Lecture 10

Numerical Solutions-Poorman's Quantum Mechanics

Study Goal of This Lecture

- Schrödinger equation in matrix form
- Quantum dynamics
- Matlab demo(slide)

10.1 Schrödinger Equation in 1-D

Following the principle that once a "basis " is given, the wave function can be written as a vector.

$$\text{basis: } \{\phi_n\},\ \Psi = \sum_n C_n \phi_n. \tag{10.1}$$

Hereafter for simplicity, we assume the basis functions are orthonormal. In Dirac notation, the wave function is a ket, i.e. a column vector

$$|\Psi\rangle = \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ . \\ . \\ C_n \end{pmatrix},\ \text{write in } \{\phi_n\} \text{ basis, and the length is N.(truncated)} \tag{10.2}$$

Note that in principle a ket has infinite dimensions, but in reality one must always truncate at a certain number $N \Rightarrow N$ coefficients. Then, an operator, which transforms a vector to another vector, is an $N \times N$ matrix. The transformation is linear. So, solving Schrödinger equation means we construct the Hamiltonian matrix $\hat{H}$, then find the eigenvector and eigenvalues of the matrix.

$$\underbrace{\hat{H}}_{matrix} |\psi_n\rangle = E_n \underbrace{|\psi_n\rangle}_{vector} . \tag{10.3}$$

Now, we ask: Given $\{|\phi_n\rangle\}$ basis set, how do we write down $\hat{H}$ in $\{|\phi_n\rangle\}$?
The matrix element!

$$\hat{H} = \begin{array}{c} \\ \langle\phi_1| \\ \langle\phi_2| \\ \langle\phi_3| \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccc} |\phi_1\rangle & |\phi_2\rangle & |\phi_3\rangle & \cdots \end{array} \\ \begin{pmatrix} \langle\phi_1|\hat{H}|\phi_1\rangle & \langle\phi_1|\hat{H}|\phi_2\rangle & \langle\phi_1|\hat{H}|\phi_3\rangle & \cdots \\ \langle\phi_2|\hat{H}|\phi_1\rangle & \langle\phi_2|\hat{H}|\phi_2\rangle & \cdots & \cdots \\ \vdots & \vdots & \ddots & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \end{array}, \tag{10.4}$$

$$H_{nm} = \langle\phi_n|\hat{H}|\phi_m\rangle = \int \phi_n^* \hat{H} \phi_m d\tau. \tag{10.5}$$

Note that if $\{\phi_n\}$ are eigenvalue of $\hat{H}$, then the matrix element is

$$H_{nm} = \langle\phi_n|\hat{H}|\phi_m\rangle = \langle\phi_n|\epsilon_m|\phi_m\rangle = \epsilon_m \langle\phi_n|\phi_m\rangle = \epsilon_m \delta_{nm}, \tag{10.6}$$

then the Hamiltonian:

$$\hat{H} = \begin{pmatrix} \epsilon_1 & 0 & 0 & \cdots \\ 0 & \epsilon_2 & 0 & \cdots \\ 0 & 0 & \epsilon_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{10.7}$$

$\hat{H}$ is diagonal in the eigenbasis of $\hat{H}$. This is why solving eigenvalue problem is also called diagonalization of a matrix in linear algebra. In computer, solving eigenvalue problem/diagonizing a martix is a routine procedure. (In matlab ,the command is eig().)

10.2 Poorman's Discrete Value Representation(Grid method)

Now if we can find a matrix representation for Hamiltonian, a general one particle Hamiltonian in 1-D is

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \hat{V}(x) = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}(x). \tag{10.8}$$

To write the matrix form, we only need to find a suitable basis. If the 1-D harmonic oscillator basis is adapted, we may transform:

$$\begin{cases} \hat{x} \longrightarrow \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}), \\ \hat{p} \longrightarrow i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}^\dagger - \hat{a}), \end{cases} \tag{10.9}$$

and use the occupation number basis $\{|n\rangle\}$ to construct the Hamiltonian. This is actually often used. But we may also adopt a even more intuitive/simple basis. i.e. discrete grid points! Think about how do you "plot" the function?

$$\phi_0 = \phi_0(x) = \frac{m\omega}{\pi\hbar}^{\frac{1}{4}} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}. \tag{10.10}$$

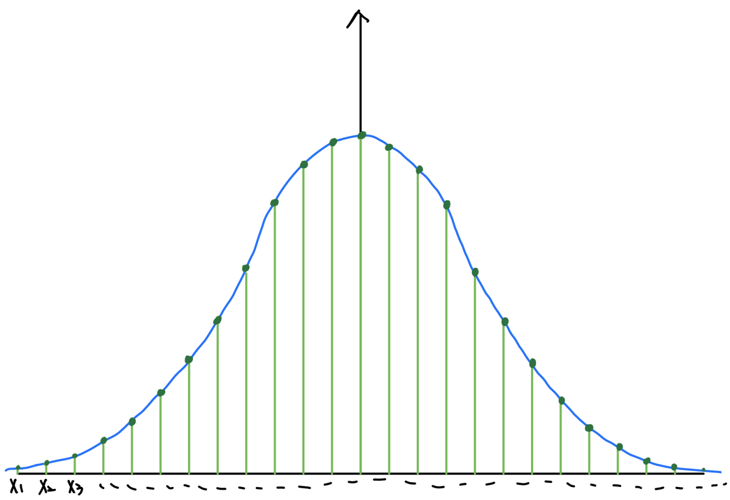

Figure 10.1: Wave function of harmonic oscillator $n = 0$

We can choose an equally spaced "grid": of N points on x: $(x_1, x_2, x_3, \cdots, x_N)$ and represent

$$|\phi_0\rangle = \begin{pmatrix} \phi_0(x_1) \\ \phi_0(x_2) \\ \phi_0(x_3) \\ \phi_0(x_4) \\ . \\ . \\ \phi_0(x_N) \end{pmatrix}. \tag{10.11}$$

This is a discrete representation of the function, actually, when we save the function in a computer, this is done all the time. But how about the Hamiltonian? consider the potential energy part firstly, and it is trivial:

$$\hat{V}\Psi = V(x)\Psi, \ \therefore \hat{V}\Psi\Big|_{x=x_n} = V(x_n)\psi(x_n), \tag{10.12}$$

$$\hat{V} = \begin{pmatrix} V(x_1) & 0 & 0 & \cdots \\ 0 & V(x_2) & 0 & \cdots \\ 0 & 0 & V(x_3) & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}. \tag{10.13}$$

then how about the kinetic energy operator? If $\Delta = x_n - x_{n-1}$ is the uniform grid spacing, then we know

$$\frac{d}{dx}\psi(x)\Big|_{x=x_n} \simeq \frac{\psi(x_n) - \psi(x_{n-1})}{\Delta}, \tag{10.14}$$

$$\frac{d^2}{dx^2}\psi(x)\Big|_{x=x_n} \simeq \frac{1}{\Delta^2}[\psi(x_{n+1}) + \psi(x_{n-1}) - 2\psi(x_n)]. \tag{10.15}$$

Therefore

$$\frac{d^2}{dx^2}|\psi(x)\rangle = \frac{d^2}{dx^2}\begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ . \\ . \\ \psi(x_N) \end{pmatrix} = \frac{1}{\Delta^2}\begin{pmatrix} -2\psi(x_1) + \psi(x_2) \\ -2\psi(x_2) + \psi(x_1) + \psi(x_3) \\ -2\psi(x_3) + \psi(x_2) + \psi(x_4) \\ . \\ . \end{pmatrix}, \tag{10.16}$$

so

$$\frac{d^2}{dx^2} = \frac{1}{\Delta^2}\begin{pmatrix} -2 & 1 & 0 & 0 & \cdots \\ 1 & -2 & 1 & 0 & \cdots \\ 0 & 1 & -2 & 1 & \cdots \\ 0 & 0 & 1 & -2 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}, \tag{10.17}$$

and $\hat{T} =$

$$\hat{T} = \begin{pmatrix} -2k & k & 0 & 0 & \cdots \\ k & -2k & k & 0 & \cdots \\ 0 & k & -2k & k & \cdots \\ 0 & 0 & k & -2k & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}, \text{ where k } = \frac{\hbar^2}{2m\Delta^2}. \tag{10.18}$$

See slide for demo and extra info.

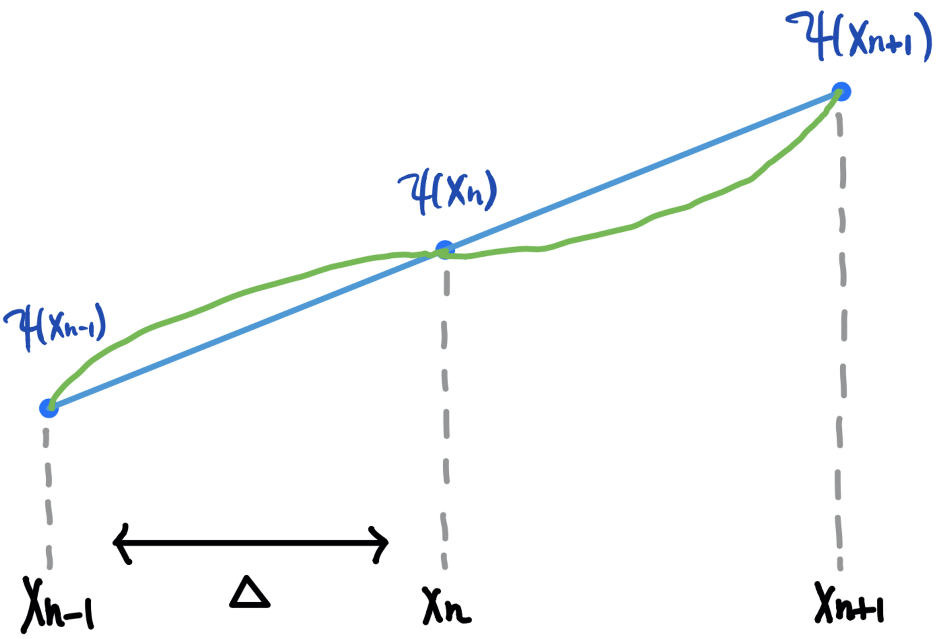

Figure 10.2: Taylor expansion of an arbitrary function.