$P_{[a,b]}$ are good operators, and diagonalize into ON basis w/ evalues 1 or $\emptyset$.

QM breaks down at some scale > 10^{-33} cm, but can use $P_{[a,b]}$ for any current expts.

Problem : This approach, while mathematically correct, introduces unnecessary complications from physical point of view.

Most operators of interest cannot be diagonalized in $\mathcal{H}$.

Ex. position x

momentum $p = -i\hbar\, \partial/\partial x$

Energy $H = p^2/2m + V(x)$ (for example)

estates of x $\longrightarrow$ support at a point, $|\psi|^2 = 0$ except at x.

" " p $\Rightarrow$ support everywhere, $\int |\psi|^2 = \infty$

Solution (Dirac) : Ignore this problem. Treat all these operators as acceptable and include their eigenvectors formally, even if not in $\mathcal{H}$.

["" Quote from Von Neumann]

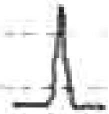
Dirac's approach:

Replace discrete basis $|a_i\rangle$ with continuous basis $|\xi\rangle$, ξ in continuous domain (like $(-\infty, \infty)$).

$$A|a_i\rangle = a_i|a_i\rangle \Longrightarrow \Xi|\xi\rangle = \xi|\xi\rangle$$

$$\langle a_i|a_j\rangle = \delta_{ij} \Longrightarrow \langle\xi|\xi'\rangle = \delta(\xi-\xi')$$

$$\sum_i |a_i\rangle\langle a_i| = \mathbb{1} \Longrightarrow \int d\xi\, |\xi\rangle\langle\xi| = \mathbb{1}.$$

[Brief review of Dirac δ function:  "distribution"

$$\delta(\xi) = 0, \quad \text{when } \xi \neq 0$$

$$\int_{-a}^{a} \delta(\xi)\, d\xi = 1, \quad \forall\, a > 0.$$

~~Can~~ Property: $\displaystyle\int_{-\infty}^{\infty} \delta(\xi) f(\xi)\, d\xi = f(0)$ for smooth f.

Can realize $\delta(\xi)$ as a limit of smooth functions

e.g. $\displaystyle\delta(\xi) = \lim_{a\to\infty} \sqrt{\frac{a}{\pi}}\, e^{-a\xi^2}$]

$$= \lim_{\varepsilon\to 0} \frac{1}{\pi}\frac{\varepsilon}{x^2+\varepsilon^2} = \frac{1}{2\pi}\int dk\, e^{ikx}$$

Generally, can allow operators with partly continuous & partly discrete spectrum.

Example: "position basis".

$$\boxed{X|x'\rangle = x'|x'\rangle}$$

[Notation: X is always operator. $x', x'', \ldots$ are eigenvalues]

$$\boxed{\langle x'|x''\rangle = \delta(x'-x''), \quad \int_{-\infty}^{\infty} dx'\, |x'\rangle\langle x'| = \mathbb{1}}$$

$|x'\rangle$ is <u>not in $\mathcal{H}$</u>, but can still treat as state for most operations; justifiable in terms of appropriate limits.

Note: x is not measurable to arbitrary precision experimentally! (can [illegible]) So not really an observable, but a convenient formal tool.

Working with x, p:

Write

$$|\psi\rangle = \int dx' \, |x'\rangle\langle x'|\psi\rangle$$

$$= \int dx' \, \psi(x') \, |x'\rangle$$

so $\psi(x') = \langle x'|\psi\rangle$.

The probability that $a \leq x \leq b$ is given by

$$\int_a^b dx' \, |\psi(x')|^2 = \int_a^b dx' \, \langle\psi|x'\rangle\langle x'|\psi\rangle$$

$$= \langle\psi|P_{[a,b]}|\psi\rangle.$$

<u>Momentum operator</u>

$$\boxed{p = -i\hbar \frac{\partial}{\partial x}}$$

<u>p is generator of translation</u>

$$e^{iap/\hbar} f(x) = e^{a\,\partial/\partial x} f(x) = f(x+a).$$

Commutation relation $\boxed{[x, p] = i\hbar}$ [recall $[A, B] = \mathbb{1}$ imp. for finite dim]

[Related to $\{x, p\} = 1$ through classical - quantum correspondence, foundation of "matrix mechanics" of Bohr, Jordan, etc... (more later)]

From general uncertainty relation,

$$\boxed{\langle \Delta x^2 \rangle \langle \Delta p^2 \rangle \geq \hbar^2/4.}$$

So wavefunctions can't be localized in x and in p.

<u>Momentum basis</u>

~~Brief review of Fourier transforms in QM notation~~

Construct a basis of states with

$$\boxed{p|p'\rangle = p'|p'\rangle.}$$

know $\quad -i\,\partial/\partial x' \langle x'|p'\rangle = p'\langle x'|p'\rangle$

so $\quad \langle x'|p'\rangle = N e^{ip'x'/\hbar}$

want $\quad \boxed{\langle p'|p''\rangle = \delta(p' - p'')}$

so

$$\int dx' \langle p'|x'\rangle\langle x'|p''\rangle = \int dx' |N|^2 e^{ix'(p''-p')/\hbar}$$

$$= |N|^2 \cdot 2\pi\hbar \cdot \delta(p' - p'')$$

so $\quad |N|^2 = \dfrac{1}{2\pi\hbar},$

$$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ip'x'/\hbar}.$$

Completeness for momentum states

$$\int dp' \, |p'\rangle\langle p'|$$

$$= \int dx' \, dx'' \, dp' \, |x'\rangle\langle x'|p'\rangle\langle p'|x''\rangle\langle x''|$$

$$= \int dx' \, dx'' \, dp' \, |x'\rangle \frac{1}{2\pi\hbar} e^{ip'(x''-x')/\hbar} \langle x''|$$

$$= \int dx' \, |x'\rangle\langle x'| = \mathbb{1}.$$

Fourier transforms

$$|\psi\rangle = \int dp' \, |p'\rangle\langle p'|\psi\rangle$$

$$= \int dp' \, \phi(p') \, |p'\rangle$$

$$\phi(p') = \langle p'|\psi\rangle$$

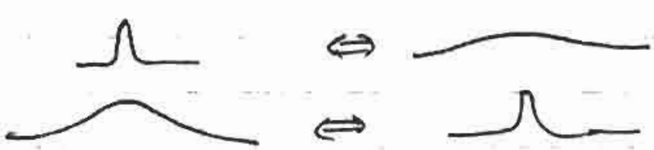
$$= \int dx' \, \langle p'|x'\rangle\langle x'|\psi\rangle$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int dx' \, e^{-ip'x'/\hbar} \, \psi(x')$$

similarly

$$\psi(x') = \frac{1}{\sqrt{2\pi\hbar}} \int dp' \, e^{ip'x'/\hbar} \, \phi(p')$$

Uncertainty principle $\langle \Delta x^2 \rangle\langle \Delta p^2 \rangle \geq \hbar^2/4$ relates width of wavefunction $\psi(x')$ and Fourier transform $\phi(p')$



[Example: inequality saturated for Gaussian e^{-x^2/d^2}]

Generalize to 3D

$$\mathcal{H} = \mathcal{H}^{(x)} \otimes \mathcal{H}^{(y)} \otimes \mathcal{H}^{(z)}$$

$$|\psi\rangle = \int dx\,dy\,dz \;\; \psi(x,y,z)\; |x,y,z\rangle$$

$|x,y,z\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle$ is basis for $\mathcal{H}$

Translation group

$$T(\vec{a})\,|\vec{x}\rangle = |\vec{x}+\vec{a}\rangle \, , \qquad \vec{a} \in \mathbb{R}^3 .$$

$\mathbb{R}^3$ forms a group under addition $\vec{a}+\vec{b}$.
(closed, associative, identity ϕ, inverse $-\vec{a}$).

A representation of a group G on $\mathcal{H}$ is a map R from G to linear operators on $\mathcal{H}$ so that $R(\text{identity}) = \mathbb{1}$, $R(ab) = R(a)R(b)$.

T is a unitary representation of the 3D translation group on $\mathcal{H}$.

$$T^{\dagger}(\vec{a}) = T^{-1}(\vec{a}) = T(-\vec{a})$$
$$T(\vec{a}+\vec{b}) = T(\vec{a})\,T(\vec{b})$$
$$T(0) = \mathbb{1}$$

Realization: $T(\vec{a}) = e^{-i\vec{a}\cdot\vec{p}/\hbar}$ $\quad [p_i, p_j] = 0 \Rightarrow T(\vec{a})T(\vec{b}) = T(\vec{b})T(\vec{a})$

Active picture :

Passive picture : $\quad \psi(\vec{x}) \Longrightarrow \psi(\vec{x}-\vec{a})$
(peak at $\vec{a}$)

$$T(\vec{a}) \int \psi(\vec{x}')\,|\vec{x}'\rangle\, d\vec{x}' = \int \psi(\vec{x}')\,|\vec{x}'+\vec{a}\rangle\, d\vec{x}'$$
$$= \int \psi(\vec{x}''-\vec{a})\,|\vec{x}''\rangle\, d\vec{x}''$$

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 $\hat{H} = X\mathbb{1} - H$ 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.]

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 solution

Solution by operator method

(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

$$a^{+}a = \frac{m\omega}{2\hbar} x^2 + \frac{p^2}{2\hbar m\omega} + \frac{i}{2\hbar}[x,p]$$

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

similarly

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

so

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

Writing $N = a^{+}a$,

$$\boxed{H = \hbar\omega\,(N + 1/2)}$$

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

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 $\langle 0|0\rangle = 1$, $C = \sqrt[4]{\frac{m\omega}{\hbar}}\,\pi^{-1/4}$.

So

$$a|0\rangle = 0$$

$$\Rightarrow N|0\rangle = a^+ a|0\rangle = 0.$$

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

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

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

Gives normalized states by induction.

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

$$\boxed{\begin{aligned} a^\dagger|n\rangle &= \sqrt{n+1}\ |n+1\rangle \\ a\ |n\rangle &= \sqrt{n}\ \ |n-1\rangle \end{aligned}}$$

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 $a|\tilde{n}\rangle = \sqrt{n}\ |\widetilde{(n-1)}\rangle$
$a^\dagger|\widetilde{(n-1)}\rangle = |\tilde{n}\rangle$, but $|0\rangle$ unique.

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

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

All operators can be expressed as (infinite) matrices wrt this countable ON basis

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

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

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

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

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

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

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

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

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

Today: more on solving Eigenvalue problems

Many ways to solve diff. eq's — focus on those giving physical insight.
Only some can be solved exactly
- Today: some approximate methods for low-dimensional systems
[next week: Quantum MC by ...]

Symmetry:
A key principle is to exploit any available symmetry.

Unitary representation $\mathcal{R}$ of gp. G on $\mathcal{H}$:

$$
\begin{aligned}
&\mathcal{R}(g) \text{ is a linear op. on } \mathcal{H} \qquad \forall g \in G. \\
&\mathcal{R}(gh) = \mathcal{R}(g)\mathcal{R}(h) \\
&\mathcal{R}^\dagger(g) = \mathcal{R}(g^{-1}) \\
&\mathcal{R}(id) = \mathbb{1}
\end{aligned}
$$

If $H = \mathcal{R}^\dagger(g)\, H\, \mathcal{R}(g) \qquad \forall g \in G$
then G is a group of symmetries of the physical system.

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

then
$$
\begin{aligned}
H\mathcal{R}(g)|\psi\rangle &= \mathcal{R}(g)\left(\mathcal{R}^\dagger(g)\, H\, \mathcal{R}(g)\right)|\psi\rangle \\
&= E\,\mathcal{R}(g)\,|\psi\rangle.
\end{aligned}
$$

so $\mathcal{R}|\psi\rangle$ has same energy as $|\psi\rangle$.

Example: $\mathbb{Z}_2$ parity symmetry

Group $\mathbb{Z}_2$ has 2 elements: $1,\ a.$
mult. rule $\quad a^2 = 1.$

Representation of parity $\mathbb{Z}_2$ on $\mathcal{H}$ for single particle:

<u>Parity operator</u> $\Pi = \mathcal{B}_\pi(a)$

$$\Pi|x\rangle = |-x\rangle \qquad \text{(note: phase is convention)}$$

$$\Pi^2 = \mathbb{1}.$$

<u>Theorem</u>: If $[\pi, H] = 0$ $\quad (\pi H \pi = H)$

then when $H|\psi_n\rangle = E_n|\psi_n\rangle$, E_n nondegenerate,

then $\psi_n(x) = \pm\psi_n(-x)$. (parity even / odd)

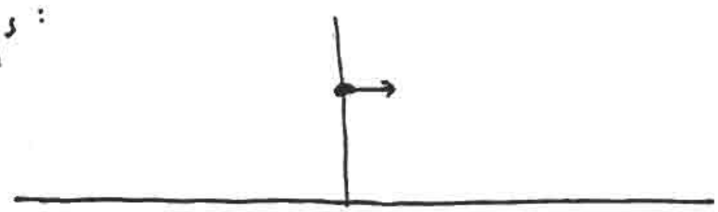
<u>Pf.</u> Can choose $\psi_n(x)$ phase to be real,
$\pi|\psi_n\rangle = \pm|\psi_n\rangle$.

(Euler-Crane)
"Shooting method" for solving 1D problems

$$\left(\frac{p^2}{2m} + V(x)\right)|\psi\rangle = E|\psi\rangle,$$

where $V(x) = V(-x)$ (even potential)

Even states:
$(\psi(x) = \psi(-x))$



Fix E, solve $\psi''(x) = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi(x)$
with initial conditions

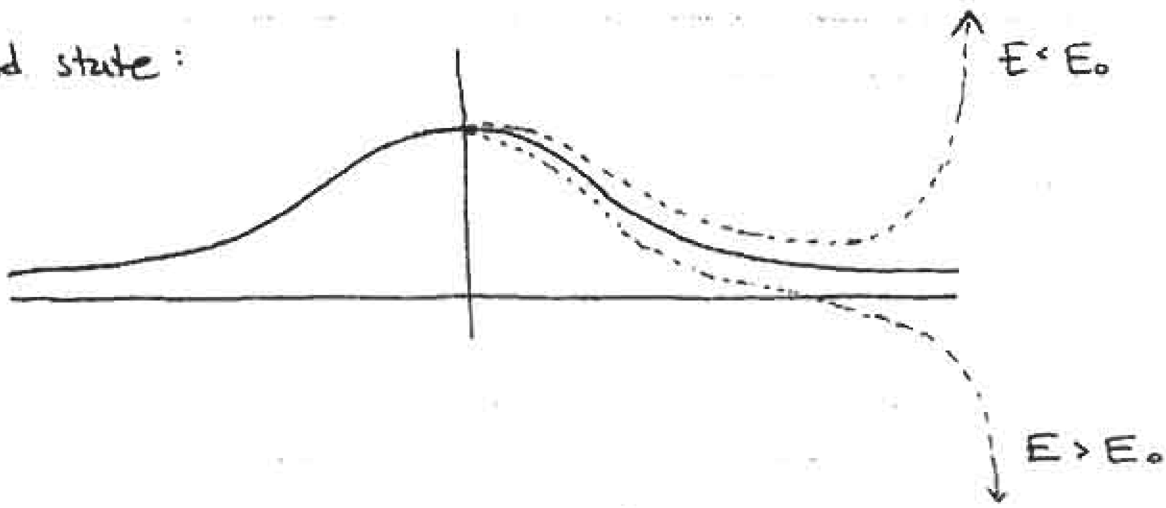
$$\psi(0) = 1, \quad \psi'(0) = 0$$

Naive Newton algorithm:

$$\psi^{(0)}(x+\Delta x) = \psi^{(0)}(x) + \Delta x\, \psi^{(1)}(x)$$
$$\psi^{(1)}(x+\Delta x) = \psi^{(1)}(x) + \Delta x \frac{2m}{\hbar^2}\left(V(x+\Delta x/2) - E\right)\psi^{(0)}(x)$$

[Can use Runge-Kutta, etc... to be more exact]

Ground state:

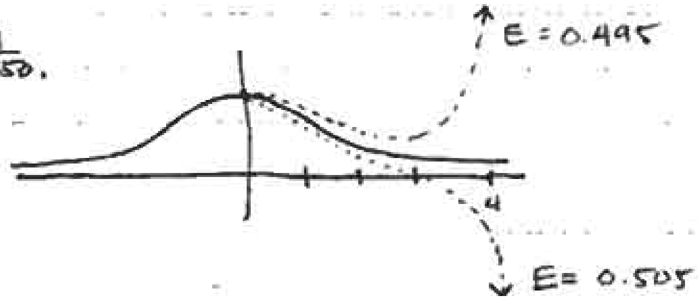


Can triangulate quickly on E_0.
Increased accuracy as $\Delta x \to 0$.

Ex. SHO

$$-\frac{1}{2}\psi'' + \left(\frac{1}{2}x^2 - E\right)\psi = 0 \qquad (\hbar = m = \omega = 1)$$

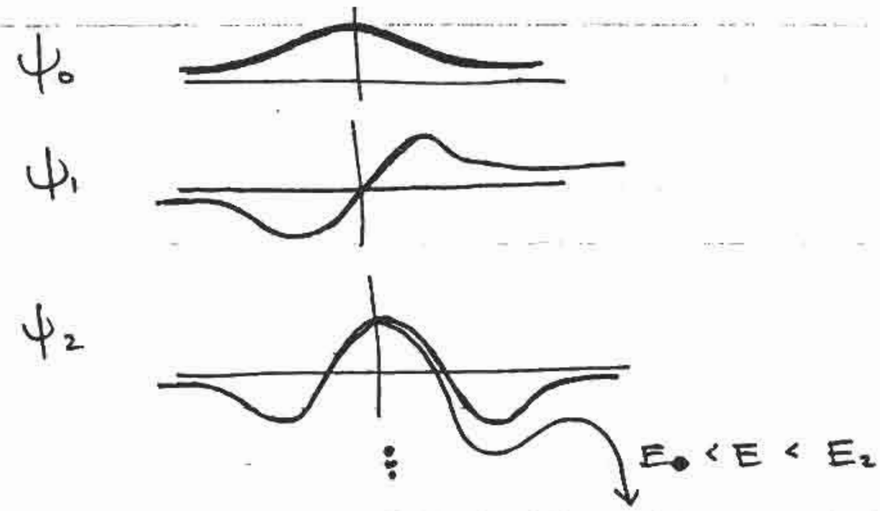
with $\Delta x = \frac{1}{250}$.



1000 steps $\rightarrow$ within 1% of E_0.

Similar story for n^{th} excited state.

Can show: n^{th} excited state has n ϕ's.



Shooting method works well in 1D, not in higher dimensions.

Variational method (Rayleigh - Ritz)

Basic theorem: define $\overline{H} = \dfrac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$ for any $|\psi\rangle \in \mathcal{H}$.

If E_0 is the ground state energy then $\overline{H} \geq E_0$

Proof:

Suffices to show when $\langle\psi|\psi\rangle = 1$.

Write $|\psi\rangle = \sum c_n |n\rangle$, $H|n\rangle = E_n|n\rangle$

$(\sum |c_n|^2 = 1)$ (note: not SHO basis necessarily)

$$\langle\psi|H|\psi\rangle = \sum E_n |c_n|^2$$
$$= E_0 + \sum (E_n - E_0)|c_n|^2 \geq E_0.$$

Variational method for finding upper bound on E_0:

A) Define a multi-parameter space of "trial functions" $|\psi(\lambda_1, \lambda_2, \ldots, \lambda_k)\rangle$

B) Calculate $\overline{H}(\lambda_1, \lambda_2, \ldots \lambda_k)$

C) Minimize $\overline{H}$ by solving $\partial\overline{H}/\partial\lambda_i = 0 \quad i=1,\ldots,k.$

Can often get very good approx. to E_0 with a few parameters

Helpful to use physical intuition to pick states.

<u>Ex of variational method</u> (others in book: pp. 313–316)

Consider SHO

$$H = \tfrac{1}{2}p^2 + 2x^2 \qquad [\hbar = m = 1, \ \omega = 2]$$

Use linear combination of $\omega = 1$ eigenstates $|n\rangle$ as trial function:

$$|\psi\rangle = \sum c_n|n\rangle, \qquad \sum |c_n|^2 = 1.$$

$$\langle n|H|m\rangle = \langle n|\,[N + 1/2] + \tfrac{3}{2}x^2\,|m\rangle$$

$$= \tfrac{5}{2}(n + 1/2)\,\delta_{n,m} + 3/4\sqrt{m(m-1)}\;\delta_{m,n+2} + 3/4\sqrt{n(n-1)}\;\delta_{n,m+2}$$

In even sector, including $|0\rangle$, $|2\rangle$, $|4\rangle$, for example:

$$H = \begin{pmatrix} 5/4 & \frac{3}{2\sqrt{2}} & 0 \\ \frac{3}{2\sqrt{2}} & 25/4 & \frac{3\sqrt{3}}{2} \\ 0 & \frac{3\sqrt{3}}{2} & 45/4 \end{pmatrix}$$

Exact energy: $E_0 = \frac{\omega}{2} = 1.$

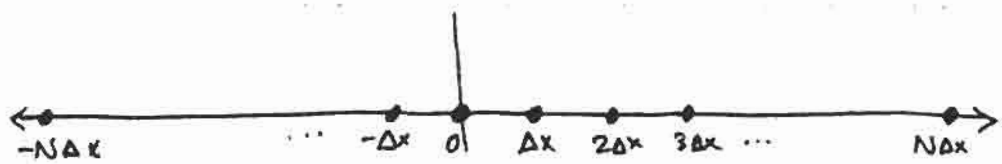
Keeping:

1	state:	$E_{min} = 5/4 = 1.25$
2	states:	$E_{min} \cong 1.0343$
3	states:	$E_{min} \cong 1.00471$
4	"	$E_{min} \cong 1.000615$
5	"	$E_{min} \cong 1.0000773$
		$\vdots$

Converges rapidly.

Compare with simple numerical finite difference method

Divide space into gridpoints (1D example; easy to generalize to higher D)



Sample wavefunction at gridpoints $\psi(k\Delta x)$, $-N \le k \le N$.

(Assume $\psi = 0$ for $|k| > N$).

$V(x)$ is diagonal matrix

$$V_{kk'} = V(k\Delta x)\,\delta_{kk'}$$

$$\partial/\partial x\, f \rightarrow \frac{1}{\Delta x}\left(f((k+1/2)\Delta x) - f((k-1/2)\Delta x)\right)$$

$-\dfrac{\partial^2}{\partial x^2}$ is tridiagonal matrix (in 1D)
(pentadiagonal in 2D, etc)

$$D_{kk'} = \begin{cases} \dfrac{2}{\Delta x^2}, & k = k' \\ -1/\Delta x^2, & |k-k'| = 1 \\ 0, & \text{otherwise} \end{cases}$$

Ex. 1D SHO $H = \frac{1}{2}p^2 + \frac{1}{2}x^2$ $(\hbar = m = \omega = 1)$

$$H = \begin{pmatrix} \frac{1}{\Delta x^2} + 2\Delta x^2 & -1/2\Delta x^2 & 0 & & & \cdots \\ -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + \frac{1}{2}\Delta x^2 & -1/2\,\Delta x^2 & 0 & & \\ 0 & -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + \cdot & -\frac{1}{2\Delta x^2} & 0 & \\ & 0 & -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + \frac{1}{2}\Delta x^2 & -\frac{1}{2\Delta x^2} & \\ & & 0 & -\frac{1}{2\Delta x^2} & \frac{1}{\Delta x^2} + 2\Delta x^2 & \\ \cdots & & & 0 & 0 & \ddots \end{pmatrix}$$

Sample results

Δx	$N_{\Delta x}$	$2N+1$	E_{min}	$E_{(2)}$
0.5	1	5	0.674	2.304
0.2	2	21	0.517	1.635
0.1	5	101	0.4997	1.4984
		note:		
0.05	5	201	0.49992	1.4996
0.1	10	201	0.4997	1.4984

=

- Useful to sample points more carefully when wf is large
- Generally, variational method much more efficient.

Some other approximation methods:

- Bohr - Sommerfeld $\oint p\,dq = n h$

- WKB (will discuss in later lecture)

- Pert. theory (later in course).

- Quantum Monte Carlo (next week)
  [Good for realistic, high-dimensional systems]

Quantum Monte Carlo method

Want to solve $H\psi = E\psi$ for ψ fn in high-dim space.

consider diff. equation

$$\frac{\partial \psi(\tau)}{\partial \tau} = -H\psi(\tau) \qquad \text{(Im time Schrödinger equation)}$$

if $H\psi^{(0)} = E\,\psi^{(0)}$

$$\psi(\tau) = e^{-E\tau}\,\psi(0)$$

if $\psi(0) = \sum c_n^{(0)}|\psi_n\rangle \qquad H|\psi_n\rangle = E_n|\psi_n\rangle$

$$\psi(\tau) = \sum c_n(\tau)\,|\psi_n\rangle \qquad c_n(\tau) = c_n(0)\,e^{-E_n\tau}.$$

~~at large~~ ground state dominates. $\psi(\tau) \to c_0(0)\,e^{-E_0\tau}\,|\psi_0\rangle$

So want to simulate

$$\frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,\tau)}{\partial x^2} - V(x)\,\psi(x,\tau)$$

In high dim, can't do finite difference-type methods

N^d large (10^{12}) for $10\times \cdots \times 10$ in Helium

If $V=0$, just diffusion equation

$$\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2m}\,\frac{\partial^2\psi}{\partial x^2}.$$

Can solve by random walks.

Assume $\psi(x,0)$ is a prob. distribution. (≥ 0 everywhere)

$$\psi(x,\Delta\tau) = \int K(y)\,\psi(x-y,0)$$

each particle moves from x to $x+y$ with prob $K(y)$

describes a step of a random walk. ~~$\int K(y)\,dy = 1$~~

$K(y)$ = prob. step from $x-y$ to x

$$\int K(y) = 1$$

$$\int K(y)\,y = 0$$

$$\int K(y)\tfrac{1}{2}y^2 = \alpha$$

$$\frac{\partial\psi}{\partial t} \sim \frac{\psi}{\Delta t}$$

$$\begin{aligned}
\psi(x,\Delta\tau) = {} & \int K(y)\,\psi(x,0) \\
& - \int K(y)\,y\,\frac{\partial\psi}{\partial x}(x,0) \\
& + \frac{1}{2}\int K(y)\,y^2\,\frac{\partial^2\psi}{\partial x^2}(x,0) + \dots \\
= {} & \psi(x,0) \\
& + \alpha\,\frac{\partial^2\psi}{\partial x^2}(x,0)
\end{aligned}$$

$\Rightarrow$ diffusion eqn

~~FeP $\psi(x,t)$ ... add~~

scale $\Delta\tau \sim \varepsilon$

$\alpha \sim \frac{\hbar^2}{2m}\varepsilon$, higher order terms negligible

$$\frac{\partial\psi}{\partial\tau} \approx \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

For example, $K(y) = \frac{1}{2}\left(\delta(y-\sqrt{2\varepsilon}) + \delta(y+\sqrt{2\varepsilon})\right)$

prob. $\frac{1}{2}$ $x \to x \pm \sqrt{2\varepsilon}$

$$\int K = 1 \qquad \frac{1}{2}\int K y^2 = \varepsilon$$

prob. distribution under random walk $\Rightarrow$ $\frac{\partial\psi}{\partial\tau} = \frac{\partial^2\psi}{\partial x^2}$.

[note error in GT: $\frac{\partial\psi}{\partial\tau} = D\frac{\partial^2\psi}{\partial x^2}$, $D = \frac{1}{2}\frac{\Delta x^2}{\Delta\tau}$]

so, to solve diff. equation, start w/ distribution of "~~a~~ random walkers", w/ distrib given by $\psi(x,0)$. perform random walks K_ε for T/ε steps. get solution $\psi(X,T)$ w/ correct distribution

Adding source terms

$$(\ast) \quad \frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,\tau)}{\partial x^2} - V(x)\, \psi(x,\tau)$$

If only had V, just treat as
~ radioactive decay → exponential birth / death.

@ each time step:

if $V > 0$, prob. $V \Delta \tau$ particle "dies"
if $V < 0$, prob. $V \Delta \tau$ particle doubles.

Naive Algorithm to solve $(\ast)$

1. Place N walkers in space
2. randomly move according to pdist $K(y)$ ($x \to x + y$)
3. Kill / double walker based on $V(x)$ @ new position.

Problem: even ground state decays as

$$\psi(x,\tau) \sim e^{-E_0 \tau} \psi_0(x)$$

Solution: use reference energy.

Related problem: how to extract E_0?

Difficult to fit $e^{-E_0 \tau}$ using prob. distribution

But $E_0 = \langle V \rangle = \dfrac{\sum_{i=1}^{N} V(x_i)}{N}$

Pf. $\dfrac{\partial \psi(x,\tau)}{\partial \tau} = \dfrac{\hbar^2}{2m} \dfrac{\partial^2 \psi(x,\tau)}{\partial x^2} - V(x)\,\psi(x,\tau)$

$\Rightarrow \displaystyle\int \frac{\partial \psi}{\partial \tau}\, dx = -\int V(x)\,\psi(x,\tau)\, dx$

but asymptotically $\psi \to c_0\, \phi_0(x)\, e^{-E_0 \tau}$

$\dfrac{\partial \psi}{\partial \tau} = -E_0\, \psi$

$\Rightarrow -E_0 \displaystyle\int \psi\, dx = -\int V(x)\,\psi(x,\tau)\, dx$

$\Rightarrow E_0 = \dfrac{\int V(x)\,\psi(x,\tau)}{\int \psi(x,\tau)}$ as $\tau \to \infty$.

Improved algorithm

1. Place N_0 walkers in space randomly @ positions X_i

2. Compute $V_{ref} = \frac{1}{N_0} \sum V(X_i)$

3. Random walk with kernel K_c for each walker

4. For each walker
Compute $\Delta V = \left[V(x) - V_{ref}\right] \Delta\tau$, random $r \in [0,1]$
   if $\Delta V > 0$, $r < \Delta V$, remove
   if $\Delta V < 0$, $r < -\Delta V$, add a new walker.

5. Change to new $V_{ref} = \langle V \rangle - \frac{1}{N_0}(N - N_0)\Delta\tau$

repeat 3-5 many times,
asymptotically, $V_{ref} \sim$ ground state energy.

Even better: use initial guess (importance sampling)

$\Rightarrow$ Fokker-Planck eqn (drift term)