1.5 Eigenvalue problems

For finite-dimensional $\mathcal{H}$, operators (like H) are matrices.

For ∞-dimensional $\mathcal{H}$, have operators like $H = H(x,p)$.

Fundamental problem:

* Solve $H|\psi\rangle = \lambda|\psi\rangle$

1) Find spectrum of eigenvalues λ_n [discrete + cts spectrum]
2) Find eigenstates $|\psi_n\rangle$

Sometimes have simpler problem:

1b) Find smallest eigenvalue λ_0
2b) Find associated eigenstate $|\psi_0\rangle$ ("ground state" for H)

How to solve?

For finite-dimensional systems,

$\det(H - \lambda \mathbb{1}) = 0$ degree N polynomial.

$\lambda_0, \ldots, \lambda_{N-1}$ are roots.

Solve $H|\psi\rangle = \lambda|\psi\rangle$ by linear algebra.

Difficult for large matrices.

Trick: For matrix H, with all $\lambda > 0$, can get largest λ_{max} by looking at

$$H^n |V\rangle \xrightarrow[n \to \infty]{} \lambda_{max}^n |V_{max}\rangle\langle V_{max}|V\rangle + \text{smaller terms.}$$

for large n, generic $|V\rangle$. Fit to linear form: $\ln c\lambda^n = n \underline{\underline{\ln \lambda}} + \ln c$.

To get λ_0, take $\tilde{H} = X\mathbb{1} - H$ for large X.

How about when $\dim \mathcal{H} = \infty$?

$$\det(H - \lambda \mathbb{1}) \text{ not a polynomial.}$$

Must solve differential equation.

For example, in 1D:

$$H = \frac{p^2}{2m} + V(x)$$

$$H|\psi\rangle = E|\psi\rangle$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x).$$

Need to find values of E, solutions.

Many methods exist. [some appropriate for large D, some for small D.]

$H|\psi\rangle = E|\psi\rangle$

1D: $H = \frac{p^2}{2m} + V(x)$

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

find allowed E, sol'ns ψ w/ $\psi \in \mathcal{H}$
(include BC's)

Diff eq + BC's

ex. $V(x) = V_0$ constant

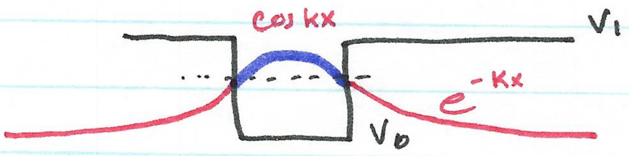
$$\frac{d^2}{dx^2}\psi(x) = \underbrace{\frac{2m}{\hbar^2}(V_0 - E)}_{\text{const}}\psi(x)$$

$E > V_0$, $\psi \sim \underline{e^{ikx}}$ (lin comb of sin, cos)

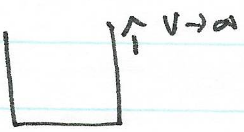
$E < V_0$ $\psi \sim e^{\pm \kappa x}$
(tunneling)

$V_0 = \infty \Rightarrow \psi = 0$

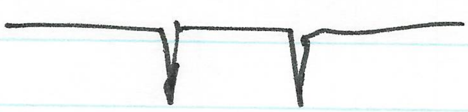
e.g.



pset ∞ square

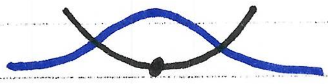


δ fun potentials



Example: Simple Harmonic Oscillator (SHO)

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2$$



Want to solve equation of form

$$-\psi''(x) + x^2 \psi(x) = E\,\psi(x)$$

For simple diff eq's like this: can find (or look up) analytic solutions

Solution by operator method [ref. e.g. Cohen-Tannoudji]

(basic idea: $a^2 + b^2 = (a+ib)(a-ib)$)

Define
$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right)$$
$$a^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

So
$$a^+ a = \frac{m\omega}{2\hbar} x^2 + \frac{p^2}{2\hbar m\omega} + \frac{i}{2\hbar} \underbrace{[x,p]}_{i\hbar \mathbb{1}}$$

* $$= \frac{H}{\hbar\omega} - \frac{1}{2}$$

similarly
$$a a^+ = \frac{H}{\hbar\omega} + \frac{1}{2}$$

So
$$\boxed{[a, a^+] = 1}$$

Writing $N = a^+ a$,

$$\boxed{H = \hbar\omega\left(N + \tfrac{1}{2}\right)}$$

Define $|0\rangle$ by $\quad a|0\rangle = 0.$

("ground state")
[will prove]

State is unique

$$\left(x' + \frac{\hbar}{m\omega}\frac{d}{dx'}\right)\psi_0(x') = 0$$

$$\Rightarrow \psi_0(x') = \langle x'|0\rangle = c\,e^{-\frac{m\omega}{2\hbar}x^2}$$

for $\langle 0|0\rangle = 1$, $c = \sqrt[4]{\frac{m\omega}{\hbar\pi}}$

So

$$a|0\rangle = 0$$

$$\Rightarrow N|0\rangle = a^+a|0\rangle = 0.$$ $\Rightarrow H|0\rangle = \hbar\omega/2$ (ground state energy)

Now, if $N|n\rangle = n|n\rangle$

$$N(a^+|n\rangle) = a^+a\,a^+|n\rangle$$

$$= (a^+a^+a + a^+)|n\rangle$$

$$= (n+1)\,a^+|n\rangle$$

(equivalently $[N, a^+] = a^+$).

So we have a tower of states

$$|0\rangle$$
$$|1\rangle = c_1\,a^+|0\rangle$$
$$|2\rangle = c_2\,(a^+)^2|0\rangle$$
$$\vdots$$

with $N|n\rangle = n|n\rangle$

If $\langle n|n\rangle = 1$,

$$\langle n|a\, a^+|n\rangle = \langle n|(N+1)|n\rangle = n+1,$$

so $|n+1\rangle = \frac{1}{\sqrt{n+1}}\, a^+|n\rangle$ gives $\langle n+1|n+1\rangle = 1$.

Gives normalized states by induction.

Generally, $|n\rangle = (a^+)^n/\sqrt{n!}\,|0\rangle$.

$$\boxed{\begin{aligned} a^+|n\rangle &= \sqrt{n+1}\,|n+1\rangle \\ a|n\rangle &= \sqrt{n}\,|n-1\rangle \end{aligned}}$$ "ladder operators"

and $\langle n|n'\rangle = \delta_{n,n'}$.

Energy of n^{th} state:

$$H|n\rangle = E_n|n\rangle$$

$$\boxed{E_n = \hbar\omega(n+1/2)}$$

$E_0 = \hbar\omega/2$
$E_1 = 3\hbar\omega/2$
$E_2 = 5\hbar\omega/2$
$\vdots$

Can there be other eigenstates?

$|\tilde{n}\rangle$, $\tilde{n}$ integer, $|n\rangle \neq |\tilde{n}\rangle$?

* no, since $a|\tilde{n}\rangle = \sqrt{n}\,|\widetilde{(n-1)}\rangle$
$a^+|\widetilde{(n-1)}\rangle = |\tilde{n}\rangle$, but $|0\rangle$ unique.

$|\alpha\rangle$, α non integer? no, since
$a^k|\alpha\rangle \sim |\alpha-k\rangle$, $\alpha-k<0$
but $(\langle\alpha-k|a^+a|\alpha-k\rangle) = \alpha-k \geq 0$.
contradiction

Upshot: $|n\rangle$ form a complete ON basis for $\mathcal{H} = \mathcal{L}^2(\mathbb{R})$

(note: $n \neq n' \Rightarrow \langle n|n'\rangle = 0$ since $\langle n|H|n'\rangle = E_n\langle n|n'\rangle = E_{n'}\langle n|n'\rangle$)

All operators can be expressed as (infinite) matrices wrt this <u>countable</u> ON basis

$$\langle n'|x|n\rangle = \langle n'|\sqrt{\frac{\hbar}{2m\omega}}(a+a^+)|n\rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left[\delta_{n,n'+1}\sqrt{n} + \delta_{n+1,n'}\sqrt{n'}\right]$$

$$\left(\sqrt{\frac{\hbar}{2m\omega}}\begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & \sqrt{2} & & \\ & \sqrt{2} & 0 & \sqrt{3} & \\ & & \sqrt{3} & \ddots & \ddots \end{bmatrix}\right)$$

similarly

$$* \quad \langle n'|p|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left[-\delta_{n,n'+1}\sqrt{n} + \delta_{n+1,n'}\sqrt{n'}\right]$$

$$\left(i\sqrt{\frac{m\hbar\omega}{2}}\begin{bmatrix} 0 & -1 & & & \\ 1 & 0 & -\sqrt{2} & & \\ & \sqrt{2} & 0 & -\sqrt{3} & \\ & & \sqrt{3} & 0 & \ldots \end{bmatrix}\right)$$

check: $[x,p] = i\hbar$

Can calculate position basis for all states

$$\langle x'|n\rangle = \left(\frac{1}{\pi^{1/4}\sqrt{2^n n!}}\right)\left(\frac{m\omega}{\hbar}\right)^{\frac{n+1/2}{2}}\left(x' - \frac{\hbar}{m\omega}\frac{d}{dx}\right)^n e^{-\frac{m\omega}{2\hbar}x'^2}$$

– Hermite polynomials $\times\ \psi_0(x)$

$$\psi_n = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{\frac{-m\omega x^2}{2\hbar}} H_n(\ldots$$

$$H_n = (-1)^n e^{z^2}\frac{d^n}{dz^n}\left(e^{-z^2}\right)$$

[Homework: write $|x\rangle$ in $|n\rangle$ basis as "squeezed state"
$e^{\alpha + \beta a^+ + \gamma a^{+2}}|0\rangle$]

Useful exercise: show in state $|n\rangle$

$$\langle\Delta x^2\rangle\langle\Delta p^2\rangle = (n+1/2)^2\hbar^2.$$