Lecture2

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Laplacian operator

- Laplacian operator (∇^2) in 3D
  - In the cartesian coordinate, it is given by

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

- Laplacian operator (∇^2) in 1D
  - In this case, it is reduced to

$$\nabla^2 = \frac{d^2}{dx^2}$$

  - It is simply the second order differentiation.

Where can we find it?

- The infinte potential well problem

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$$

  - Therefore, solving the Schrödinger equation is just to calculate the eigenvalue/eigenfunction of the Laplacian operator.
  - Analytic solutions ($\cos kx$ and $\sin kx$) are known.
  - Our goal is *<u>its discretization</u>*.

Discretization

- Let us assume that we have N points in $[0, a]$.
  - When they are uniformly distributed, the i-th point is given by
$$x_i = \frac{i-1}{N-1}a = (i-1)\Delta x$$
  - Then, the wavefunction, $\psi(x)$, can be described with a vector of $[\psi_2 \quad \psi_3 \quad \psi_4 \quad \psi_5 \quad \cdots \quad \psi_{N-4} \quad \psi_{N-3} \quad \psi_{N-2} \quad \psi_{N-1}]^T$.
  - Of course, $\psi_i = \psi(x_i)$ and the boundary conditions are imposed.
  - In such a case, the second derivative can be approximated by
$$\left.\frac{d^2\psi}{dx^2}\right|_{x=x_i} \approx \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1})}{\Delta x^2}$$

Matrix form

- Consider a case of $N = 5$.
  - Then, $\psi(x)$, can be described with a small vector of $[\psi_2 \quad \psi_3 \quad \psi_4]^T$.
  - The Laplacian operator maps the above vector into

$$\frac{1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix}\begin{bmatrix} \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

  - It can be regarded as a discretized version of $\frac{d^2\psi(x)}{dx^2}$.

Eigenvalue problem

- Assume a natural number, N (≥ 2).
  - For a square matrix, A, whose size is $N \times N$, an eigenvalue (λ) and the corresponding eigenvector (x) satisfy

$$Ax = \lambda x$$

  - Example)

$$A = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

It is found that $\lambda = 3$ or $\lambda = 1$. Also corresponding eigenvectors are $[1 \quad -1]^T$ and $[1 \quad 1]^T$, respectively.

Infinite potential well ($N = 5$)

- Recall that the problem looks like:

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

- In a matrix form (with the boundary conditions),
  - It is simply given by

$$\frac{1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix}\begin{bmatrix} \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = -k^2\begin{bmatrix} \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

where $\Delta x = \frac{a}{4}$.

  - How can we solve it numerically?

MATLAB example

- MATLAB is just one possible way to do it.
  - You can use any language of your preference!
- First, set the matrix, A.

```
A = [-2.0 1.0 0.0; 1.0 -2.0 1.0; 0.0 1.0 -2.0];
```

- Calculate the eigenvalues.

```
[V,D] = eig(A)
```

  - Each diagonal component of D represents an eigenvalue.
  - Each column of V represents the corresponding eigenvector.
  - For more information, see the MATLAB manual for a function, eig.

Physical interpretation

- Eigenvalues are -3.4142, -2.0000, and -0.5858.
  - Which one is for the ground state energy?
  - It is noted that the eigenvalue is $-k^2(\Delta x)^2$.
  - Therefore, -0.5858 is for the smallest k^2.
  - In an analytic solution, the smallest k^2 is $\left(\frac{\pi}{a}\right)^2$.
  - The energy is obtained from $E = \frac{\hbar^2}{2m}k^2$.

Practical number

- Example)
  - Assume a = 5 nm and $m = 0.91\, m_0$. (m_0 is the electron rest mass.)
  - Then, Δx = 1.25 nm and $k^2(\Delta x)^2$ = 0.5858.
  - So, k^2 = 3.749X10^{17} m^{-2}. ← Compare it with the analytic solution!
  - Finally, $E = \frac{\hbar^2}{2m} k^2 = 2.5148 \times 10^{-21}\ \mathrm{J} = 0.0157\ \mathrm{eV}$.
- Of course, a higher N value gives a better result.
  - Draw the error of the ground state energy as a function of N.

Homework#2

- Due: AM08:00, September 10
- Problem#1
  - Write a simple code for solving the infinite potential well problem.
  - In this case, the effective mass is $0.19\,m_0$.
  - Use three different values of N. (5, 50, and 500)
  - Upload your code.
  - Upload your report, too.