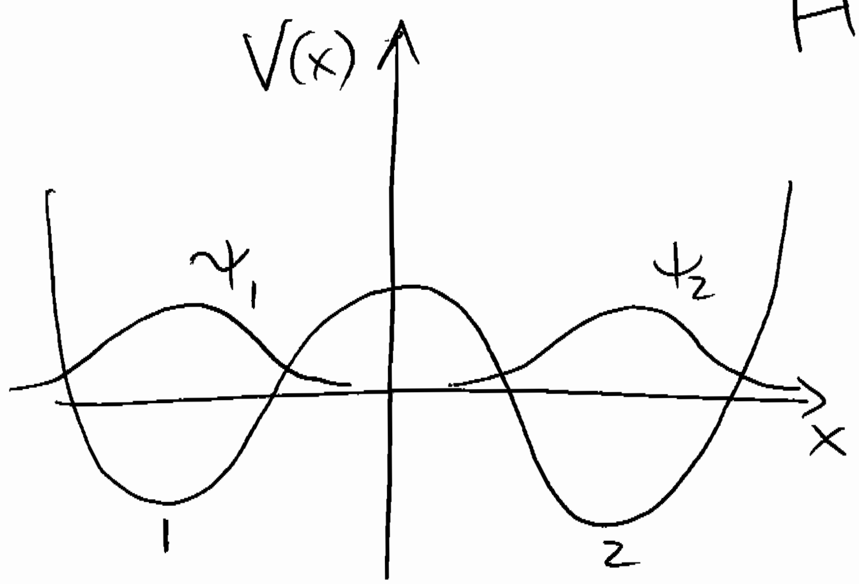
Matrix mechanics

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



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

ψ_1 = ground state of well 1

ψ_2 = g.s. of well 2

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

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

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

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

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

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

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

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

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

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

$$\langle\psi|\psi\rangle = |c_1|^2 \int dx\, |\psi_1(x)|^2$$
$$+ |c_2|^2 \int dx\, |\psi_2(x)|^2$$
$$+ c_1^* c_2 \int dx\, \psi_1^*(x)\, \psi_2(x) \to 0$$
$$+ c_1 c_2^* \int dx\, \psi_2^*(x)\, \psi_1(x) \to 0$$
$$= |c_1|^2 + |c_2|^2$$

or

$$\langle\psi|\psi\rangle = \begin{pmatrix} c_1^* & c_2^* \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = |c_1|^2 + |c_2|^2.$$

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

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

<u>Proof:</u> $E\,\psi(x) = \hat{H}\,\psi(x)$

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

$$E\left[c_1 \overbrace{\int dx\, \psi_1^*(x)\,\psi_1(x)}^{=1} + \cancel{c_2 \int dx\, \psi_1^*(x)\,\psi_2(x)}^{\,0}\right]$$

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

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

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

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

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

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

has a non-trivial solution only if the determinant

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

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

$$\boxed{E_\pm = \varepsilon \pm |\Delta|.}$$

energy eigenvalues

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

The energy eigenstates are

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

Check:

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

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

In other words,

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

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

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

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 $\hat{H} = \varepsilon \mathbb{1} + \Delta \hat{P}$.

Another operator of interest is σ_z, defined by

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

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

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

$$= c_+ \psi_+(x) + c_- \psi_-(x)$$

represent valid physical states of the system.

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

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

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

Postulate 3

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

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} \varepsilon & \Delta \\ \Delta & \varepsilon \end{pmatrix} \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$$

or

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

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

Postulate 4

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

are linear, Hermitian operators.

If one measures the energy E of the system:

$$E \longleftrightarrow \hat{H} \longrightarrow \begin{cases} \varepsilon + \Delta \\ \varepsilon - \Delta \end{cases}$$

are the possible outcomes.

If one measures the parity

$$P \longleftrightarrow \sigma_x \longrightarrow \begin{cases} +1 \\ -1 \end{cases}$$ are the possible outcomes

After such a measurement, the 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:

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

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 $E_\pm = \varepsilon \pm \Delta$ is obtained, with probability

$$P_\pm = |C_\pm|^2$$ (assuming ψ is normalized.)

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

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

$$R: \quad P_R = |C_2|^2.$$

<u>Example</u> Suppose we measure σ_z @ $t=0$ and obtain the result $\sigma_z = 1$ (particle to the left of $x=0$).

After the measurement

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

$C_2(0) = 0$.

The system evolves under

$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$ for a time t:

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

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

$$C_1(t) = \frac{1}{\sqrt{2}} \left(C_+(t) + C_-(t) \right)$$

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

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

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

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

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

<u>If we measure the energy</u>
<u>E @ time t</u> possible
outcomes are $E_\pm = \varepsilon \pm \Delta$

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

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

(indep. of time!)