22/10/2025 Lec. 27. **Separable Hamiltonians**

Consider a Hamiltonian $\hat{H}$ for a system such that $\hat{H} = \hat{H}_1 + \hat{H}_2 + \cdots + \hat{H}_N$ — (1)
where $\hat{H}_1, \hat{H}_2, \ldots$ are Hermitian operators.

If $[\hat{H}_i, \hat{H}_j] = 0 \quad \forall\, i,j$ — (2)
and $\{\varphi^{(1)}_{m_1}, \varphi^{(2)}_{m_2}, \ldots \varphi^{(N)}_{m_N}\}$ are eigenfunction of $\hat{H}_1, \hat{H}_2, \ldots, \hat{H}_N$, respectively, then any product

$$\Phi_{m_1 m_2 \ldots} = \varphi^{(1)}_{m_1} \varphi^{(2)}_{m_2} \cdots \varphi^{(N)}_{m_N} \quad \text{— (3)}$$

is an eigenfunction of $\hat{H}$.

It's easy to verify (H.W.) that the corresponding eigenvalue of $\hat{H}$ is

$$E_{m_1 m_2 \ldots m_N} = \sum_{i=1}^{N} \epsilon_{m_i} \quad \text{— (4)}$$

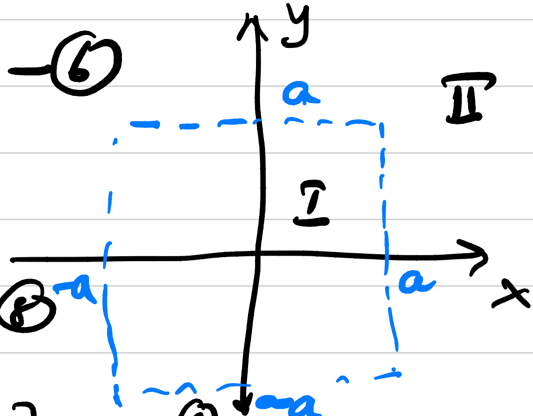
where $\hat{H}_i \varphi^{(i)}_{m_i} = \epsilon_{m_i} \varphi^{(i)}_{m_i}$ — (5)

· Particle in an infinite 2-d square well.

— $V(x,y) = \begin{cases} 0 & \text{if } |x|<a \text{ and } |y|<a \\ \infty & \text{if } |x|>a \text{ \& } |y|>a \end{cases}$

$\Rightarrow$ in region I

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} \quad \text{—(6)}$$



$$\& \quad \equiv \hat{H}_x + \hat{H}_y \quad \text{—(7)}$$

in region II

$$\Phi(x,y) = 0 \quad \text{—(8)}$$

Note that $[\hat{H}_x, \hat{H}_y] = 0$ —(9) since momenta in different directions commute.

$\therefore$ we first solve the $\hat{H}_x$ & $\hat{H}_y$ problems.

i.e.
$$-\frac{\hbar^2}{2m}\frac{\partial^2 \phi^{(x)}(x)}{\partial x^2} - E\phi^{(x)}(x) = 0 \quad \text{—(10)}$$

&
$$-\frac{\hbar^2}{2m}\frac{\partial^2 \phi^{(y)}(y)}{\partial y^2} - E\phi^{(y)}(y) = 0 \quad \text{—(11)}$$

But each of these is just the corresponding particle-in-a-1d-square well problem.

$\therefore$ The corresponding eigen solutions are:

$$\text{(12)} \begin{cases} \varphi^{(x)}_{n_1}(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{n_1\pi}{2a}(x+a)\right) \\ \mathcal{E}_{n_1} = \frac{n_1^2 h^2}{16ma^2} \qquad n_1 = 1, 2, 3, \ldots \\ \varphi^{(y)}_{n_2}(y) = \sqrt{\frac{1}{a}} \sin\left(\frac{n_2\pi}{2a}(y+a)\right) \qquad n_2 = 1, 2, 3, \ldots \\ \mathcal{E}_{n_2} = \frac{n_2^2 h^2}{32ma^2} \end{cases}$$

$$\text{where } \sin\left(\frac{n\pi}{2a}(x+a)\right) = \begin{cases} \sin\left(\frac{n\pi x}{2a}\right) & \text{if } n \text{ even} \\ (-1)^{[n/2]} \cos\left(\frac{n\pi x}{2a}\right) & \text{if } n \text{ odd,} \end{cases} \qquad (13)$$

we ignore the extra minus sign the formula brings as it does not change the state.

$\therefore$ The solutions to the 2D problem are:

$$\Phi_{n_1,n_2}(x,y) = \frac{1}{a}\sin\left(\frac{n_1\pi(x+a)}{2a}\right)\sin\left(\frac{n_2\pi(y+a)}{2a}\right)$$

$$E_{n_1,n_2} = \frac{h^2}{32ma^2}\left(n_1^2 + n_2^2\right) \quad (14)$$

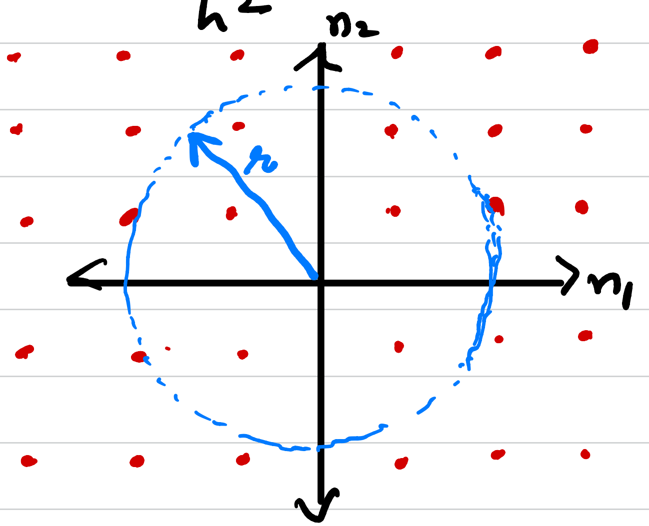
Degeneracies:

We can rewrite (14) as:

$$n_1^2 + n_2^2 = r^2 \quad (15)$$

$$\text{where} \quad r = \frac{32ma^2 E_{n_1,n_2}}{h^2} \quad (16)$$

This is just the equation for a circle. In the figure on the RHS, the allowed quantum numbers are plotted as a grid of points.



All degenerate states yielding energy $E = E_{n_1 n_2}$, will fall on a circle of radius r. Clearly, the possibility for such events increases with the radius r or the energy E.

Particle in a 3-d square well

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m} \quad \text{—(17)}$$

Applying the same separability principle we get the eigenstates as.

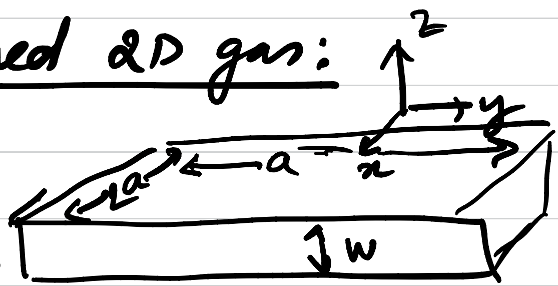
$$\left.\begin{aligned} \Phi_{n_1 n_2 n_3}(x,y,z) &= \left(\frac{1}{a}\right)^{3/2} \sin\left(\frac{n_1\pi}{2a}(x+a)\right) \\ &\quad \sin\left(\frac{n_2\pi}{2a}(x+a)\right) \\ &\quad \sin\left(\frac{n_3\pi}{2a}(x+a)\right) \\ E_{n_1 n_2 n_3} &= \frac{h^2}{32ma^2}\left(n_1^2 + n_2^2 + n_3^2\right) \end{aligned}\right\} \quad (18)$$

$n_1, n_2, n_3 = 1, 2, 3, \ldots$

Both these models come in handy to understand the electronic levels available in quantum wells and dots.

A harmonically confined 2D gas:

If $w \ll 2a$ we can model it as a 2D box.



More realistically, we either model it as a

(i) 3-d box with one direction different from others

(ii) Use harmonic confinement in z direction and assume x & y directions to be free. i.e.

$$V(x,y,z) = \frac{1}{2} m\omega^2 z^2 \quad — (19)$$

some frequency ω.

HW: Solve the problem both ways to obtain eigenvalues & eigenfunctions. Compare the eigenfunctions in the limit of $a \to \infty$, $W/a \to 0$.

$$\Rightarrow \langle \hat{x} \rangle_t = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, x\, \psi(x) \quad \text{—(21)}$$

The RHS can be evaluated (converges) if $\psi(x)$ is a bound state.

$$\Rightarrow \frac{d\langle \hat{x} \rangle_t}{dt} = 0 \quad \text{for such a state!} \quad \text{—(22)}$$

$$\therefore \langle \hat{p}_x \rangle = 0 \quad \text{from (15)} \rightarrow (23)$$

$\therefore$ For a stationary bound state the expectation value of momentum is 0 at all times.

Hypervirial Theorem :

Now consider a QM system of N (1-d) particles or 1 particle and N-d.

We define the generalized coordinates and momenta $\{\hat{q}_i, \hat{p}_i\}_{i=1,N}$ to describe the dynamic variables, such that

$$\left.\begin{aligned} [\hat{q}_i, \hat{p}_j] &= i\hbar\,\delta_{ij} \\ [\hat{q}_i, \hat{q}_j] &= [\hat{p}_i, \hat{p}_j] = 0 \end{aligned}\right\} \quad (24)$$

i.e. they still obey the same commutation relations part of our postulates.

The Hamiltonian would then be

$$\hat{H} = \sum_{i=1}^{N} c_i\,\hat{p}_i^2 + V(q_1, q_2, q_3 \cdots q_N) \quad (25)$$

where c_i are some constants that depend on the choice of coordinates.

For instance if $\{q_i\}$ were just Cartesian coordinates $C_i = 1/2m_i$

$\hat{p}_i \leftrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x_i}$

Now consider the operator

$$\hat{A} = \sum_{i=1}^{N} \hat{q}_i \hat{p}_i \quad — (26)$$

and a stationary bound state $|\Psi(t)\rangle$.

Then,

$$\frac{d\langle \hat{A}\rangle}{dt} = 0 \quad — (27)$$

as we saw in (22).

But $\frac{d\langle \hat{A}\rangle}{dt} = \frac{i}{\hbar}\langle [\hat{A}, \hat{H}]\rangle$ by (8)

$$\Rightarrow \langle [\hat{A}, \hat{H}]\rangle = 0 \quad — (9)$$

for A given by (28)

$$[\hat{A}, \hat{H}] = \sum_{i=1}^{N} [\hat{q}_i \hat{p}_i, \hat{H}]$$

$$= \sum_{i=1}^{N} C_i \, [\hat{q}_i \hat{p}_i, \hat{p}_i^2] + [\hat{q}_i \hat{p}_i, V(q)] \quad \text{—(27)}$$

where we have used the fact that $[q_i p_i, \hat{p}_j^2] = 0$ if $i \neq j$.

$$\therefore [\hat{A}, \hat{H}] = \sum_{i=1}^{N} \left\{ C_i \, [\hat{q}_i, \hat{p}_i^2] \, \hat{p}_i + q_i [\hat{p}_i, V(q)] \right\}$$

(using $[\hat{A}B, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$)

$$= \sum_{i=1}^{N} \left\{ C_i \cdot 2i\hbar \, \hat{p}_i^2 + \frac{\hbar}{i} \hat{q}_i \frac{\partial \hat{V}}{\partial q_i} \right\}$$

$$= i\hbar \left\{ 2\hat{T} - \sum_{i=1}^{N} \hat{q}_i \frac{\partial \hat{V}}{\partial q_i} \right\} \quad \text{—(28)}$$

$\therefore \langle [\hat{A}, \hat{H}] \rangle = 0$

$$\Rightarrow \boxed{2\langle \hat{T} \rangle = \left\langle \sum_{i=1}^{N} \hat{q}_i \frac{\partial \hat{V}}{\partial q_i} \right\rangle} \quad \text{(29)}$$

This is called the Hypervirial theorem. Since $|\Psi(t)\rangle$ is a stationary bound state, (29) is especially true for eigenfunction.

The RHS is like a virial

$$\vec{r}.\underbrace{\vec{F}}_{\text{force}}$$

Virial Theorem: Now consider a special class of potential energy functions called homogenous fns.

$V(q_1, q_2 .. q_N)$ is said to be homogenous of degree n if

$$V(\lambda q_1, \lambda q_2 .. \lambda q_N) = \lambda^n V(q_1, q_2, q_3 \ldots q_N) \quad \text{— (30)}$$

for some $\lambda \in \mathbb{C}$

Then, differentiation of (30) with respect to λ yields

$$LHS = \sum_{i=1}^{N} \frac{\partial V(\lambda q_i)}{\partial(\lambda q_i)} \cdot \frac{\partial(\lambda q_i)}{\partial \lambda}$$

$$= \sum_{i=1}^{N} \frac{\partial V(\lambda q_1, \lambda q_2 \cdots)}{\partial(\lambda q_i)} q_i \quad \text{— (31)}$$

$$RHS = n \lambda^{n-1} V(q_1, q_2 \cdots q_N) \quad \text{— (32)}$$

Since (30), (31) & (32) are true for any λ, we can set $\lambda = 1$ which yields

$$\boxed{\sum_{i=1}^{N} \frac{\partial V}{\partial q_i} \cdot q_i = n V(q_1, q_2 \cdots q_N)}$$

— (33)