the *finite difference method*, the discretized version of the second derivative is:

$$\frac{d^2\Psi}{dt^2} \to \frac{1}{a^2}(\Psi(x_{n+1}) - 2\Psi(x_n) + \Psi(x_{n-1})) \tag{6}$$

The potential discretization is simple,

$$U(x)\Psi(x) \to U(x_n)\Psi(x_n) \tag{7}$$

Thus, we can write the Schrodinger equation as follow:

$$\begin{aligned}
i\hbar\frac{d\Psi_n}{dt} &= [H_{op}\psi]_{x=x_n} && (8)\\
&= -\frac{\hbar}{2m}\frac{1}{a^2}[\Psi(x_{n+1}) - 2\Psi(x_n) + \Psi(x_{n-1})] + U(x_n)\Psi(x_n) && (9)\\
&= \left(U(x_n) + 2\frac{\hbar}{2m}\frac{1}{a^2}\right)\Psi(x_n) - \frac{\hbar}{2m}\frac{1}{a^2}\Psi(x_{n+1}) - \frac{\hbar}{2m}\frac{1}{a^2}\Psi(x_{n-1}) && (10)\\
&= (U_n + 2t_0)\Psi_{x_n} - t_0\Psi_{x_{n+1}} - t_0\Psi_{x_{n-1}} && (11)\\
&= \sum_m (U_n + 2t_0)\delta_{n,m} - t_0\delta_{n,m+1} - t_0\Psi_{n,m-1} && (12)
\end{aligned}$$

Note: $t_0 = \frac{\hbar}{2m}\frac{1}{a^2}$ and $U_n = U(x_n)$

It is easy to see that the element of the Hamiltonian matrix is,

$$H_{n,m} = (U_n + 2t_0)\delta_{n,m} - t_0\delta_{n,m+1} - t_0\Psi_{n,m-1} \tag{13}$$

The matrix representing H looks like a tridiagonal matrix of form:

$$\begin{bmatrix}
2t_0 + U_n & -t_0 & 0 & 0 & \cdots & 0 \\
-t_0 & 2t_0 + U_n & -t_0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & -t_0 & 2t_0 + U_n & -t_0 & 0 \\
0 & 0 & 0 & 0 & -t_0 & 2t_0 + U_n
\end{bmatrix} \tag{14}$$

> For a given potential function U(x) it is straightforward to setup this matrix, once we have chosen an appropriate lattice spacing a.

2.3 Examples

2.3.1 Particles in a box

2.3.2 Particle in a 3D "box"