Lecture 3 – Time-Independent Perturbation Theory

02/04/16

Wrapping up Time-Reversal

example: Non-invariant $\mathcal{H}$ under time-reversal

– charged particle in a magnetic field

$\vec{p}$ changes sign under time-reversal

$$\mathcal{H} = \frac{(\vec{p} - e\vec{A})}{2m}$$

the potential $\vec{A}$ is invariant under time-reversal

If we were to also change $\vec{B} = \vec{\nabla} \times \vec{A}$, it would be invariant.

Time-Independent Perturbation Theory

For a Hamiltonian (not solvable)

$$\mathcal{H} = H_0 + V$$

there is a family of Hamiltonians

real parameter

$$\mathcal{H}(\lambda) = H_0 + \lambda V$$

Hermitian operator

solvable Hamiltonian

→ Taylor expanding about λ to solve $\mathcal{H}$

e.g. $\mathcal{H}(1) = H_0 + V$

gives a good approximation of the eigenvalues & eigenstates of $\mathcal{H}$

examples:

① H_0 = simple harmonic oscillator

$\lambda V = \underbrace{\lambda x^4}_{\text{creates the anharmonic oscillator}}$

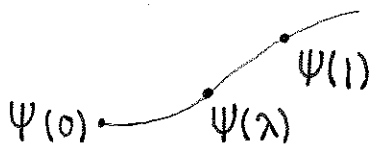
② $H_0 = \frac{p^2}{2m} - \frac{e^2}{r}$ the Coulomb potential

$\lambda V = f(r)\vec{L}\cdot\vec{S},\ p^4,\ \delta^3(\vec{r})$ valid perturbations, all

Constraints on the approximation:

$$\underbrace{\mathcal{H}(\lambda)}_{H_0 + \lambda V}|\Psi(\lambda)\rangle = E(\lambda)|\Psi(\lambda)\rangle$$

→ require that when λV "turns on" ($\lambda \geq 1$), the wavefunction Ψ does not become discontinuous



– a continuous function, even when the perturbation is "on"

$(\mathcal{H}-E)|\Psi\rangle = 0$

└ λ suppressed for ease

Take the derivative with respect to λ (want to expand about $\lambda=0$, that is, the $\mathcal{H}=H_0$ case)

let $\bullet \equiv \frac{d}{d\lambda}$

$(\dot{\mathcal{H}}-\dot{E})|\Psi\rangle + (\mathcal{H}-E)|\dot{\Psi}\rangle = 0$

$-\ddot{E}|\Psi\rangle + 2(\dot{\mathcal{H}}-\dot{E})|\dot{\Psi}\rangle + (\mathcal{H}-E)|\ddot{\Psi}\rangle = 0$

⋮ etc.

$\dot{\mathcal{H}} = V$, $\mathcal{H}(0) = H_0$

$$E(\lambda) = \overbrace{E(0)}^{\varepsilon \text{ – an eigenvalue of } H_0} + \underbrace{\dot{E}(0)\lambda}_{E^{(1)}} + \underbrace{\tfrac{1}{2}\ddot{E}(0)\lambda^2}_{E^{(2)}} + \ldots$$

└ higher order terms for approximation

$|\dot{\Psi}\rangle \equiv |\dot{\Psi}(0)\rangle$

now, plug in proper order terms ⤵

$\underbrace{(H_0-\varepsilon)}_{=0}|\Psi\rangle = 0$

$(V-E^{(1)})|\Psi\rangle + \underbrace{\cancel{(H_0-\varepsilon)|\dot{\Psi}\rangle}}_{\to 0} = 0$

$-E^{(2)}|\Psi\rangle + (V-E^{(1)})|\dot{\Psi}\rangle + (H_0-\varepsilon)|\ddot{\Psi}\rangle = 0$

→ $\langle\Psi|(V-E^{(1)})|\Psi\rangle = 0$

└ an expression for the first-order correction on the energy

$\Rightarrow E^{(1)} = \langle\Psi|V|\Psi\rangle$

*only correct when ε is <u>non-degenerate</u>

ex: **Harmonic oscillator**

$(\hbar = m = \omega = 1)$

$\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}x^2$

*to restore units, $x_0 = \sqrt{\hbar/m\omega}$:
dimensions of length; the spread of the ground state wavefunction
→ the Hamiltonian can be rewritten using the raising and lowering operators, $\hat{a}^\dagger$ and $\hat{a}$

$$\hat{a} = \frac{(\hat{x}+i\hat{p})}{\sqrt{2}} \equiv \frac{(x/x_0) + (ix_0 p/\hbar)}{\sqrt{2}}, \quad \hat{a}^\dagger = \frac{(\hat{x}-i\hat{p})}{\sqrt{2}}$$

$[x, p] = i$, $[a, a^\dagger] = 1$

$$\mathcal{H} = \underbrace{aa^\dagger}_{} + \tfrac{1}{2} = H_0$$

number operator; eigenvalues $N = 0, 1, 2, 3, \ldots$
so the spectrum of this Hamiltonian can be seen to be equally-spaced levels starting at 1/2 (fixed spacing for all n)

New $\mathcal{H}$:

$$\mathcal{H} = H_0 + \underbrace{\beta x^4}_{V}$$

$E^{(1)} = \langle\psi|\beta x^4|\psi\rangle$ to be a good approximation, the next-order correction term should be smaller than this

first-order eigenvalue corrections:

$$E_n^{(1)} = \beta\langle n|x^4|n\rangle$$

→ expand in terms of a & $a^\dagger$

$$= (\beta/4)\langle n|(a+a^\dagger)(a+a^\dagger)(a+a^\dagger)(a+a^\dagger)|n\rangle$$

since $x = 1/\sqrt{2}\,(a+a^\dagger)$
where $a|n\rangle = \sqrt{n}\,|n-1\rangle$; $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$

$$= (3\beta/4)(\underline{2n^2} + 2n + 1)$$

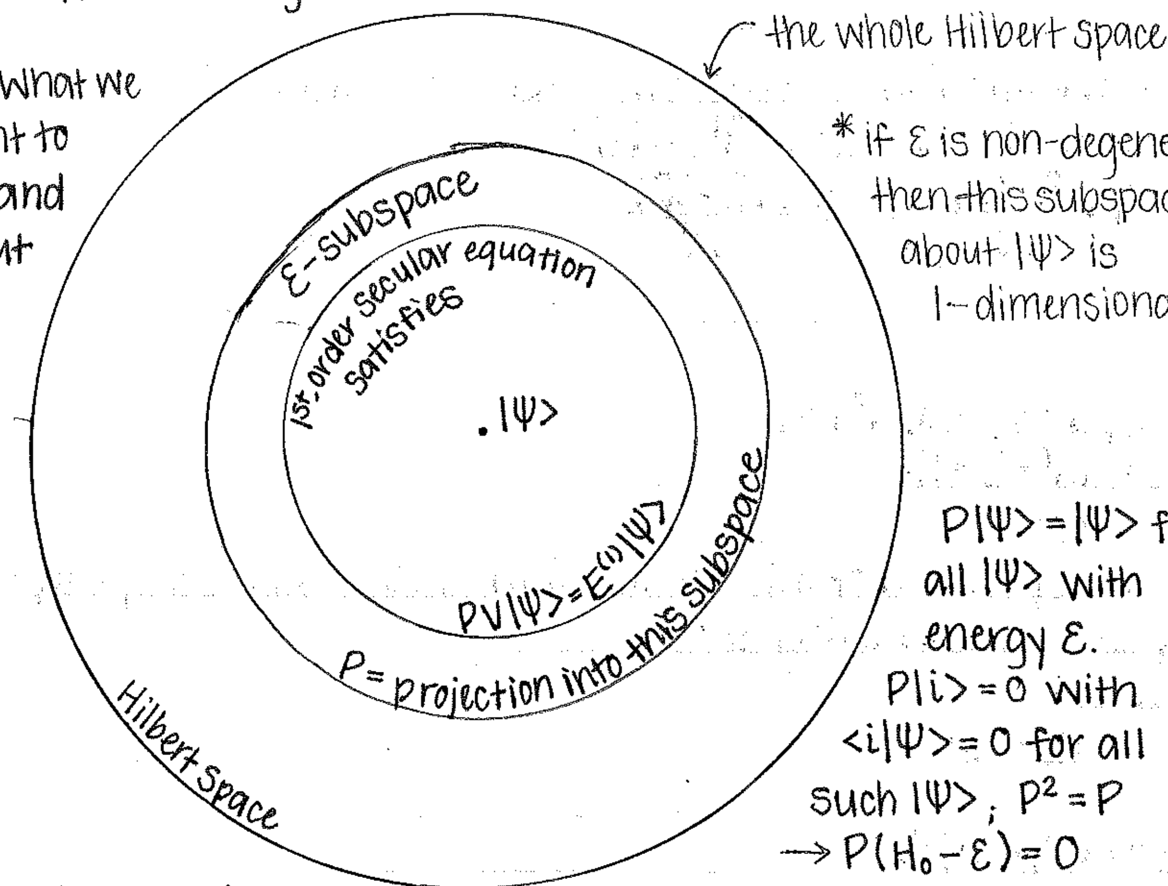
as n grows, our correction term grows like n^2, thus at higher-lying states, this is not as good of an approximation since the original spacing is fixed for n.

$E^{(1)}$ grows as n^2, which is small compared to V which grows as x^4, so this is a good approximation for low n-values.

→

What happens for degenerate values of $\mathcal{E}$?

$|\psi\rangle$ - what we want to expand about



* if $\mathcal{E}$ is non-degenerate, then this subspace about $|\psi\rangle$ is 1-dimensional

$P|\psi\rangle = |\psi\rangle$ for all $|\psi\rangle$ with energy $\mathcal{E}$.
$P|i\rangle = 0$ with $\langle i|\psi\rangle = 0$ for all such $|\psi\rangle$; $P^2 = P$
$\rightarrow P(H_0 - \mathcal{E}) = 0$

Let $|m\rangle$ label the basis of states with energy $\mathcal{E}$; let $|i\rangle$ label an orthonormal basis.

$$\mathbb{1} = \underbrace{\sum_m |m\rangle\langle m|}_{P} + \underbrace{\sum_i |i\rangle\langle i|}_{\mathbb{1}-P}$$

$\mathbb{1}-P$ - projects into the orthogonal subspace

$$P(H_0 - \mathcal{E}) = \sum_m |m\rangle\langle m|(H_0 - \mathcal{E}) = 0$$

So for the first-order correction...

$$P(V - E^{(1)})|\psi\rangle = 0$$

first-order secular equation

$$\underbrace{PV|\psi\rangle}_{} = E^{(1)}|\psi\rangle$$ where $|\psi\rangle$ is an eigenstate of H_0

P is an operator that sends a degenerate subspace back into itself

ex. $H_0 = \mathcal{E}\mathbb{1}$, $V = \lambda\sigma_x$

($\mathcal{H} = \mathbb{C}^2$; Hilbert space is real space)

$$\mathcal{H} = H_0 + V$$
$$= \mathcal{E}\mathbb{1} + \lambda\sigma_x$$

exact solution:

eigenvalues $\varepsilon \pm \lambda$

eigenstates $\underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}}_{\sigma_x}$

let $|\psi\rangle = \begin{pmatrix}1\\0\end{pmatrix}$

then $\langle\psi|V|\psi\rangle = (1,0)\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0$ — this shows the first-order correction is 0, which we know is not true!

This form fails here because ε is degenerate → the Hamiltonian is discontinuous when λ is "turned on"

for degenerate ε values, you must use the 1st order secular equation to send the degenerate subspace back into itself

→ The 1st Order secular equation tells us which states to start with at zero^n order perturbation

the collection of states/ preferred basis

$PV|\psi\rangle = E^{(1)}|\psi\rangle$

→ go to m eigenbasis

insert identity

$\langle m|PV|\psi\rangle = E^{(1)}\langle m|\psi\rangle$

$\sum_{m'}|m'\rangle\langle m'| + \underbrace{\sum_i |i\rangle\langle i|}$

P on $|m\rangle$ does nothing because it is already in the degenerate subspace

but this can be left out because $\langle i|\psi\rangle = 0$

$\sum_{m'}\langle m|V|m'\rangle\langle m'|\psi\rangle = E^{(1)}\langle m|\psi\rangle$

↑ matrix form of 1st order secular equation

(projects into $|m\rangle$ such that $E^{(1)}$ will not be 0)

To get the 2nd order correction for the energy, we will first need to determine the first order correction to the state, $|\dot{\psi}\rangle$.

2nd Order Energy Perturbation:

$-E^{(2)}|\psi\rangle + (V - E^{(1)})|\dot{\psi}\rangle + (H_0 - \varepsilon)|\ddot{\psi}\rangle = 0$

$$\langle\psi|\left(-E^{(2)}|\psi\rangle + (V-E^{(1)})|\dot\psi\rangle + \overbrace{(H_0-\varepsilon)}^{\to 0}|\ddot\psi\rangle\right) = 0$$

$$\Rightarrow E^{(2)} = \langle\psi|(V-E^{(1)})|\dot\psi\rangle$$

Instead of following this path, let's project into the orthogonal subspace before we take the inverse.

$$(\mathbb{1}-P)\left((V-E^{(1)})|\psi\rangle + (H_0-\varepsilon)|\dot\psi\rangle\right)$$
$$= (\mathbb{1}-P)(V-E^{(1)})|\psi\rangle + (\mathbb{1}-P)\underbrace{(H_0-\varepsilon)}|\dot\psi\rangle = 0$$

in this subspace, $(H_0-\varepsilon)$ is NOT 0

$$\Rightarrow (\mathbb{1}-P)|\dot\psi\rangle = -(H_0-\varepsilon)^{-1}(\mathbb{1}-P)(V-E^{(1)})|\psi\rangle$$

we can take the inverse because we are no longer in a subspace where this equals zero

We could use this equation if we can get away with inserting a $(\mathbb{1}-P)$ into the equation for $E^{(2)}$:

$$E^{(2)} = \langle\psi|(V-E^{(1)})\overset{(\mathbb{1}-P)}{\vee}|\dot\psi\rangle$$

but if we restrict $|\psi\rangle$ to not only be in the ε subspace, but the subspace where the 1st order secular equation is satisfied, then we indeed <u>CAN</u> do this.
(the extra term goes to zero under satisfaction of the 1st secular equation, so it's no different)

If $|\psi\rangle$ satisfies the 1st order secular equation, then

$$E^{(2)} = \langle\psi|(V-E^{(1)})\overset{(P+(\mathbb{1}-P))}{\vee}(\varepsilon-H_0)^{-1}(V-E^{(1)})|\psi\rangle$$
$$= \sum_i \frac{\langle\psi|(V-\cancel{E^{(1)}})|i\rangle\langle i|(V-\cancel{E^{(1)}})|\psi\rangle}{\varepsilon-\varepsilon_i}$$

cancels out; just numbers

where $|i\rangle$ was defined to be orthogonal to the original degenerate subspace, $|m\rangle$

$$E^{(2)} = \sum_i \frac{\langle\psi|V|i\rangle\langle i|V|\psi\rangle}{\underbrace{\varepsilon-\varepsilon_i}_{\text{the difference in energy levels}}}$$