# 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 Ven]

**Symmetry:**

A key principle is to exploit any available symmetry.

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

$\mathcal{R}(g)$ is a linear op. on $\mathcal{H}$ $\quad \forall g \in G$.

$$\mathcal{R}(gh) = \mathcal{R}(g)\,\mathcal{R}(h)$$
$$\mathcal{R}^\dagger(g) = \mathcal{R}(g^{-1})$$
$$\mathcal{R}(id) = \mathbb{1}$$

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

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

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 $a^2 = 1$.

| $\cdot$ | 1 | a |
|---|---|---|
| 1 | 1 | a |
| a | a | 1 |

mult table for $\mathbb{Z}_2$

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

<u>Parity operator</u> $\quad \Pi = B_\pi(a)$

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

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

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

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

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

<u>Pf.</u> $\quad$ Can choose $\psi_n(x)$ phase to be real,

$\Pi|\psi_n\rangle = \pm|\psi_n\rangle$.

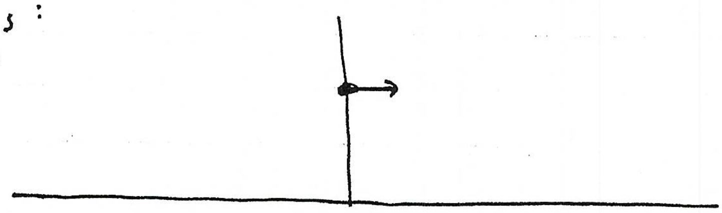
$\Rightarrow \psi_n(-x) = \pm\psi_n(x)$

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

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

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

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



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

with initial conditions

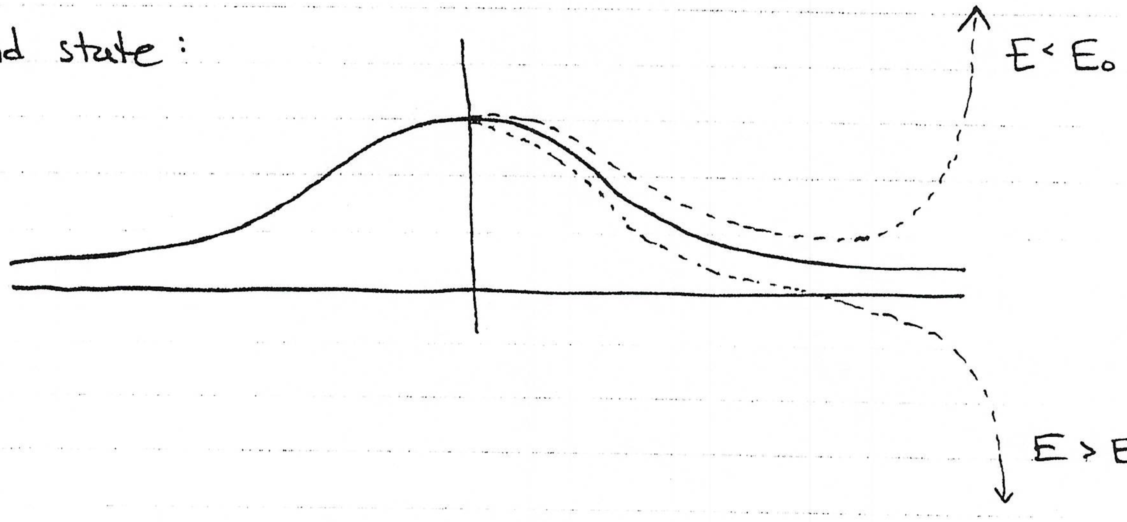
$\psi(0) = 1, \qquad \psi'(0) = 0$

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:

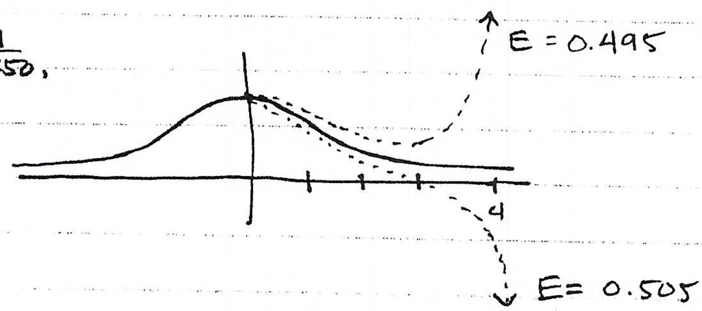



Can triangulate quickly on $E_0$.
Increased accuracy as $\Delta x \to 0$.

Ex. SHO

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

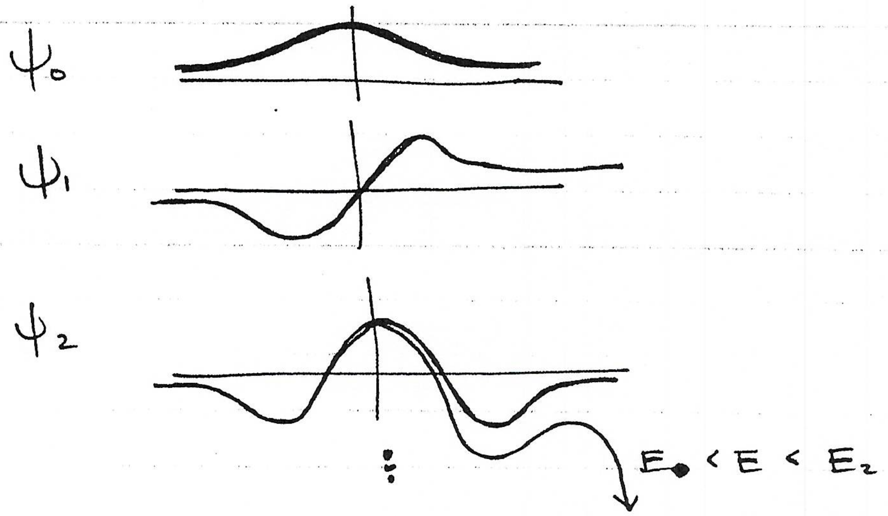
with $\Delta x = \frac{1}{250}$,




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

Similar story for $n^{th}$ excited state.

Can show: $n^{th}$ excited state has $n$ $\phi$'s.




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

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<u>Variational method</u> (Rayleigh - Ritz)

<u>Basic theorem</u>:

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 $\overline{H} \geq E_0$

<u>Proof</u>:

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.

Ex of variational method (others in book: pp. 313–316)

Consider SHO

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

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

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

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

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

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.

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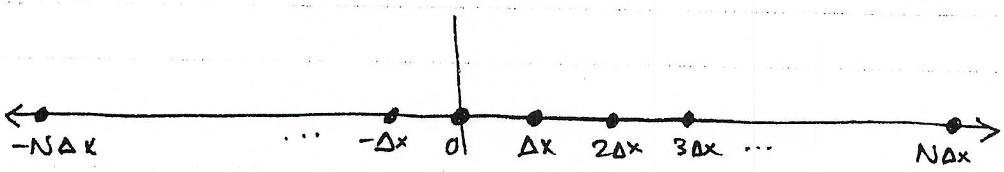
Compare with simple numerical finite difference method

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




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

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

$V(x)$ is diagonal matrix

~~$\partial/\partial x f \to \frac{1}{\Delta x}(f((k+1/2)\Delta x) - f((k-1/2)\Delta x))$~~

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

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

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

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

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

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

Sample results

| $\Delta x$ | $N\Delta x$ | $2N+1$ | $E_{min}$ | $E_{(2)}$ |
|---|---|---|---|---|
| 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:

| $\Delta x$ | $N\Delta x$ | $2N+1$ | $E_{min}$ | $E_{(2)}$ |
|---|---|---|---|---|
| 0.05 | 5 | 201 | 0.49992 | 1.4996 |
| 0.1 | 10 | 201 | 0.4997 | 1.4984 |

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

# 2. Time evolution (Quantum dynamics)

## 2.1 Time evolution & the Schrödinger equation

Time in QM is a parameter ($|\psi(t)\rangle \in \mathcal{H}$).
not an observable like $X$.

Note: SR relates $x, t$; restored in relativistic QFT, where $X$ is no longer an observable.

Question: how does a state $|\psi(t)\rangle$ evolve in time?

Postulate (Schrödinger eqn.)

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

Write ~~In~~ terms of time-evolution operator $\mathcal{U}(t, t_0)$;

If state at time $t_0$, $|\alpha, t_0\rangle \in \mathcal{H}$
becomes at time $t$ $|\alpha, t_0; t\rangle \in \mathcal{H}$,

write $|\alpha, t_0; t\rangle = \mathcal{U}(t, t_0)\, |\alpha, t_0\rangle$.

Properties of $\mathcal{U}(t, t_0)$:

i) Unitary – conserves probability, norm

$$\boxed{\mathcal{U}^\dagger(t, t_0)\, \mathcal{U}(t, t_0) = \mathbb{1}}$$

$$\langle \alpha, t_0; t \,|\, \alpha, t_0; t\rangle = \langle \alpha, t_0 | \mathcal{U}^\dagger(t, t_0)\, \mathcal{U}(t, t_0) | \alpha, t_0\rangle$$
$$= \langle \alpha, t_0 | \alpha, t_0\rangle .$$

ii) composition law

$$\boxed{\mathcal{U}(t,t_1)\,\mathcal{U}(t_1,t_0) = \mathcal{U}(t,t_0)}$$

$$|\alpha,t_0;t\rangle = \mathcal{U}(t,t_1)\,|\alpha,t_0;t_1\rangle$$

$$= \mathcal{U}(t,t_1)\,\mathcal{U}(t_1,t_0)\,|\alpha,t_0\rangle.$$
$$= \mathcal{U}(t,t_0)\,|\alpha,t_0\rangle$$

iii) identity at $t=t_0$

$$\boxed{\lim_{t\to t_0} \mathcal{U}(t,t_0) = \mathbb{1}}$$ since $\lim_{t\to t_0} |\alpha,t_0;t\rangle = |\alpha,t_0\rangle$.

Properties i) — iii) satisfied when infinitesimal form is

$$\mathcal{U}(t_0+dt,\,t_0) = 1 - \frac{iH(t_0)dt}{\hbar}$$

(equivalent to Schrödinger.)

Appearance of $\hbar$ — needed on dimensional grounds.
— discuss further in context of classical - quantum correspondence

Schrödinger for $\mathcal{U}(t,t_0)$

$$\boxed{i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0) = H(t)\,\mathcal{U}(t,t_0)} \qquad (*)$$

$$i\hbar\frac{\partial}{\partial t}|\alpha,t_0;t\rangle = i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0)\,|\alpha,t_0\rangle$$

$$= H(t)\,\mathcal{U}(t,t_0)\,|\alpha,t_0\rangle$$

$$= H(t)\,|\alpha,t_0;t\rangle$$

Solutions of (*).

1) Time-independent $H(t) = H$

$$\lim_{N\to\infty}\left[1 - \frac{i}{\hbar} H \frac{(t-t_0)}{N}\right]^N = e^{-\frac{iH}{\hbar}(t-t_0)}$$

so

$$\boxed{\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}}$$

(can easily verify solves $i\hbar \frac{d}{dt}\mathcal{U}(t,t_0) = H\,\mathcal{U}(t,t_0)$).

2) Time-dependent, but $[H(t), H(t')] = 0$.

(Ex: particle in magnetic field, constant direction, varying strength
$H = \frac{p^2}{2m} + B(t) S_z$ )

similar solution but now

$$\boxed{\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'}}$$

verify: $i\hbar\frac{d}{dt}\mathcal{U}(t,t_0) = \frac{d}{dt}\left[\int_{t_0}^{t} H(t')dt'\right]\mathcal{U}(t,t_0)$

$= H(t)\,\mathcal{U}(t,t_0)$

3) Time-dependent $H(t)$, $[H(t), H(t')] \neq \emptyset$.

(Ex: particle in B field, direction changes in time.)

Solve iteratively

$$\int_{t_0}^{t} dt' \left[\frac{d}{dt'} \mathcal{U}(t',t_0)\right] = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\, H(t')\,\mathcal{U}(t',t_0)$$

$$\Rightarrow \quad \mathcal{U}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt' \cdot H(t')\,\mathcal{U}(t',t_0)$$

defines $\mathcal{U}(t,t_0)$ in terms of $\mathcal{U}(t',t_0)$, $t' \leq t$.

iterating:

$$\mathcal{U}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, H(t')$$

$$+ \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt^{(1)} \int_{t_0}^{t^{(1)}} dt^{(2)}\, H(t^{(1)})H(t^{(2)})\,\mathcal{U}(t^{(2)},t_0)$$

$$\vdots$$

$$= 1 + \sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n\, H(t_1)\cdots H(t_n)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \mathcal{T}\left(\int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n\, H(t_1)H(t_2)\cdots H(t_n)\right)$$

(Dyson series)

where $\mathcal{T}$ is time-ordering operator – orders following ops so time goes up to left.

can write answer in compact form

$$\boxed{\mathcal{U}(t,t_0) = \mathcal{T}\left[e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, H(t')}\right]}$$

(looks same as (2), but $\mathcal{T}$ carries extra info above)