— Not a good name since diagonalization isn't a perturbation method

↳ But on the other hand diagonalization to handle degenerate states can be combined with non-degenerate ~~that~~ perturbation to handle non-degenerate states — in an unholy combination which probably is used.

Also you can probably derive non-degenerate perturbation from diagonalization at least to some order.

— I think for 2-d. Hilbert space this ~~follows easy~~ is proven easily

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Diagonalization

Say you have Hamiltonian H for a system, but not a solution

~~Ordi~~ I'm thinking of H in operator form.

But say you also ~~Ho~~ had Hamiltonian H_0 for the same Hilbert space as H, but not the same system.

And you have the stationary state solutions for H_0

We are assuming quantized states — a discrete but usually infinite set

$$H_0 |\chi_{0i}\rangle = E_{0i} |\chi_{0i}\rangle$$

and $\sum |\chi_{0i}\rangle \langle$ and E_{0i} known

is a complete orthonormal set.

If you have a complete set that is not orthonormal, you can always, in principle, derive ~~a set~~ an orthonormal complete set by linear combination of the first set.

The Gram-Schmidt procedure is the brute force way (which incidently proves it can be done), but there are usually better ways.

There can be degeneracies.

No problem with that for diagonalization.

Now consider

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

the eigen problem for which you do NOT know the solution.

Now I know what you are thinking; expand $|\psi\rangle$ in the set $\{|\psi_0\rangle\}$ and solve for the coefficients

$$|\psi\rangle = \sum_j c_j |\psi_{0j}\rangle$$

For an infinite dimension Hilbert space, the sum is in general, an infinite sum.

So

$$\sum_j c_j H|\psi_{oj}\rangle = E\sum_j c_j|\psi_{oj}\rangle$$

Now what do we do to isolate the c_j's?

Operate on this equation by $\langle\psi_{oi}|$ to get

$$\sum_j c_j \langle\psi_{oi}|H|\psi_{oj}\rangle = E\sum_j c_j\langle\psi_{oi}|\psi_{oj}\rangle$$

$$= \delta_{ij}$$

by orthonormality.

6-40

Do one bra

$$\sum_j c_j \langle \psi_{0i} | H | \psi_{0j} \rangle = E c_i$$

This is the matrix element of H in the H_0 representation.

In one-dimension for example

$$\langle \psi_{0i} | H | \psi_{0j} \rangle = \int_{-\infty}^{\infty} \psi_{0i}^* H \psi_{0j} \, dx$$

In general the matrix elements have to be evaluated numerically.

So

$$H \sum_j c_j |\psi_j\rangle = E \sum_j c_j |\psi_j\rangle$$

$$\sum_j c_j H |\psi_j\rangle = E \sum_j c_j |\psi_j\rangle$$

We want solutions for the c_j.

Obvious inner product with $|\psi_{oi}\rangle$

$$\sum_j c_j \langle \psi_{oi} | H | \psi_{oj} \rangle = E \sum_j c_j \langle \psi_{oi} | \psi_{oj} \rangle$$

$\langle \psi_{oi} | \psi_{oj} \rangle = \delta_{ij}$

$$= E c_i$$

$$H_{ij} = \langle \psi_{oi} | H | \psi_{oj} \rangle$$

is called the matrix element of H in the $\{|\psi_{oi}\rangle\}$ representation.

for 1-d, x-space

$$H_{ij} = \langle \psi_{oi} | H | \psi_{oj} \rangle = \int_{-\infty}^{\infty} \psi_{oi}^{*} H \psi_{oj} \, dx$$

In any case H_{ij} can be evaluated analytically or numerically.

We now have a set of linear equations for the c_i's

$$\sum_j H_{ij} c_j = E c_i$$

which can be assembled into a matrix equation

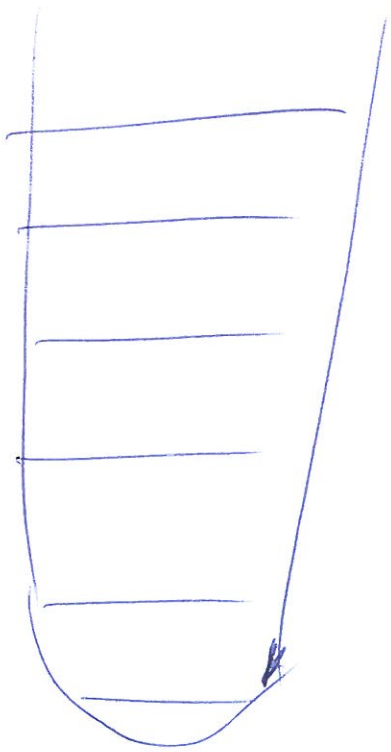
$$H_{\text{matrix}} \, \underline{c} = E \underline{c}$$

which is a matrix eigenvalue problem.

For a finite Hilbert space, of dimension N, it is an $N \times N$ problem.

What if $N = \infty$?

In this case, you must truncate.



potential well with infinite discrete states $|\chi_{0i}\rangle$

~~Let assume that~~

The $|\chi_{i0}\rangle$'s are mixtures of the $|\chi_{0i}\rangle$ states.

6-68

Now Non-degenerate perturbation theory

gives us a clue.

Recall p. 6-36a - 6-36c

The ~~state~~ perturbation (original state) correction to the unperturbed state decrease in size as the ~~the~~ energy difference between the original state and the mixed in other state decreases.

So state j remote in energy from a given state i are less mixed in in creating the perturbed state.

This suggests ~~We assume~~ (but I think it can proven) that if you are interested only in a certain energy range, you

~~only~~ need only to some approximation to include in the Matrix H_{mat} states $|\psi_{oi}\rangle$ from that range and for greater accuracy states $|\psi_{oi}\rangle$ from near it.

In fact, usually people want the ground state up to some energy. Quantum systems of interest are often in ground or low excitation states.

So you would assemble H_{mat} for the lowest N states of $\Sigma|\psi_{oi}\rangle$

If that is NOT accurate enough, you can always increase N and hope for large enough N that the lowest energy states at least are sufficiently accurate.

We note that we've shown the equivalence/relationship/commonality of Sch. Wave mechanics and Heisenberg ~~Wave~~ matrix mechanics

both were discovered ~1926 independently

(Sch. discovered the Sch. equation over the 1925-1926 Christmas

The playboy physicist is NOT a contradiction in terms.

season while on a skiing vacation with a lady not his wife

— Sch took his vacations seriously and commented this was the only time in his life when he worked on ~~this~~ a vacation)

We've sort of gone from wave mechanics to matrix mechanics, but if you knew the matrix first you could just have wave matrices.

But actually both approaches are needed.

We conceive of potentials as functions of space

— ~~they~~ are I think

So the Hamiltonian in operator form is pretty fundamental.

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But computers hate differential equations

→ You have to turn them into difference equations and risk instabilities and all kinds of ~~arbitrary~~ choices to get best form.

But computers love matrices.

So the matrix formulation allows a good solution procedure, once the matrix elements have been evaluated using H in operator form usually.

But there are systems like ~~spin~~ pure spin cases

where matrix operations are fundamental — and so the matrix formulation is fundamental too, not just a numerical convenience.

To return

$$H_{mat}\,\underline{c} = E\,\underline{c}$$

is a matrix eigenvalue problem.

The solution procedure is simple in principle

$$(H - E I_{mat})\,\underline{c} = 0$$

I_{mat} is a unit matrix of dimension N.

For a non-trivial solution
(one where $\underline{c} \neq 0$),

$$\det | H - E 1_{mat} | = 0$$

for an N-dimension matrix
this determinant equation
gives a degree N.
— and so has N solutions
for eigenvalues E.

The H_{mat} is a Hermitian matrix,
H is a Hermitian operator

$$(H_{ij})^\dagger = (H_{ij}^*)^T = H_{ji}^*$$

Hermition conjugation of a matrix,

$$= \langle \chi_{oj} | H | \chi_{oi} \rangle^*$$
$$= \langle \chi_{oi} | H^\dagger | \chi_{oj} \rangle$$

by Hermition conjugate

$$= \langle \psi_{oi} | H | \psi_{oj} \rangle \quad \text{since } H = H^{\dagger}$$

$$= H_{ij}$$

$$\therefore \quad H_{mat}^{\dagger} = H_{mat}$$

The matrix is a Hermitian matrix.

We should really have known this since the abstract vector formalism of QM treats operators generally whether matrix or differentiating or other.

It can be shown (in fact we shown) that the eigenvalues of H_{mat} must be pure real and ~~for~~

non-degenerate ones have orthoganal ~~states~~ eigenvectors.

Degenerate state vector can be linearly combined to create an orthoganal set of equivalent independent states.

Now for each eigenvalue E_i plug into matrix equation

$$H \underset{\sim}{c}_i = E \underset{\sim}{c}_i$$

and solve $\underset{\sim}{c}_i$

So you get the set of E_i and $\underset{\sim}{c}_i$.

These are the complete solution of the (truncated) matrix problem

$$|\psi_i\rangle = \sum_j c_{ij} |\psi_{0j}\rangle$$

ith state

2 x 2 cases can be done by hand easily (we'll look at this case)

3 x 3 cases can be done by hand easily in special cases. (we'll look at examples)

— higher dimension cases we leave to the computer

— standard packages (e.g., LAPACK) kick out eigenproblem solutions efficiently

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Why is diagonalization called diagonalization?

Brief foray into unitary ~~matrices.~~ operators (which could be matrices)

— They are transformations with the following property

$$U^{\dagger} = U^{-1}$$

and so they are NOT Hermitian (unless $U^{-1} = U$ which implies $1 = UU^{-1} = U^2$ $U = \pm 1_{op}$)

Unitary matrices can be used both for physical evolution operators and thus represent physical properties or coordinate transformations

Consider inner product

$$\langle a | b \rangle$$

Now consider $|b'\rangle = U|b\rangle$

and $|a'\rangle = U|a\rangle$

and so $\langle a'| = \langle a|U^\dagger$

$$\langle a'|b'\rangle$$

$$= \langle a|U^\dagger U|b\rangle$$

$$= \langle a|U^{-1}U|b\rangle$$

by unitarity

$$= \langle a|b\rangle$$

$\langle a'|\alpha\rangle = \langle \alpha|a'\rangle^* = \langle \alpha|U|a\rangle^*$

$= (\langle a|U^\dagger|\alpha\rangle)^*$

$= \langle a|U^\dagger|\alpha\rangle$

since $|\alpha\rangle$ is general

$\langle a'| = \langle a|U^\dagger$

So Unitary transformations preserve inner products and normalization

Now consider our set of N eigenvectors

$$\{\underset{\sim}{c}_i\}$$

Define $U = \begin{pmatrix} \underset{\sim}{c}_1 \\ \underset{\sim}{c}_2 \\ \vdots \end{pmatrix}^*$

a matrix where the rows are the complex conjugates of eigenvectors

and $U^+ = \begin{pmatrix} \underset{\sim}{c}_1 & \underset{\sim}{c}_2 & \underset{\sim}{c}_2 \end{pmatrix}$

is the matrix where the columns are the eigenvectors.

$U U^+ = 1_{mat}$ using orthonormality.

$\therefore U^+ = U^{-1}$ and U is unitary.

Now $H \underset{\sim}{c}_i = E_i \underset{\sim}{c}_i$

Operate on with U

$$U H \underset{\sim}{c}_i = E_i U \underset{\sim}{c}_i$$

$$U H U^{-1} U \underset{\sim}{c}_i = E_i U \underset{\sim}{c}_i$$

$$U H U^{-1} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = E_i \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

a unit vector with 1 in the ith location all other elements zero.

Now $H' = U H U^{-1}$

is the transformed Hamiltonian of H.

It is H in it's own representation.

$$H'_{ij} = \sum_{k} \sum_{l} U_{ik} H_{kl} U^{-1}_{lj}$$

Werner Heisenberg

6-82

$$H'_{ij} = \sum_{k,\ell} U_{ik} H_{k\ell} U^{+}_{\ell j}$$

$$= \sum_{k} U_{ik} E_j U^{+}_{kj}$$

$$= \sum_{k} E_j U_{ik} U^{-1}_{kj}$$

$$= E_j \delta_{ij}$$

If you think about it

$$\therefore H' = \begin{pmatrix} E_1 & & & 0 \\ & E_2 & & \\ & & E_3 & \\ 0 & & & \ddots \; E_N \end{pmatrix}$$

The matrix Hamiltonian in it's own representation,

is a diagonal matrix whose diagonal elements are the eigen energies

— We've diagonalized the matrix

Actually, I don't think people explicitly form the diagonalized matrix much — but one could — and hence the name "diagonalizing the matrix."

Diagonalization is the standard, ~~probably the standard~~

{ Even I have done it in long ago summer undergrad research work

Non-perturbative approach to solving for eigen state and eigen energies.

It's can be exact for finite Hilbert spaces and for infinite ones it must

be approximate.

How does one choose set $\{|\psi_{0i}\rangle\}$ if one has choice (and one often does)?

Well as close as one can conveniently to the exact set $\{|\psi_i\rangle\}$.

Intuitively, it should be clear that truncation of $\infty \times \infty$ matrix to an $N \times N$ matrix is a better approximation if $\{|\psi_{0i}\rangle\}$ is like $\{|\psi_i\rangle\}$ or H_0 is ~~like~~ like H

If $\{|\psi_{0i}\rangle\}$ were exactly right and $H = H_0$ then truncation would give exact solutions, of course.