4. Perturbation theory

Previously discussed various approaches to solving eigenvalue problems:

- Exact solution (∞-dim: diff. eq's, operator methods; finite dim: explicit diagonalization)
- Shooting method (1D)
- Variational method (need good trial wf's in large D)
- Finite difference methods (small D)
- WKB
- Q. Monte Carlo

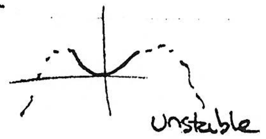
If H close to H_0 where answer known: use perturbation theory

Idea: write $H = H_0 + \lambda V$

solve $H|\psi\rangle = E|\psi\rangle$ as power series in λ.

Method often gives good approx — but must be careful, particularly when small pert $\rightarrow$ qualitative change

(e.g. $H_0 = \frac{p^2}{2m} + \frac{1}{2}x^2$, $V = -\lambda x^4$



)

This semester: time-independent pert. theory
Next semester: time-dependent " "

Nondegenerate time-independent pert. theory (Rayleigh - Schrödinger)

$H = H_0 + \lambda V$

unperturbed

$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$

$\langle n^{(0)} | m^{(0)}\rangle = \delta_{nm}$

exact

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

choose $\langle n^{(0)} | n\rangle = 1$ (convenient)

Assume $E_n^{(0)}$ are nondegenerate ($E_n^{(0)} \neq E_m^{(0)}$, $n \neq m$)

Expand

$$|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \ldots$$
$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots$$

Normalization: $\langle n^{(0)} | n\rangle = 1$ for all λ

$\Rightarrow \langle n^{(0)} | n^{(k)}\rangle = 0 \quad \forall \; k \neq 0.$

– all corrections orthogonal to $|n^{(0)}\rangle$

Convenient, but $\langle n | n\rangle \neq 1$

so must normalize again @ end.

Setup: expand $H|n\rangle = E_n |n\rangle$, collect terms @ each order in λ

$$(H_0 + \lambda V)[|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \ldots]$$
$$= [E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots][|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \ldots]$$

λ^0: $H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$ ✓

λ^1: $H_0 |n^{(1)}\rangle + V|n^{(0)}\rangle = E_n^{(1)} |n^{(0)}\rangle + E_n^{(0)} |n^{(1)}\rangle$

λ^k: $H_0 |n^{(k)}\rangle + V |n^{(k-1)}\rangle$

$$= E_n^{(0)} |n^{(k)}\rangle + E_n^{(1)} |n^{(k-1)}\rangle + \ldots + E_n^{(k)} |n^{(0)}\rangle$$

Take inner product with $\langle n^{(0)}|$ @ each order

$$\langle n^{(0)}|H_0|n^{(k)}\rangle + \langle n^{(0)}|V|n^{(k-1)}\rangle = E_n^{(k)}$$

$$\Rightarrow \quad \boxed{E_n^{(k)} = \langle n^{(0)}|V|n^{(k-1)}\rangle}$$

Take inner product with $\langle m^{(0)}|$, $m\neq n$ @ each order

$$\langle m^{(0)}|E_n^{(0)} - H_0|n^{(k)}\rangle = \langle m^{(0)}|\left[(V-E_n^{(1)})|n^{(k-1)}\rangle - E_n^{(2)}|n^{(k-2)}\rangle \cdots - E_n^{(k-1)}|n^{(1)}\rangle\right]$$

Define $\quad Q_n = 1 - |n^{(0)}\rangle\langle n^{(0)}| = \sum_{m\neq n} |m^{(0)}\rangle\langle m^{(0)}|$

(projects onto space orthog. to $|n^{(0)}\rangle$)

$\sum |m^{(0)}\rangle \cdot$ above, define $\frac{Q_n}{E_n^{(0)}-H_0} = \sum_{m\neq n} \frac{|m^{(0)}\rangle\langle m^{(0)}|}{E_n^{(0)} - E_m^{(0)}}$

$\Downarrow$

$$\boxed{|n^{(k)}\rangle = \frac{Q_n}{E_n^{(0)}-H_0}\left[(V-E_n^{(1)})|n^{(k-1)}\rangle - E_n^{(2)}|n^{(k-2)}\rangle \cdots - E_n^{(k-1)}|n^{(1)}\rangle\right]}$$

Low-order calculations:

E^1) $\quad E_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$

so $\quad E_n = E_n^{(0)} + \lambda\langle n^{(0)}|V|n^{(0)}\rangle + \mathcal{O}(\lambda^2)$

Note: consistent with Feynman-Hellman

$$\frac{\partial E}{\partial \lambda} = \langle \psi|\frac{\partial H}{\partial \lambda}|\psi\rangle.$$

$|1\rangle$) $$|n^{(1)}\rangle = \sum_{m\neq n} \frac{|m^{(0)}\rangle\langle m^{(0)}|}{E_n^{(0)} - E_m^{(0)}} \left(V - E_n^{(1)}\right) |n^{(0)}\rangle$$

$$= \sum_{m\neq n} |m^{(0)}\rangle \frac{\langle m^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} = \sum_{m\neq n} |m^{(0)}\rangle \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}}$$

(writing $V_{mn} = \langle m^{(0)}|V|n^{(0)}\rangle$).

So

$$|n\rangle = |n^{(0)}\rangle + \lambda \sum_{m\neq n} |m^{(0)}\rangle \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} + \mathcal{O}(\lambda^2)$$

E^2) $$E_n^{(2)} = \sum_{m\neq n} \frac{V_{nm}V_{mn}}{E_n^{(0)} - E_m^{(0)}}$$ etc...

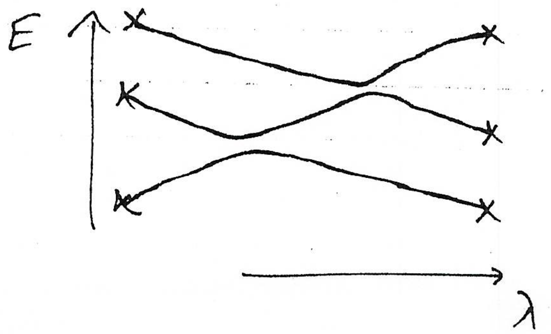
Notes: * 2nd order correction to ground state energy $E_0^{(2)}$ always negative (since $E_0^{(0)} < E_m^{(0)}$)

* More generally - levels repel if coupled.

If E_n, E_m are close, $E_n < E_m$ $(E_m - E_n \sim \varepsilon)$

$$E_n^{(2)} = -\frac{|V_{nm}|^2}{\varepsilon} \qquad E_m^{(2)} = \frac{|V_{nm}|^2}{\varepsilon}$$

General phenomenon: no level-crossing when states coupled



General structure of equations:

Abbreviate
$$E^k = \langle 0 | V | k-1 \rangle$$
$$|k\rangle = \frac{Q}{\Delta}\left[(V-E^1)|k-1\rangle - E^2|k-2\rangle \cdots - E^{k-1}|1\rangle\right]$$

$$E^1 = \langle 0|V|0\rangle = \langle V \rangle$$

$$|1\rangle = \frac{Q}{\Delta} V |0\rangle$$

$$E^2 = \langle 0|V|1\rangle = \langle V \frac{Q}{\Delta} V \rangle$$

$$|2\rangle = \frac{Q}{\Delta}(V-E^1)|1\rangle = \frac{Q}{\Delta}(V-\langle V\rangle)\frac{Q}{\Delta} V|0\rangle$$

$$E^3 = \langle 0|V|2\rangle = \langle V \frac{Q}{\Delta}(V-\langle V\rangle)\frac{Q}{\Delta} V |0\rangle$$

$$|3\rangle = \frac{Q}{\Delta}(V-E^1)|2\rangle - E^2|1\rangle$$
$$= \frac{Q}{\Delta}\left[(V-\langle V\rangle)\frac{Q}{\Delta}(V-\langle V\rangle) - \langle V\frac{Q}{\Delta}V\rangle\right]\frac{Q}{\Delta}V|0\rangle$$

$$E^4 = \langle V \frac{Q}{\Delta}\left[(V-\langle V\rangle)\frac{Q}{\Delta}(V-\langle V\rangle) - \langle V\frac{Q}{\Delta}V\rangle\right]\frac{Q}{\Delta} V|0\rangle$$

$$\vdots$$

systematic expansion, but complicated structure.

- recursion easy to implement, though.

Alternative approach: Brillouin – Wigner
→ simpler structure but nonlinear eqn for E_n.

Wavefunction renormalization

define $|n\rangle_N = Z_n^{1/2} |n\rangle$, $\quad Z_n = \frac{1}{\langle n|n\rangle}$

so $\;{}_N\langle n|n\rangle_N = 1$

$$Z_n^{-1} = \langle n|n\rangle = 1 + \lambda^2 \langle n^{(1)}|n^{(1)}\rangle + \dots$$

$$= 1 + \lambda^2 \sum_{m\neq n} \frac{V_{nm}V_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)^2} + \dots$$

Note: $Z_n = |\langle n^{(0)}|n\rangle_N|^2$ is prob. of finding perturbed state in original eigenstate

$$Z_n \sim 1 - \underbrace{\lambda^2 \sum_{m\neq n} \frac{V_{nm}V_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)^2}}_{\text{prob. for "leakage" into other states, to order } \mathcal{O}(\lambda^2).} + \dots$$

Example:

$$H = \frac{p^2}{2} + \frac{1}{2}x^2 + \lambda x. \qquad (m = \hbar = \omega = 1)$$

Exact solution:

$$H = \frac{1}{2}p^2 + \frac{1}{2}(x+\lambda)^2 - \frac{\lambda^2}{2}$$

so all energies shift by $-\lambda^2/2$

Perturbation calculation

$$E_n^{(1)} = \langle n^{(0)} | x | n^{(0)} \rangle = 0 \quad \checkmark$$

$$\left\{ \langle n' | x | n \rangle = \frac{1}{\sqrt{2}} \left[\delta_{n,n'+1} \sqrt{n} + \delta_{n+1,n'} \sqrt{n'} \right] \right\}$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{\langle n^{(0)} | x | m^{(0)} \rangle \langle m^{(0)} | x | n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}}$$

since $E_n^{(0)} = n + 1/2$,

$$E_n^{(2)} = -\frac{n+1}{2} + \frac{n}{2} = -\frac{1}{2} \quad \checkmark$$

Convergence of perturbation series:

In general, perturbation series do not converge for most useful problems — anharmonic oscillator, QED, etc.

BUT — for small perts, series usually converges near correct answer to some order, then diverges.

Example: anharmonic oscillator.

Real example of QM in HW.
Here: consider pert. expansion of integral

$$Z(\lambda) = \int_{-\infty}^{\infty} dx \, e^{-\frac{1}{2}x^2 - \frac{\lambda}{4}x^4}$$

Can do perturbative expansion of $Z(\lambda)$

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$$Z(\lambda) = \sum_k \int_{-\infty}^{\infty} dx \, e^{-\frac{1}{2}x^2} \left[(-1)^k \frac{\lambda^k x^{4k}}{4^k k!} \right]$$

$$= \sum_k \lambda^k Z_k .$$

$$Z_k = \sqrt{2\pi} \, \frac{(-1)^k (4k-1)!!}{4^k \, k!} = \sqrt{2\pi} \, \frac{(-1)^k \, (4k)!}{k! \, 16^k \, (2k)!}$$

$$Z(\lambda) = \sqrt{2\pi} \left[1 - \frac{3}{4}\lambda + \frac{105}{32}\lambda^2 - \frac{3465}{128}\lambda^3 + \frac{675675}{2048}\lambda^4 - \dots \right]$$

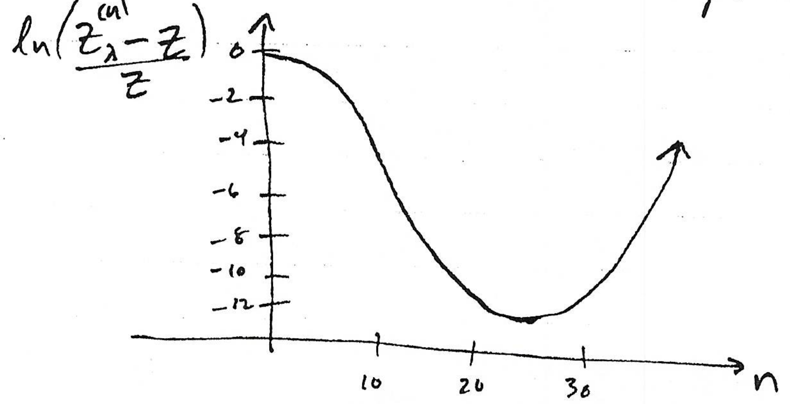
note: power series non-analytic @ 0, since problematic for $\lambda < 0$

Stirling: $n! \sim \sqrt{2\pi} \, n^{n+1/2} e^{-n}$

$$Z_k \sim \sqrt{2} \left(-\frac{4\lambda k}{e} \right)^k$$ diverges badly.

but convergent for small $k \ll \frac{e}{4\lambda}$.

For example, @ $\lambda = 0.01$,
12 terms gives $\sim 10^{-10}$ accuracy.
25 terms " $\sim 10^{-12}$ " (best approx)
then blow up.



$\sum \lambda^k Z_k$ poorly behaved for large λ.

$Z(1) \cong 1.93525$

Successive approx's give

$\sqrt{2\pi}\,(1) \cong 2.5$
$\sqrt{2\pi}\,(1/4) \cong 0.627$
$\sqrt{2\pi}\,(113/32) \cong 8.851$
$\sqrt{2\pi}\,(-3013/64) \cong -59.004$
$\vdots$

worse & worse.

Can we use Z_k's to get an accurate estimate of $Z(\lambda)$ for large λ?

Yes: Padé approximants

$$P^n_n = \frac{a_0 + a_1\lambda + \dots + a_n\lambda^n}{b_0 + b_1\lambda + \dots + b_n\lambda^n}$$

defined uniquely by cond $= Z_0 + \lambda Z_1 + \dots + \lambda^{2n} Z_{2n} + O(\lambda^{2n+1})$

$$P^1_1(\lambda) = \frac{1 + \frac{29}{8}\lambda}{1 + \frac{35}{8}\lambda} = 1 - \frac{3}{4}\lambda + \frac{105}{32}\lambda^2 + \dots$$

$$P^1_1(1) = 2.1569$$

$$P^2_2(\lambda) = \frac{1 + \frac{3939}{248} z + \frac{54525}{1984} z^2}{1 + \frac{4125}{248} z + \frac{72765}{1984} z^2} \Rightarrow P^2_2(1) = 2.04768$$

... gives systematic approx scheme for any λ

Padé's may not always work, but often very effective.