

Perturbation Theory

Not so many QM problems can be completely solved. Fortunately, many very important problems involve adding a smaller piece to Hamiltonian of a solvable problem

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}$$

\nearrow solvable \nwarrow small

Before deriving "perturbation theory" let's guess what happens. Suppose we have a gm system in a state $\psi(x)$. What would our guess be for the energy shift of an additional small $\lambda V(x)$?

Reasoning: $P(x) = |\psi(x)|^2 dx$ is probability particle is between x and $x+dx$

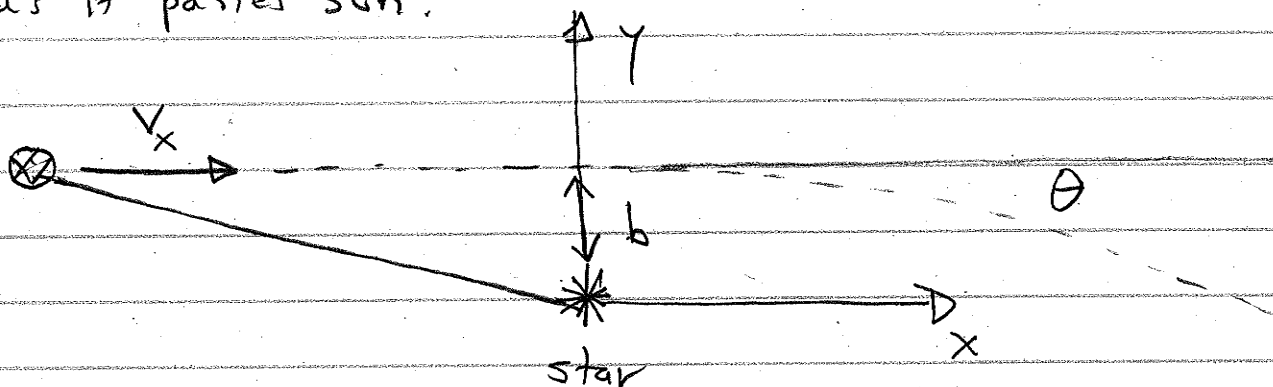
Its energy if at x is $\lambda V(x)$

$$\delta E = \int dx P(x) \lambda V(x) = \int |\psi(x)|^2 \lambda V(x) dx$$

PT-CM1

An example of perturbation theory in classical mechanics, From qualifying exam!

By what angle is a very fast comet deflected as it passes sun?



Assume path is unperturbed

Q: What is b called?
A: "Impact parameter"

$$(x, y) = (-v_x t, b)$$

$$\frac{dp_y}{dt} = F_y = \frac{GMm}{b^2 + v_x^2 t^2} \frac{b}{(b^2 + v_x^2 t^2)^{1/2}}$$

$$\Delta p_y = \int_{-\infty}^{+\infty} dt \frac{GMm b}{(b^2 + v_x^2 t^2)^{3/2}}$$

$$v_x t = b \tan \theta$$

$$t = -\infty \rightarrow \theta = -\pi/2$$

$$t = +\infty \rightarrow \theta = +\pi/2$$

$$v_x dt = b \sec^2 \theta d\theta$$

PT-CM2

$$\Delta p_y = \int_{-\pi/2}^{\pi/2} \frac{-GMm b \sec^2 \theta d\theta}{b^3 \sec^3 \theta} / v_x$$

$$= -\frac{GMm}{b v_x} \int_{-\pi/2}^{\pi/2} \cos \theta d\theta = -2GMm / b v_x$$

$$v_y = -2GM / b v_x$$

at large t

$$\tan \theta = \frac{v_y}{v_x} = \frac{-2GM}{b v_x^2}$$

Most elegantly written

$$\tan \theta = -\frac{2GMm}{b} / \frac{1}{2} m v_x^2$$

↑
grav PE at
closest approach

↑
KE

PT2

Q: What went into this result?

A: We assumed $\lambda V(x)$ doesn't change $\psi(x)$. (λ small)

We will now derive this result more formally, and

extend it!

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}$$

$$\hat{H}_0 |\phi_{n0}\rangle = E_{n0} |\phi_{n0}\rangle$$

↑
↑
Eigenvectors/values of \hat{H}_0

$$E_n = E_{n0} + \lambda E_{n1} + \lambda^2 E_{n2} + \dots$$

$$|\phi_n\rangle = |\phi_{n0}\rangle + \lambda |\phi_{n1}\rangle + \lambda^2 |\phi_{n2}\rangle + \dots$$

$$(\hat{H}_0 + \lambda \hat{V}) \{ |\phi_{n0}\rangle + \lambda |\phi_{n1}\rangle + \lambda^2 |\phi_{n2}\rangle + \dots \}$$

$$= (E_{n0} + \lambda E_{n1} + \lambda^2 E_{n2} + \dots) \{ |\phi_{n0}\rangle + \lambda |\phi_{n1}\rangle + \dots \}$$

Matching term-by-term

$$\hat{H}_0 |\phi_{n0}\rangle = E_{n0} |\phi_{n0}\rangle \quad \text{as expected!}$$

PT 3

$$\hat{H}_0 |\phi_{n1}\rangle + \hat{V} |\phi_{n0}\rangle = E_{n1} |\phi_{n0}\rangle + E_{n0} |\phi_{n1}\rangle$$

Take dot product with $|\phi_{n0}\rangle$

$$Q: \langle \phi_{n0} | \hat{H}_0 | \phi_{n1} \rangle = ?$$

$$A: E_{n0} \langle \phi_{n0} | \phi_{n1} \rangle \quad \text{since } \hat{H}_0 \text{ can "act back" on } \langle \phi_{n0} |$$

$$\text{so } \langle \phi_{n0} | \hat{V} | \phi_{n0} \rangle = E_{n1}$$

This is just what we guessed

$$E_{n1} = \int dx |\phi_{n0}(x)|^2 v(x)$$

in position representation.

$$E_n = E_{n0} + \lambda \langle \phi_{n0} | \hat{V} | \phi_{n0} \rangle$$

PT4

If instead we dot with $\langle \phi_m |$ $m \neq n$

$$\langle \phi_m | \hat{H}_0 | \phi_n \rangle + \langle \phi_m | \hat{V} | \phi_n \rangle$$

$$= E_n \langle \phi_m | \phi_n \rangle + E_m \langle \phi_m | \phi_n \rangle$$

Q: What is this?

A: $E_m \langle \phi_m | \phi_n \rangle$

Q: What is this? A: ϕ

$$\langle \phi_m | \phi_n \rangle = \frac{\langle \phi_m | \hat{V} | \phi_n \rangle}{E_n - E_m}$$

Q: What is wrong with this formula?

A: $E_m = E_n$ for $m \neq n$
"Need to discuss"

"degenerate perturbation theory"

$$|\phi_n\rangle = |\phi_n\rangle + \lambda \sum_{m \neq n} \frac{\langle \phi_m | \hat{V} | \phi_n \rangle}{E_n - E_m} |\phi_m\rangle$$

Interesting physics: $|\phi_n\rangle$ is shifted from $|\phi_n\rangle$,

picking up components in direction of $|\phi_m\rangle$

which are larger if $\langle \phi_m | \hat{V} | \phi_n \rangle$ larger, i.e. if

" \hat{V} connects n to m "

What might be less expected is energy denominator.

Almost like "resonance" if state m close to n in energy shift in $|\phi_n\rangle$ is more pronounced,

PT 5

Finish by getting E_{n2}

$$\hat{H}_0 |\phi_{n2}\rangle + \hat{V} |\phi_{n1}\rangle = E_{n0} |\phi_{n2}\rangle + E_{n1} |\phi_{n1}\rangle + E_{n2} |\phi_{n0}\rangle$$

Dot with $\langle \phi_{n0} |$

$$E_{n0} \langle \phi_{n0} | \phi_{n2} \rangle + \langle \phi_{n0} | \hat{V} | \phi_{n1} \rangle$$

cancel

$$= E_{n0} \langle \phi_{n0} | \phi_{n2} \rangle + E_{n1} \langle \phi_{n0} | \phi_{n1} \rangle + E_{n2} \langle \phi_{n0} | \phi_{n0} \rangle$$

zero

1

since

$$|\phi_{n1}\rangle = \sum_{m \neq n} \frac{\langle \phi_{m0} | \hat{V} | \phi_{n0} \rangle}{E_{n0} - E_{m0}} |\phi_{m0}\rangle$$

$$E_{n2} = \langle \phi_{n0} | \hat{V} | \phi_{n1} \rangle$$

$$= \sum_{m \neq n} \frac{|\langle \phi_{n0} | \hat{V} | \phi_{m0} \rangle|^2}{E_{n0} - E_{m0}}$$

PT 6

Now we will do a ton of problems.

Let's start with a very simple matrix problem

$$\hat{H}_0 = A \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} \quad \hat{V} = a \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\phi_{10} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\phi_{20} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$E_{10} = 2A$$

$$E_{20} = 3A$$

Solve exactly $\hat{H} = \hat{H}_0 + \hat{V} = \begin{pmatrix} 2A & a \\ a & 3A \end{pmatrix}$

$$(2A - E)(3A - E) - a^2 = 0$$

$$E^2 - 5AE + 6A^2 - a^2 = 0$$

$$E = \frac{1}{2} \left\{ 5A \pm \sqrt{25A^2 - 4(6A^2 - a^2)} \right\}$$

$$= \frac{1}{2} \left\{ 5A \pm \sqrt{A^2 - 4a^2} \right\} \leftarrow \text{Exact energies}$$

$$(A^2 - 4a^2)^{1/2} = A \left(1 - 4a^2/A^2 \right)^{1/2}$$

$$= A \left(1 - 2a^2/A^2 + \dots \right)$$

PT 7

So exact soln, when expanded, gives

$$E = \frac{1}{2} \left\{ 5A \pm A \mp \frac{2a^2}{A} \right\}$$

get

$$\begin{array}{c} \overbrace{2A} \\ 3A \end{array} \quad \uparrow$$

no first order shift

second order shifts are $\mp \frac{a^2}{A}$.

Check against formalism,

first order shifts $(10)a \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

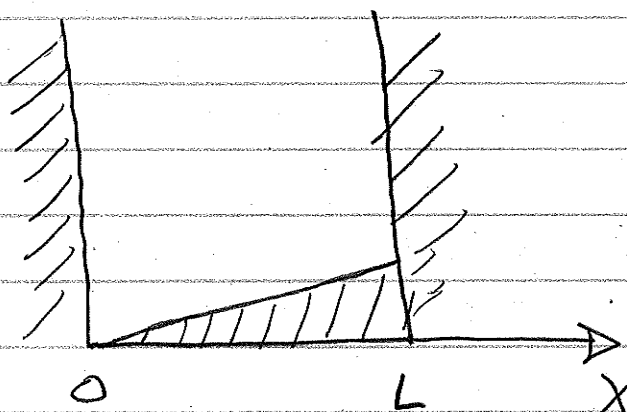
$$= a(10) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \phi \quad \checkmark$$

second order shift $\frac{\left\{ (10)a \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}^2}{2A - 3A} = \frac{-a^2}{A}$

HW: similar problem check eigenvectors

PT8

Less trivial add ϵx to infinite square well



$$\phi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$\langle E_{n1} \rangle = \int_0^L \epsilon x \frac{2}{L} \sin^2 \frac{n\pi x}{L} dx$$

$$= \frac{2\epsilon}{L} \int_0^L x \left(\frac{1}{2} \right) \left(1 - \cos \frac{2n\pi x}{L} \right) dx$$

$$= \frac{2\epsilon}{L} \frac{1}{2} \frac{x^2}{2} \Big|_0^L - \frac{2\epsilon}{L} \frac{1}{2} \int_0^L x \cos \frac{2n\pi x}{L} dx$$

$$= \frac{\epsilon L}{2}$$

$$\frac{L}{2n\pi} x \sin \frac{2n\pi x}{L} \Big|_0^L - \int_0^L \frac{L}{2n\pi} \sin \frac{2n\pi x}{L} dx$$

Q: Interpretation

A: Average position

$$\langle x \rangle = L/2$$

vanishes

also vanishes

so this is whole story!

PT.9

Perturb Quantum oscillator by linear potential.

This calculation / problem illustrates how useful raising + lowering operators are!

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 + \lambda x \right) \psi(x) = E \psi(x)$$

↑

↓

$$\Delta E_{n1} = \langle n | \lambda x | n \rangle$$

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

$$a |n\rangle = \sqrt{n} |n-1\rangle$$

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

$$E_{n1} = 0$$

$$E_{n2} = \sum_{m \neq n} \frac{\langle n | \lambda x | m \rangle \langle m | \lambda x | n \rangle}{E_n - E_m}$$

Q: which m contribute?

↑
"intermediate states"

$$A: m = n+1 \quad \langle n | \lambda x | m \rangle = \lambda \sqrt{n+1} \sqrt{\frac{\hbar}{2m\omega}}$$

$$m = n-1 \quad \langle n | \lambda x | m \rangle = \lambda \sqrt{n} \sqrt{\frac{\hbar}{2m\omega}}$$

PT 10

$$E_{n2} = \lambda^2 \frac{\hbar}{2m\omega} \left[\frac{n+1}{-\hbar\omega} + \frac{n}{\hbar\omega} \right]$$
$$= -\frac{\lambda^2}{2m\omega^2}$$

You may have done this problem a different way in 215A?

$$\frac{1}{2} m\omega^2 x^2 + \lambda x$$
$$= \frac{1}{2} m\omega^2 \left(x + \frac{\lambda}{m\omega^2} \right)^2 - \frac{1}{2} m\omega^2 \frac{\lambda^2}{(m\omega^2)^2}$$

↗
shifted oscillator
equilibrium
position

$-\frac{\lambda^2}{2m\omega^2}$
↖
our 2nd order
answer.

Imagine trying to do these with Hermite polynomials

$$\Delta E_{n1} = \int \psi_{n0}(x) \Delta X \psi_{n0}(x) dx$$

$$\psi_{n0}(x) = A_n H_n(\xi) e^{-\xi^2/2} \quad \xi \equiv \sqrt{\frac{m\omega}{\hbar}} x$$

$(2^n n! \sqrt{\pi})^{-1/2}$ ↗

$n=5 \quad H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi$

PT 11

Coming up: Very imp case of Hydrogen atom
in electric field ("Stark effect"), magnetic field, etc

Also: How about Heisenberg model problems
perturbatively

eg
$$\hat{H} = +J (S_1 \cdot S_2 + S_2 \cdot S_3 + S_3 \cdot S_4 + S_4 \cdot S_1)$$
$$+ J' (S_1 \cdot S_3 + S_2 \cdot S_4)$$

treat as \hat{V} .

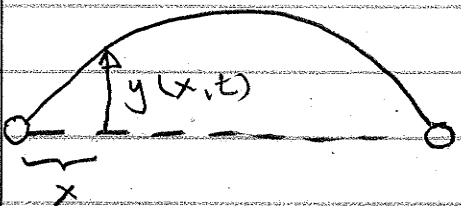
This one might be hard since need
actual wave functions of \hat{H}_0

But how about
$$\hat{H} = J S_1 \cdot S_2 - B(S_{1z} + S_{2z})$$

where we do know wave functions?

Actually, perturbation theory has other classical mechanics applications besides the scattering problem we began with

Consider an oscillating string. How does its frequency change if you place a small bead on it.



Wave eqn $\frac{d^2 y}{dx^2} = \frac{1}{v^2} \frac{d^2 y}{dt^2}$ $v^2 = T/\mu$

Separation of variables (just like time dep sch Eqn

\rightarrow time indep sch Eqn!) $y(x,t) = f(x)g(t)$

$$\frac{d^2 f}{dx^2} g = \frac{1}{v^2} \frac{d^2 g}{dt^2} f$$

$$\frac{1}{f} \frac{d^2 f}{dx^2} = \frac{1}{v^2} \frac{d^2 g}{dt^2} = -k^2$$

$$\frac{d^2 f}{dx^2} = -k^2 f \quad \frac{d^2 g}{dt^2} = -k^2 v^2 g$$

$$f = e^{\pm ikx}$$

$$g = e^{\pm i\omega t} \quad \omega \equiv kv$$

All together linear combination of solis

$$\int dk \left[a(k) e^{ik(x-vt)} + b(k) e^{ik(x+vt)} \right]$$

For fixed end point string k becomes discrete

$$y(x,t) = \sum_n \sin \frac{n\pi x}{L} \left(a_n \sin \frac{n\pi \omega t}{L} + b_n \cos \frac{n\pi \omega t}{L} \right)$$

Q: How do you determine a_n, b_n ?

A: Initial conditions $y(x,0)$ and $\frac{dy}{dt}(x,0)$.

and Fourier series.

After that review, perturbation theory

$$\frac{T}{\mu} \frac{d^2}{dx^2} f = -\omega^2 f$$

\uparrow

$$\rightarrow \frac{T}{\mu + \Delta\mu} \approx \frac{T}{\mu} - \frac{T\Delta\mu}{\mu^2}$$

"Perturbation" = $\frac{T\Delta\mu}{\mu^2}$

fundamental

"wave function"

$n=1$

$$y_1(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$$

PT-14

According to first order perturbation theory

change in eigenvalue is

$$E_1 = \Delta(-\omega^2) = \int_0^L \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \left(-\frac{T}{\mu^2} \Delta \mu \right) \frac{dL}{dx} \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} dx$$

suppose $\Delta \mu = m_0 \delta(x - L/2)$

$$-\sqrt{\frac{2}{L}} \frac{\pi^2}{L^2} \sin \frac{\pi x}{L}$$

↑
bead at string center

Q: Does this have right units $[\mu] = M/L$?!

A: Yes!

Q: Before doing algebra, do you expect ω to increase or decrease?

A: Decrease (move mass.)

$$\Delta(-\omega^2) = \frac{2}{L} \frac{T}{\mu^2} m_0 \frac{\pi^2}{L^2} \int_0^L \delta(x - L/2) \sin^2 \frac{\pi x}{L} dx$$

+ 1

$$\omega_0^2 = \frac{T}{\mu} \frac{\pi^2}{L^2}$$

$$\omega^2 \approx \omega_0^2 \left[1 - \frac{2m_0}{\mu L} \right]$$

↑
 $M = \mu L =$ total mass of string



Q: What is $\Delta \omega^2$ of first harmonic?

We have done a few examples.

Let's turn back to theory for a moment and

see how to deal with degeneracy:

$$E_{n2} = \sum_{m \neq n} \frac{|\langle \phi_{n0} | \hat{V} | \phi_{m0} \rangle|^2}{E_{n0} - E_{m0}}$$

↑
trouble!

But even $E_{n1} = \langle \phi_{n0} | \hat{V} | \phi_{n0} \rangle$

is problematic because ϕ_{n0} is not well defined,

can be linear combination of degenerate states.

$$\hat{H}_0 \phi_{a0} = E_{a0} \phi_{a0} \quad \begin{array}{l} \text{assume} \\ \text{equal! call it } E_0 \end{array}$$

$$\hat{H}_0 \phi_{b0} = E_{b0} \phi_{b0}$$

$$\text{NB: } \langle \phi_{a0} | \phi_{b0} \rangle = 0$$

$$\phi_0 = \alpha \phi_{a0} + \beta \phi_{b0}$$

even though
degenerate!

obviously $\hat{H}_0 \phi_0 = E_0 \phi_0$

As before $\hat{H} = \hat{H}_0 + \lambda \hat{V}$

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \dots$$

$$\phi = \phi_0 + \lambda \phi_1 + \lambda^2 \phi_2 + \dots$$

(will suppress subscript "n")

Much of calculation is same as before

$$\hat{H} \phi = E \phi$$

$$\lambda^0 \quad \hat{H}_0 \phi_0 = E_0 \phi_0 \quad \checkmark$$

$$\lambda^1 \quad \hat{H}_0 \phi_1 + \hat{V} \phi_0 = E_0 \phi_1 + E_1 \phi_0$$

Take inner product with $\langle \phi_{a0} |$ $\alpha |\phi_{a0}\rangle + \beta |\phi_{b0}\rangle$

$$\begin{aligned} & \langle \phi_{a0} | \hat{H}_0 \phi_1 \rangle + \langle \phi_{a0} | \hat{V} \phi_0 \rangle \\ & = E_0 \langle \phi_{a0} | \phi_1 \rangle + E_1 \langle \phi_{a0} | \phi_0 \rangle \end{aligned}$$

First terms on lhs + rhs cancel

$$\alpha \langle \phi_{a0} | \hat{V} | \phi_{a0} \rangle + \beta \langle \phi_{a0} | \hat{V} | \phi_{b0} \rangle = \alpha E_1$$

obviously we also have (inner product with $\langle \phi_{b0} |$):

$$\alpha \langle \phi_{b0} | \hat{V} | \phi_{a0} \rangle + \beta \langle \phi_{b0} | \hat{V} | \phi_{b0} \rangle = \beta E_1$$

PT-17

In Matrix form:

$$\begin{bmatrix} \langle \phi_{a0} | \hat{V} | \phi_{a0} \rangle & \langle \phi_{a0} | \hat{V} | \phi_{b0} \rangle \\ \langle \phi_{b0} | \hat{V} | \phi_{a0} \rangle & \langle \phi_{b0} | \hat{V} | \phi_{b0} \rangle \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E_1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Q: what are first order shifts then

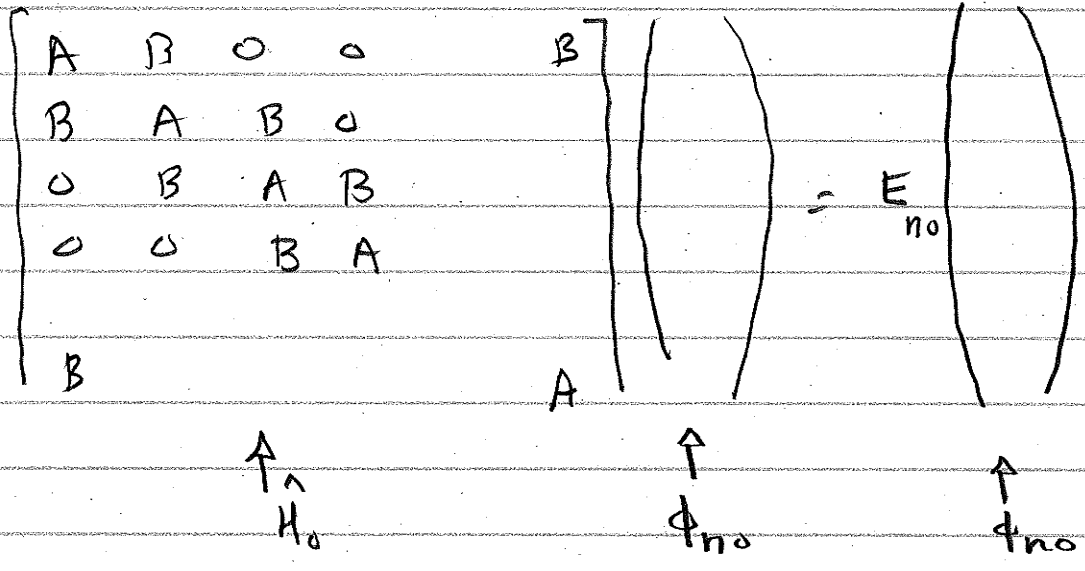
Conclusion: To get first order shifts E_1 youneed to diagonalize the matrix \hat{V} in the degenerate

subspace. Explicitly:

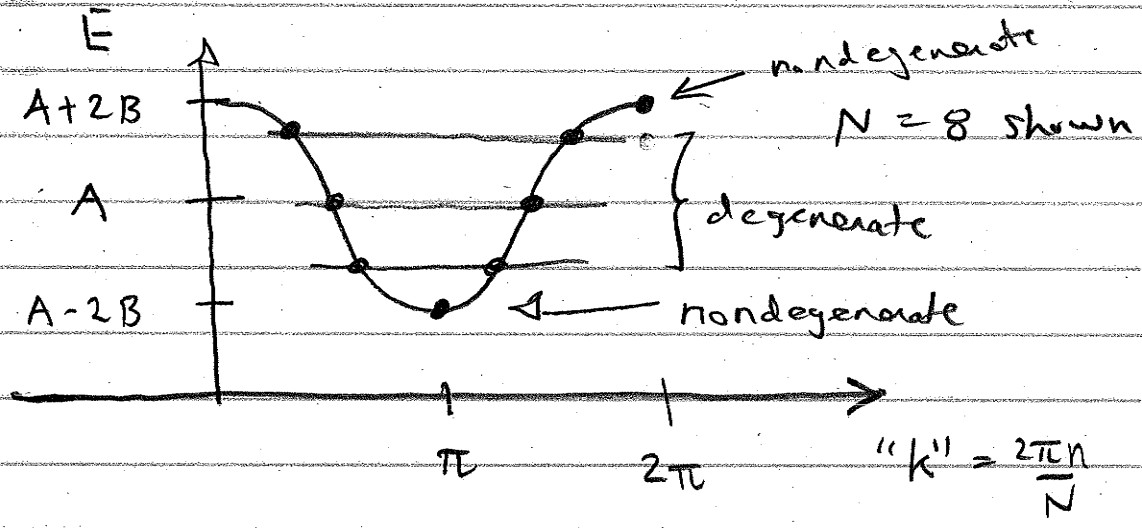
$$E_1^{\pm} = \frac{1}{2} \left[V_{aa} + V_{bb} \pm \sqrt{(V_{aa} - V_{bb})^2 + 4|V_{ab}|^2} \right]$$

denoting $V_{aa} = \langle \phi_{a0} | \hat{V} | \phi_{a0} \rangle$ etc.

An example from our tridiagonal matrix problem



$$E_{n_0} = A + 2B \cos \frac{2\pi n}{N} \quad n = 1, 2, \dots, N$$



Recall $k = 2\pi$ $\phi_{N_0} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \frac{1}{\sqrt{N}}$

$k = \pi$ $\phi_{\frac{N}{2}0} = \begin{pmatrix} 1 \\ -1 \\ \vdots \\ -1 \end{pmatrix} \frac{1}{\sqrt{N}}$

PT-19

Problem:

$$\hat{V} = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ 0 & & & & \\ \vdots & & a & & \\ \vdots & & & & \end{pmatrix} \quad \begin{array}{l} \text{very} \\ \text{Sparse!} \\ \text{Just one nonzero} \\ \text{entry} \end{array}$$

Make a small change to $A \rightarrow A' = A + a$

row/column $N/2$. How are eigenvalues shifted?

First, the nondegenerate ones

$$E_{N1} = \langle \phi_{N0} | \hat{V} | \phi_{N0} \rangle = \frac{1}{N} a$$

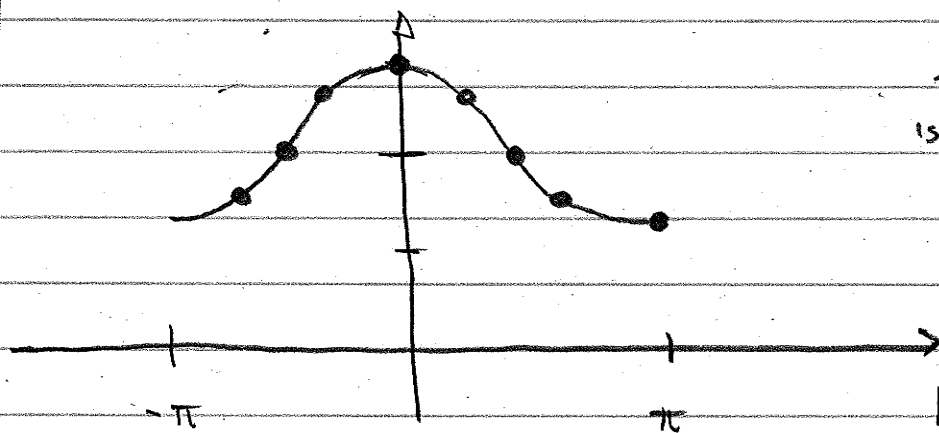
Q: say in words why $1/N$ is there

A: particle spends only $1/N$ of its time there.

$$E_{\frac{N}{2}1} = \langle \phi_{\frac{N}{2}0} | \hat{V} | \phi_{\frac{N}{2}0} \rangle = +\frac{1}{N} a \quad \text{also}$$

The degenerate ones?

It is more simple to consider equivalent labeling



equivalence
is just fact that
 λ, ϕ_n involve
 \sin, \cos (or $e^{\pm i}$)
which are invariant
under translation
by 2π .

Simpler because $\pm k$ are the degenerate levels

(Rather than symmetric around π) $\left. \begin{array}{l} a = n \\ b = -n \end{array} \right\}$ Notation.

$$V_{nn} = \langle \phi_{no} | \hat{V} | \phi_{no} \rangle = a/N$$

Hermitian conjugate

components $\frac{1}{\sqrt{N}} e^{i \frac{n2\pi}{N} l}$

$l = \frac{N}{2}$ component
is relevant one

$$V_{-n,n} = a/N$$

similarly

$$e^{i n \pi}$$

Q:

$$V_{-n,n} = ?$$

$$A: V_{-n,n} = \frac{a}{N} e^{i n \pi} = \frac{a}{N} e_{\perp}!$$

So must get eigenvalues of 2×2

$$\frac{a}{N} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \Rightarrow 0, 2 \left(\frac{a}{N} \right)$$

PT-21

Think more about this

One linear combination is unshifted

$$\frac{1}{\sqrt{N}} e^{i \frac{2\pi n l}{N}} \quad \leftarrow \text{components } \pm n \text{ degenerate}$$

↙

$$\frac{1}{\sqrt{N}} \sin \frac{2\pi n l}{N} \quad \text{can also be used}$$

↘

$$\frac{1}{\sqrt{N}} \cos \frac{2\pi n l}{N}$$

but for $\sin \frac{2\pi n l}{N}$ the wave function vanishes at $l = \frac{N}{2}$
and hence perturbation does not affect it. (like our vibrating string with bead at center and first harmonic)

Q: What about the other, non zero, shift and the factor of 2?

A: I suspect (you check!) it is normalization

probably $\sqrt{\frac{2}{N}}$ out front of $\cos \frac{2\pi n l}{N}$.