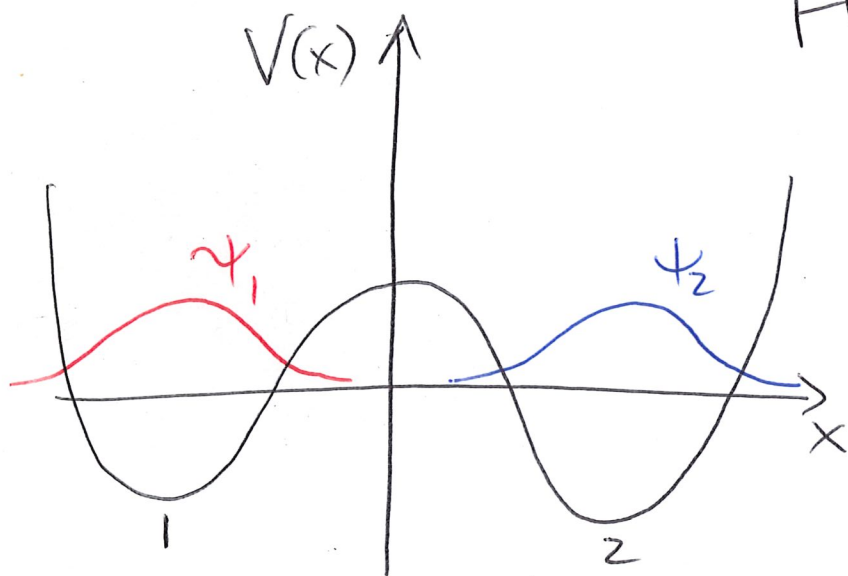


Matrix mechanics

To review the matrix approach to quantum mechanics, let us study the two-level system in detail.

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



$\psi_1 =$ ground state of well 1

$\psi_2 =$ g.s. of well 2

Suppose $\langle 1 | \hat{H} | 1 \rangle = \int dx \psi_1^*(x) \hat{H} \psi_1(x) = \epsilon$

and $\langle 2 | \hat{H} | 2 \rangle = \epsilon$

Assume $\langle 1 | 2 \rangle = \int dx \psi_1^*(x) \psi_2(x) = 0$

Define $\langle 1 | \hat{H} | 2 \rangle = \Delta$

$$\langle 2 | \hat{H} | 1 \rangle = \langle 1 | \hat{H} | 2 \rangle^* = \Delta^* \quad (2)$$

The Hamiltonian can be represented by a 2×2 matrix:

$$\hat{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix},$$

where $H_{ij} = \langle i | \hat{H} | j \rangle$.

This assumes we can neglect any higher energy states.

For the symmetric double well, we have

$$\hat{H} = \begin{pmatrix} \epsilon & \Delta \\ \Delta^* & \epsilon \end{pmatrix}.$$

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A general wavefunction of the

system $\psi(x) = c_1 \psi_1(x) + c_2 \psi_2(x)$

is represented by a column vector

$$\psi = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\psi^*(x) = c_1^* \psi_1^*(x) + c_2^* \psi_2^*(x)$$

is represented by a row vector

$$\psi^* = (c_1^* \quad c_2^*)$$

$$\langle \psi | \psi \rangle = \int dx (c_1^* \psi_1^*(x) + c_2^* \psi_2^*(x)) \times (c_1 \psi_1(x) + c_2 \psi_2(x))$$

$$\langle \Psi | \Psi \rangle = |c_1|^2 \int dx |\gamma_1(x)|^2$$

$$+ |c_2|^2 \int dx |\gamma_2(x)|^2$$

$$+ c_1^* c_2 \int dx \gamma_1^*(x) \gamma_2(x) \rightarrow 0$$

$$+ c_1 c_2^* \int dx \gamma_2^*(x) \gamma_1(x) \rightarrow 0$$

$$= |c_1|^2 + |c_2|^2$$

or

$$\langle \Psi | \Psi \rangle = (c_1^* \quad c_2^*) \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = |c_1|^2 + |c_2|^2$$

The time-indep. Schrödinger equation
 $E\Psi = \hat{H}\Psi$ may be written

$$E \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} E & \Delta \\ \Delta^* & E \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

Proof: $E \Psi(x) = \hat{H} \Psi(x)$

$$E \langle 1 | \Psi \rangle = \langle 1 | \hat{H} | \Psi \rangle$$

$$E \left[c_1 \int dx \psi_1^*(x) \psi_1(x) + c_2 \int dx \psi_1^*(x) \psi_2(x) \right]$$

$$= \int dx \psi_1^*(x) \hat{H} (c_1 \psi_1(x) + c_2 \psi_2(x))$$

$$E c_1 = c_1 H_{11} + c_2 H_{12}$$

$$E \langle 2 | \Psi \rangle = \langle 2 | \hat{H} | \Psi \rangle$$

$$\rightarrow E c_2 = c_1 H_{21} + c_2 H_{22}$$

or $E \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$



Schrödinger equation

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$$\begin{pmatrix} \epsilon - E & \Delta \\ \Delta^* & \epsilon - E \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

has a non-trivial solution only if the determinant

$$\begin{vmatrix} \epsilon - E & \Delta \\ \Delta^* & \epsilon - E \end{vmatrix} = 0$$

$$(\epsilon - E)^2 - |\Delta|^2 = 0$$

$$E_{\pm} = \epsilon \pm |\Delta|$$

energy eigenvalues

Without loss of generality, we may take $\Delta \geq 0$ (real).

The energy eigenstates are

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$$\psi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}.$$

Check:

$$\hat{H} \psi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \epsilon & \Delta \\ \Delta & \epsilon \end{pmatrix} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \epsilon \pm \Delta \\ \Delta \pm \epsilon \end{pmatrix}$$

$$= (\epsilon \pm \Delta) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = E_{\pm} \psi_{\pm}.$$

In other words,

$$\psi_{\pm}(x) = \frac{\psi_1(x) \pm \psi_2(x)}{\sqrt{2}}.$$

Parity $\hat{P} \psi_{\pm}(x) = \frac{\psi_1(-x) \pm \psi_2(-x)}{\sqrt{2}}$

By symmetry, $\psi_2(x) = \psi_1(-x)$;

$$\text{So } \hat{P} \psi_{\pm}(x) = \frac{\psi_2(x) \pm \psi_1(x)}{\sqrt{2}}$$

$$= \pm \psi_{\pm}(x).$$

The matrix representation of the parity operator is

$$\hat{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x.$$

Note that $\hat{H} = \epsilon \mathbb{1} + \Delta \hat{P}$.

Another operator of interest is

σ_z , defined by

$$\sigma_z \psi_1(x) = \psi_1(x), \quad \sigma_z \psi_2(x) = -\psi_2(x).$$

$$\text{or } \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The operator σ_z corresponds to a measurement of whether the particle is to the right or left of $x=0$.

Postulates 1 and 2

$$\begin{aligned}\psi(x) &= c_1 \psi_1(x) + c_2 \psi_2(x) \\ &= c_+ \psi_+(x) + c_- \psi_-(x)\end{aligned}$$

represent valid physical states of the system.

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \frac{c_+}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{c_-}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} \frac{C_+ + C_-}{\sqrt{2}} \\ \frac{C_+ - C_-}{\sqrt{2}} \end{pmatrix}$$

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Also $C_+ = \frac{C_1 + C_2}{\sqrt{2}}$, $C_- = \frac{C_1 - C_2}{\sqrt{2}}$

Postulate 3

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$$

$$i\hbar \frac{d}{dt} \begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix} = \begin{pmatrix} \epsilon & \Delta \\ \Delta & \epsilon \end{pmatrix} \begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix}$$

or

$$i\hbar \frac{d}{dt} \begin{pmatrix} C_+(t) \\ C_-(t) \end{pmatrix} = \begin{pmatrix} \epsilon + \Delta & 0 \\ 0 & \epsilon - \Delta \end{pmatrix} \begin{pmatrix} C_+(t) \\ C_-(t) \end{pmatrix}$$

$$C_{\pm}(t) = e^{-i \frac{E_{\pm} t}{\hbar}} C_{\pm}(0)$$

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Postulate 4

$$\hat{H} = \begin{pmatrix} \epsilon & \Delta \\ \Delta & \epsilon \end{pmatrix}, \quad \hat{P} = \sigma_x, \quad \sigma_z$$

are linear, Hermitian operators.

If one measures the energy E of the system:

$$E \leftrightarrow \hat{H} \rightarrow \begin{cases} \epsilon + \Delta \\ \epsilon - \Delta \end{cases}$$

are the possible outcomes.

If one measures the parity

$$P \leftrightarrow \sigma_x \rightarrow \begin{cases} +1 \\ -1 \end{cases} \text{ are the possible outcomes}$$

After such a measurement, the $|1\rangle$ state of the system becomes either

$$\psi_{\pm}(x) = \frac{\psi_1(x) \pm \psi_2(x)}{\sqrt{2}}$$

If one measures whether the particle is on the right or left:

$$L/R \leftrightarrow \sigma_z \rightarrow \begin{cases} 1 \\ -1 \end{cases}$$

are the possible outcomes.

After the measurement, the system is in the state

$\psi_1(x)$ or $\psi_2(x)$.

Postulate 5

If E is measured, the

value $E_{\pm} = \epsilon \pm \Delta$ is obtained, with probability

$$P_{\pm} = |C_{\pm}|^2 \quad (\text{assuming } \psi \text{ is normalized.})$$

If one measures whether the particle is right or left of $x=0$, the two possible outcomes occur with probabilities

$$L: P_L = |C_1|^2$$

$$R: P_R = |C_2|^2$$

Example Suppose we measure

σ_z @ $t=0$ and obtain

the result $\sigma_z = -1$ (particle to the left of $x=0$).

After the measurement

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$$\psi(t=0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad C_1(0) = 1 \\ C_2(0) = 0.$$

The system evolves under

$$i\hbar \frac{\partial \psi}{\partial t} = H \psi \quad \text{for a time } t:$$

$$C_+(0) = \frac{1}{\sqrt{2}}, \quad C_-(0) = \frac{1}{\sqrt{2}}$$

$$C_{\pm}(t) = \frac{1}{\sqrt{2}} e^{-i \frac{\epsilon \pm \Delta}{\hbar} t}$$

$$C_1(t) = \frac{1}{\sqrt{2}} (C_+(t) + C_-(t)) \\ = \dots e^{-i \frac{\epsilon t}{\hbar}} \cos\left(\frac{\Delta t}{\hbar}\right)$$

$$C_2(t) = \frac{1}{\sqrt{2}} (C_+(t) - C_-(t))$$

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$$= i e^{-i \frac{\epsilon t}{\hbar}} \sin\left(\frac{\Delta t}{\hbar}\right)$$

$$P_L(t) = |C_1(t)|^2 = \cos^2\left(\frac{\Delta t}{\hbar}\right)$$

$$P_R(t) = |C_2(t)|^2 = \sin^2\left(\frac{\Delta t}{\hbar}\right)$$

If we measure the energy

E @ time t Possible

outcomes are $E_{\pm} = \epsilon \pm \Delta$

$$P_{E_+}(t) = |C_+(t)|^2 = \frac{1}{2} \quad (\text{indep. of time!})$$

$$P_{E_-}(t) = |C_-(t)|^2 = \frac{1}{2}$$