PHY 742 Quantum Mechanics II
12-12:50 AM MWF Olin 103

Plan for Lecture 2
Approximate solutions for stationary states
Perturbation theory (Chap. 12 C)

1. Basic ideas
2. First order equations
3. Second order equations
4. Convergence (or lack of convergence) of analysis

Course schedule for Spring 2022

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/10/2022	Chap. 12	Approximate solutions for stationary states -- The variational approach	#1	01/14/2022
2	Wed: 01/12/2022	Chap. 12 C	Approximate solutions for stationary states -- Perturbation theory	#2	01/19/2022
3	Fri: 01/14/2022	Chap. 12 C	Approximate solutions for stationary states -- Perturbation theory		
	Mon: 01/17/2022		MLK Holiday -- no class		

PHY 742 -- Assignment #2

January 12, 2022

Read Chapter 12, part C in **Carlson's** textbook.

1. Work problem 6 at the end of chapter 12.

Methods for finding approximate solutions to the time-independent Schrödinger equation

Problem to solve – $$H\left|n\right\rangle = E_n\left|n\right\rangle$$

For a Hamiltonian of the form $$H = H^0 + \epsilon H^1$$

Here H^0 denotes a Hamiltonian whose eigenstates we know

$$H^0\left|n^0\right\rangle = E_n^0\left|n^0\right\rangle$$

H^1 denotes another contribution to the Hamiltonian scaled by a small number ϵ

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

$$H = H^0 + \epsilon H^1$$

Note that since ε is small, ε ²<< ε

Assume: $\left|n\right\rangle = \left|n^0\right\rangle + \epsilon\left|n^1\right\rangle + \epsilon^2\left|n^2\right\rangle + \ldots$

$$E_n = E_n^0 + \epsilon E_n^1 + \epsilon^2 E_n^2 + \ldots$$

Note: We will see that this methods depends on the non-degenerate zeroth order eigenvalues $E_n^0 \neq E_m^0$ for $n \neq m$

Apart from this non-degeneracy condition, the method is very powerful, since the eigenfunctions $\left\{\left|n^0\right\rangle\right\}$ form a complete set.

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

$$H = H^0 + \epsilon H^1$$

Assume: $\left|n\right\rangle = \left|n^0\right\rangle + \epsilon\left|n^1\right\rangle + \epsilon^2\left|n^2\right\rangle + \ldots$

$$E_n = E_n^0 + \epsilon E_n^1 + \epsilon^2 E_n^2 + \ldots$$

$$\Rightarrow \left(H^0 + \epsilon H^1\right)\left(\left|n^0\right\rangle + \epsilon\left|n^1\right\rangle + \epsilon^2\left|n^2\right\rangle + \ldots\right)$$

$$= \left(E_n^0 + \epsilon E_n^1 + \epsilon^2 E_n^2 + \ldots\right)\left(\left|n^0\right\rangle + \epsilon\left|n^1\right\rangle + \epsilon^2\left|n^2\right\rangle + \ldots\right)$$

Solve separately for each power of ε

$$\left(H^0+\epsilon H^1\right)\left(\left|n^0\right\rangle+\epsilon\left|n^1\right\rangle+\epsilon^2\left|n^2\right\rangle+\ldots\right)$$

$$=\left(E_n^0+\epsilon E_n^1+\epsilon^2 E_n^2+\ldots\right)\left(\left|n^0\right\rangle+\epsilon\left|n^1\right\rangle+\epsilon^2\left|n^2\right\rangle+\ldots\right)$$

Collecting terms according to their order:

$$\epsilon^0: \quad H^0\left|n^0\right\rangle=E_n^0\left|n^0\right\rangle$$

$$\epsilon^1: \quad H^0\left|n^1\right\rangle+H^1\left|n^0\right\rangle=E_n^0\left|n^1\right\rangle+E_n^1\left|n^0\right\rangle$$

$$\left\langle n^0\right|H^0\left|n^1\right\rangle+\left\langle n^0\right|H^1\left|n^0\right\rangle=\left\langle n^0\right|E_n^0\left|n^1\right\rangle+\left\langle n^0\right|E_n^1\left|n^0\right\rangle$$

$$\Rightarrow E_n^1=\left\langle n^0\right|H^1\left|n^0\right\rangle$$

Note: here we impose the condition:

$\left\langle n^0 \middle| m^1\right\rangle=0$ for all states $\left\{\left|n^0\right\rangle\right\}$ and $\left\{\left|m^1\right\rangle\right\}$.

Is this reasonable?

First order corrections -- continued

Since the eigenstates $\left|n^0\right\rangle$ for a complete set of states:

Assume $\left|n^1\right\rangle = \sum_{m\neq n} C_m \left|m^0\right\rangle$

$$H^0\left|n^1\right\rangle + H^1\left|n^0\right\rangle = E_n^0\left|n^1\right\rangle + E_n^1\left|n^0\right\rangle$$

$$C_m = \frac{\left\langle m^0\right|H_1\left|n^0\right\rangle}{E_n^0 - E_m^0} \quad \text{for } m \neq n$$

$$\boxed{\left|n^1\right\rangle = \sum_{m\neq n}\left(\frac{\left\langle m^0\right|H_1\left|n^0\right\rangle}{E_n^0 - E_m^0}\right)\left|m^0\right\rangle}$$

Second order corrections

$$\epsilon^2: \quad H^0\left|n^2\right\rangle + H^1\left|n^1\right\rangle = E_n^0\left|n^2\right\rangle + E_n^1\left|n^1\right\rangle + E_n^2\left|n^0\right\rangle$$

$$\left\langle n^0\right|H^0\left|n^2\right\rangle + \left\langle n^0\right|H^1\left|n^1\right\rangle = \left\langle n^0\right|E_n^0\left|n^2\right\rangle + \left\langle n^0\right|E_n^1\left|n^1\right\rangle + \left\langle n^0\right|E_n^2\left|n^0\right\rangle$$

$$\Rightarrow E_n^2 = \left\langle n^0\right|H^1\left|n^1\right\rangle = \sum_{m\neq n} \frac{\left\langle n^0\right|H^1\left|m^0\right\rangle\left\langle m^0\right|H^1\left|n^0\right\rangle}{E_n^0 - E_m^0}$$

(after considerable algebra --)

$$\left|n^2\right\rangle = \sum_{m\neq n}\left|m^0\right\rangle \sum_{l\neq n} \frac{\left\langle m^0\right|H^1\left|l^0\right\rangle\left\langle l^0\right|H^1\left|n^0\right\rangle}{\left(E_n^0 - E_m^0\right)\left(E_n^0 - E_l^0\right)}$$

$$-\sum_{m\neq n}\left|m^0\right\rangle \frac{\left\langle m^0\right|H^1\left|n^0\right\rangle\left\langle n^0\right|H^1\left|n^0\right\rangle}{\left(E_n^0 - E_m^0\right)^2} \quad -\frac{1}{2}\left|n^0\right\rangle \sum_{m\neq n} \frac{\left|\left\langle m^0\right|H^1\left|n^0\right\rangle\right|^2}{\left(E_n^0 - E_m^0\right)^2}$$

Due to normalization

Example – Harmonic oscillator

$$H^0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \qquad E_n^0 = \hbar\omega\left(n^0 + \frac{1}{2}\right)$$

$$H^1 = \frac{1}{2}m\Omega^2 x^2$$

Exact eigenstates: $E_n^{\text{exact}} = \hbar\sqrt{\omega^2 + \epsilon\Omega^2}\left(n + \frac{1}{2}\right)$

$$= \hbar\omega\left(1 + \frac{\epsilon}{2}\frac{\Omega^2}{\omega^2} - \frac{\epsilon^2}{8}\frac{\Omega^4}{\omega^4}\ldots\right)\left(n + \frac{1}{2}\right)$$

Perturbation theory results:

$$E_n^1 = \left\langle n^0 \middle| \tfrac{1}{2}m\Omega^2 x^2 \middle| n^0 \right\rangle = \hbar\omega\frac{\Omega^2}{2\omega^2}\left(n + \frac{1}{2}\right)$$

Example from Carlson XII C --

$$H = \frac{1}{2m}P^2 + \tfrac{1}{2}m\omega^2 X^2 + \lambda X^4$$

Using very clever harmonic oscillator operators

$$E_0 = \varepsilon_0 + \langle 0|W|0\rangle + \sum_{q\neq 0}\frac{|\langle q|W|0\rangle|^2}{\varepsilon_0 - \varepsilon_q} = \tfrac{1}{2}\hbar\omega + \frac{3\lambda\hbar^2}{4m^2\omega^2} + \frac{|\langle 2|W|0\rangle|^2}{-2\hbar\omega} + \frac{|\langle 4|W|0\rangle|^2}{-4\hbar\omega}$$

$$= \tfrac{1}{2}\hbar\omega + \frac{3\lambda\hbar^2}{4m^2\omega^2} + \left(\frac{\lambda\hbar^2}{4m^2\omega^2}\right)^2\left(-\frac{72}{2\hbar\omega} - \frac{24}{4\hbar\omega}\right) = \tfrac{1}{2}\hbar\omega + \frac{3\lambda\hbar^2}{4m^2\omega^2} - \frac{21\lambda^2\hbar^3}{8m^4\omega^5}.$$

The ground state vector, to first order, is

$$|\psi_0\rangle = |0\rangle + \sum_{q\neq 0}|q\rangle\frac{\langle q|W|0\rangle}{\varepsilon_0 - \varepsilon_q} = |0\rangle - |2\rangle\frac{\langle 2|W|0\rangle}{2\hbar\omega} - |4\rangle\frac{\langle 4|W|0\rangle}{4\hbar\omega} = |0\rangle - \frac{\lambda\hbar}{8m^2\omega^3}\left(6\sqrt{2}|2\rangle + \sqrt{6}|4\rangle\right).$$

Your homework is somewhat similar --

Example: He atom

$$H(\mathbf{r}_1,\mathbf{r}_2) = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

$$H^0(\mathbf{r}_1,\mathbf{r}_2) = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{2e^2}{r_1} - \frac{2e^2}{r_2}$$

$$H^1(\mathbf{r}_1,\mathbf{r}_2) = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

What happens when the spectrum of H^0 has degeneracy?

$$\left(H^0+\epsilon H^1\right)\left(\left|n^0\right\rangle+\epsilon\left|n^1\right\rangle+\epsilon^2\left|n^2\right\rangle+\ldots\right)$$

$$=\left(E_n^0+\epsilon E_n^1+\epsilon^2 E_n^2+\ldots\right)\left(\left|n^0\right\rangle+\epsilon\left|n^1\right\rangle+\epsilon^2\left|n^2\right\rangle+\ldots\right)$$

Collecting terms according to their order:

$$\epsilon^0: \quad H^0\left|n^0\right\rangle=E_n^0\left|n^0\right\rangle$$

$$\epsilon^1: \quad H^0\left|n^1\right\rangle+H^1\left|n^0\right\rangle=E_n^0\left|n^1\right\rangle+E_n^1\left|n^0\right\rangle$$

Since the eigenstates $\left|n^0\right\rangle$ for a complete set of states:

Assume $\left|n^1\right\rangle = \sum_{m \neq n} C_m \left|m^0\right\rangle$

$$C_m = \frac{\left\langle m^0 \middle| H_1 \middle| n^0 \right\rangle}{E_n^0 - E_m^0}$$

$$\left|n^1\right\rangle = \sum_{m \neq n} \left(\frac{\left\langle m^0 \middle| H_1 \middle| n^0 \right\rangle}{E_n^0 - E_m^0} \right) \left|m^0\right\rangle$$

➔ problem when $E^0_n = E^0_m$

➔ solution – consider the degenerate states separately

Why is degeneracy a problem for the He atom and not for the one-dimensional harmonic oscillator?

$$H(\mathbf{r}_1,\mathbf{r}_2) = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}$$

$$H^0(\mathbf{r}_1,\mathbf{r}_2) = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{2e^2}{r_1} - \frac{2e^2}{r_2}$$

$$H^1(\mathbf{r}_1,\mathbf{r}_2) = \frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}$$

➔**More discussion next time.**