Lecture 11: Time Independent Perturbation Theory

Few problems can be solved exactly:

examples
- 1D: SHO, Particle in ∞ square well
- 2D: SHO, Landau-levels, cylidrical well
- 3D: SHO, Free particle, Hydrogen, various $e^{\alpha n}$ potentials (confluent hypergeometric functions)

In principle we can solve the problem numerically, but much insight is gained through approximation methods

General problem:
- Given discrete spectrum of $\hat{H}_0$: $\hat{H}_0 |\phi_n^{(0)}\rangle = E_n^{(0)} |\phi_n^{(0)}\rangle$
- Seek $\begin{pmatrix}\text{eigenvalues}\\ \text{eigenvectors}\end{pmatrix}$ of $\hat{H} = \hat{H}_0 + \hat{H}_1$

  where $\hat{H}_1$ is a "perturbation" (i.e. small)

Example: Finestructure in Hydrogen

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} - \frac{e^2}{r}}_{\substack{\text{"Unperturbed"}\\ \text{Hydrogen atom } \hat{H}_0}} + \underbrace{\alpha^2\left(-\frac{\hat{p}^4}{8} + \frac{1}{2}\frac{\hat{\ell}\cdot\hat{s}}{r^3}\right)\frac{e^2}{a_0}}_{\text{"Perturbation" } \hat{H}_1}$$

$\alpha^2 \ll 1$

Typically we write $\hat{H} = \hat{H}_0 + \lambda \hat{H}_1$

$\uparrow$ "Book keeping" parameter to count order of perturbation

Nondegenerate case

- $E_n^{(0)} \neq E_m^{(0)}$ for $n \neq m$
- Perturbation does not introduce new degeneracies

We imagine that the perturbation can be "turned on", i.e. we treat λ as a continuous parameter.

$\Rightarrow$ Assume a Taylor series expansion of the stationary state problem:

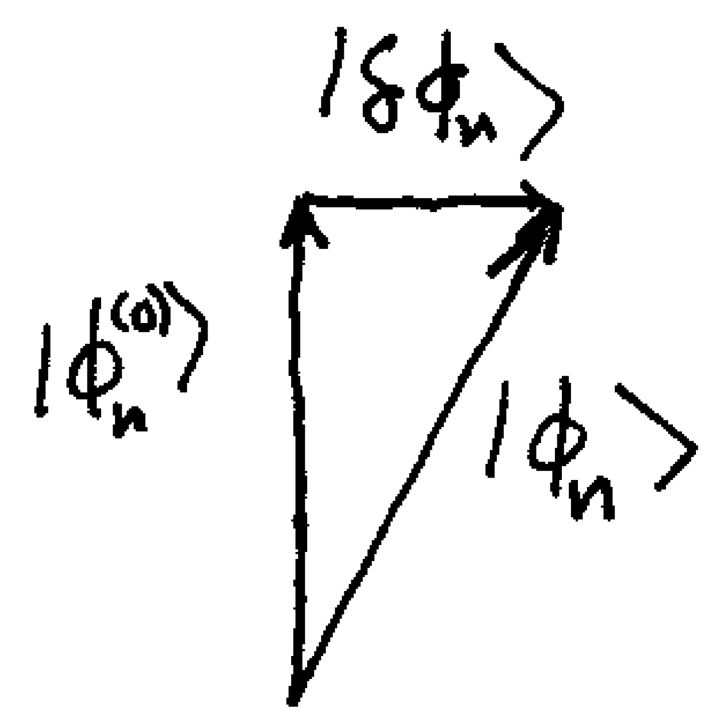
$$\hat{H}(\lambda)\,|\phi_n(\lambda)\rangle = E_n(\lambda)\,|\phi_n(\lambda)\rangle$$

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}_1 \qquad (\text{only ~~first~~ linear term})$$

$$|\phi_n(\lambda)\rangle = \sum_{k=0}^{\infty} \lambda^k |\phi_n^{(k)}\rangle = |\phi_n^{(0)}\rangle + |\delta\phi_n(\lambda)\rangle$$

$$E_n(\lambda) = \sum_{k=0}^{\infty} \lambda^k E_n^{(k)} = E_n^{(0)} + \delta E_n(\lambda)$$

Note: Because we can always normalize the state vector after the fact, we choose to define $|\delta\phi_n(\lambda)\rangle$ to be orthogonal to $|\phi_n^{(0)}\rangle$ (any other part goes into $|\phi_n^{(0)}\rangle$). Then $|\phi_n(\lambda)\rangle$ is not unit norm, and must be renormalized



$$\langle\phi_n^{(0)}|\phi_n^{(0)}\rangle = 1$$

$$\langle\delta\phi_n|\phi_n^{(0)}\rangle \equiv 0$$

$$\langle\phi_n|\phi_n\rangle \neq 1$$

but $\langle\phi_n^{(k')}|\phi_n^{(k)}\rangle \neq 0$

To find δE and $|\delta\phi\rangle$ we plug the power series expansion into the T.I.S.E.

$$\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle \Rightarrow (\hat{H}_0 + \lambda\hat{H}_1)\sum_k \lambda_k |\phi_n^{(k)}\rangle = \sum_{k,k'} \lambda^{k+k'} E_n^{(k)} |\phi_n^{(k')}\rangle$$

Collect terms $\Rightarrow$ $$\left(\hat{H}_0|\phi_n^{(0)}\rangle - E_n^{(0)}|\phi_n^{(0)}\rangle\right) + \lambda\left(\hat{H}_0|\phi_n^{(1)}\rangle + \hat{H}_1|\phi_n^{(0)}\rangle - E_n^{(0)}|\phi_n^{(1)}\rangle - E_n^{(1)}|\phi_n^{(0)}\rangle\right)$$
$$+ \lambda^2\left(\hat{H}_0|\phi_n^{(2)}\rangle + \hat{H}_1|\phi_n^{(1)}\rangle - E_n^{(0)}|\phi_n^{(2)}\rangle - E_n^{(1)}|\phi_n^{(1)}\rangle - E_n^{(2)}|\phi_n^{(0)}\rangle\right)$$
$$+ \cdots = 0$$

True for arbitrarily small $\lambda \Rightarrow$ Each term vanishes independently

Zeroth Order

$$\hat{H}_0|\phi_n^{(0)}\rangle = E_n^{(0)}|\phi_n^{(0)}\rangle$$

First Order

$$(\hat{H}_0 - E_n^{(0)})|\phi_n^{(1)}\rangle + (\hat{H}_1 - E_n^{(1)})|\phi_n^{(0)}\rangle = 0$$

Second Order

$$(\hat{H}_0 - E_n^{(0)})|\phi_n^{(2)}\rangle + (\hat{H}_1 - E_n^{(1)})|\phi_n^{(1)}\rangle - E_n^{(2)}|\phi_n^{(0)}\rangle = 0$$

Generally:

k^{th} order

$$\hat{H}_0|\phi_n^{(k)}\rangle + \hat{H}_1|\phi_n^{(k-1)}\rangle = \sum_{k'=0}^{k} E_n^{(k-k')}|\phi_n^{(k')}\rangle$$

(negative orders are zero)

We can now iterate to find eigenvalue & eigenvectors

Project equations with $\langle\phi_n^{(0)}|$

First order: $\underbrace{\langle\phi_n^{(0)}|(\hat{H}_0 - E_n^{(0)})}_{= 0}|\phi_n^{(1)}\rangle + \langle\phi_n^{(0)}|(\hat{H}_1 - E_n^{(1)})|\phi_n^{(0)}\rangle = 0$

$$\Rightarrow E_n^{(1)}\underbrace{\langle\phi_n^{(0)}|\phi_n^{(0)}\rangle}_{=1} = \langle\phi_n^{(0)}|\hat{H}_1|\phi_n^{(0)}\rangle$$

$$\Rightarrow \boxed{E_n^{(1)} = \langle\phi_n^{(0)}|\hat{H}_1|\phi_n^{(0)}\rangle}$$ Most basic eq. of perturbation theory

How do we find $|\phi_n^{(1)}\rangle$?
Use fact that $\{|\phi_n^{(0)}\rangle\}$ is a complete set

$$|\phi_n^{(1)}\rangle = \sum_{n'\neq n} c_{n'}^{(1)}|\phi_{n'}^{(0)}\rangle \qquad c_{n'}^{(1)} = \langle\phi_{n'}^{(0)}|\phi_n^{(1)}\rangle$$

because $|\delta\phi\rangle \perp |\phi^{(0)}\rangle$

Plug in this representation into first order (part of) T.I.S.E

$$(\hat{H}_0 - E_n^{(0)})\sum_{n'\neq n} c_{n'}|\phi_{n'}^{(0)}\rangle = (E_n^{(1)} - \hat{H}_1)|\phi_n^{(0)}\rangle$$

Project out component n': $\langle\phi_{n'}^{(0)}|$

$$\Rightarrow c_{n'}^{(1)}(E_{n'}^{(0)} - E_n^{(0)}) = -\langle\phi_{n'}^{(0)}|\hat{H}_1|\phi_n^{(0)}\rangle$$

$$\Rightarrow c_{n'}^{(1)} = \frac{\langle\phi_{n'}^{(0)}|\hat{H}_1|\phi_n^{(0)}\rangle}{E_n^{(0)} - E_{n'}^{(0)}}$$

(next page)

3.5

$$\Rightarrow \boxed{|\phi_n^{(1)}\rangle = \sum_{n' \neq n} |\phi_{n'}^{(0)}\rangle \frac{\langle \phi_{n'}^{(0)} | \hat{H}_1 | \phi_n^{(0)}\rangle}{E_n^{(0)} - E_{n'}^{(0)}}}$$

Lessons:

- The effect of the perturbation is to "mix in" nearby energy levels into the original bound state
- the strength of the mixing depends on the ratio of of the "coupling matrix element" to the unperturbed energy difference
- This procedure breaks down if the spectrum has degeneracies since thee resonance denominators blow up

Second order

$$\cancel{\langle \phi_n^{(0)} | \hat{H}_0 - E_n^{(0)} | \phi_n^{(2)}\rangle}^{\,0} + \langle \phi_n^{(0)} | \hat{H}_1 - E_n^{(1)} | \phi_n^{(1)}\rangle = E_n^{(2)} \underbrace{\langle \phi_n^{(0)} | \phi_n^{(0)}\rangle}_{=1}$$

$$\Rightarrow \sum_{n' \neq n} c_{n'}^{(1)} \langle \phi_n^{(0)} | \hat{H}_1 | \phi_{n'}^{(0)}\rangle = E_n^{(2)}$$

$$\Rightarrow E_n^{(2)} = \sum_{n' \neq n} \frac{\langle \phi_n^{(0)} | \hat{H}_1 | \overbrace{\phi_{n'}^{(0)}\rangle \langle \phi_{n'}^{(0)}}^{\text{"Virtual state"}} | \hat{H}_1 | \phi_n^{(0)}\rangle}{E_n^{(0)} - E_{n'}^{(0)}}$$

$$\boxed{E_n^{(2)} = \sum_{n' \neq n} \frac{|\langle \phi_{n'}^{(0)} | \hat{H}_1 | \phi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_{n'}^{(0)}}}$$

Typically we do not go beyond second order

The second order perturbation can be thought of as a two-step process.

(i) The Hamiltonian $\hat{H}_1$ mixes in "virtual states" to create a perturbed state $|\Psi_n\rangle = |\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle$

(ii) the perturbed state is level shifted by an additional order of $\hat{H}_1$

We must be careful here. Remember $E_n \neq \langle|\hat{H}|\rangle_n$ because of normalization.

$$E_n = \langle \hat{H}_n \rangle = \frac{\langle \Psi_n|\hat{H}|\Psi_n\rangle}{\langle \Psi_n|\Psi_n\rangle} = \frac{E_n^{(0)} + \lambda\langle\phi_n^{(0)}|\hat{H}_1|\phi_n^{(0)}\rangle + \lambda^2\left(\langle\phi_n^{(1)}|\hat{H}_0|\phi_n^{(1)}\rangle + \langle\phi_n^{(1)}|\hat{H}_1|\phi_n^{(0)}\rangle + \langle\phi_n^{(0)}|\hat{H}_1|\phi_n^{(1)}\rangle\right)}{1 + \lambda^2\langle\phi_n^{(1)}|\phi_n^{(1)}\rangle}$$

$$= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2\Big\{\langle\phi_n^{(1)}|\hat{H}_1|\phi_n^{(0)}\rangle + \cancel{\langle\phi_n^{(0)}|\hat{H}_1|\phi_n^{(1)}\rangle}$$
$$+ \cancel{\langle\phi_n^{(1)}|\hat{H}_0|\phi_n^{(1)}\rangle} - \cancel{E_n^{(0)}\langle\phi_n^{(1)}|\phi_n^{(1)}\rangle}\Big\}$$

So, yes, everything is consistent, but we have to be careful. We'll see the physical picture of this in the context of the quadratic Stark effect.