PHY 742 Quantum Mechanics II
1-1:50 AM MWF Olin 103

Plan for Lecture 13

Time dependent perturbation theory
Ref: Chapter 15

1. **Fermi Golden Rule for bound → continuum transition.**

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Topics for Quantum Mechanics II

Single particle analysis
- Single particle interacting with electromagnetic fields – EC Chap. 9
- Scattering of a particle from a spherical potential – EC Chap. 14
- More time independent perturbation methods – EC Chap. 12, 13
- Single electron states of a multi-well potential → molecules and solids – EC Chap. 2,6
- Time dependent perturbation methods – EC Chap. 15
- Path integral formalism (Feynman) – EC Chap. 11.C
- Relativistic effects and the Dirac Equation – EC Chap. 16

Multiple particle analysis
- Quantization of the electromagnetic fields – EC Chap. 17
- Photons and atoms – EC Chap. 18
- Multi particle systems; Bose and Fermi particles – EC Chap. 10
- Multi electron atoms and materials
  - Hartree-Fock approximation
  - Density functional approximation

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Course schedule for Spring 2020

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/13/2020	Chap. 9	Quantum mechanics of electromagnetic forces	#1	01/22/2020
2	Wed: 01/15/2020	Chap. 9	Quantum mechanics of particle in electrostatic field	#2	01/24/2020
3	Fri: 01/17/2020	Chap. 9	Quantum mechanics of particle in magnetostatic field	#3	01/27/2020
	Mon: 01/20/2020	No class	Martin Luther King Holiday		
4	Wed: 01/22/2020	Chap. 14	Scattering theory	#4	01/29/2020
5	Fri: 01/24/2020	Chap. 14	Scattering theory	#5	01/31/2020
6	Mon: 01/27/2020	Chap. 14	Scattering theory	#6	02/03/2020
7	Wed: 01/29/2020	Chap. 12	Variational methods	#7	02/05/2020
8	Fri: 01/31/2020	Chap. 12	Variational and other approximation methods	#8	02/07/2020
9	Mon: 02/03/2020	Chap. 2,6	Single particle states of molecules and solids	#9	02/10/2020
10	Wed: 02/05/2020	Chap. 2,6	H_2^+ molecular ion; Born Oppenheimer approximation	#10	02/12/2020
11	Fri: 02/07/2020	Chap. 15	Time-dependent perturbations	#11	02/14/2020
12	Mon: 02/10/2020	Chap. 15	Time-dependent perturbations	#12	02/14/2020
13	Wed: 02/12/2020	Chap. 15	Time-dependent perturbations	#13	02/17/2020
14	Fri: 02/14/2020				
15	Mon: 02/17/2020				
16	Wed: 02/19/2020				
17	Fri: 02/21/2020				
18	Mon: 02/24/2020				
19	Wed: 02/26/2020				
20	Fri: 02/28/2020				

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Summary of results of 1st order theory for a time harmonic perturbation of the form:

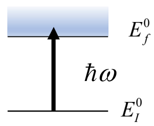
Suppose that $H^1(t) = \tilde{H}^1 h(t)$

$$\text{where} \quad h(t) \equiv \begin{cases} 0 & \text{for } t<0 \text{ and } t>T \\ 2\sin\omega t & \text{for } 0<t<T \end{cases}$$

Fermi golden rule: $\mathcal{R}_{I\to f} = \dfrac{\left|k^1_{I\to f}(t)\right|^2}{T} \approx \dfrac{2\pi}{\hbar}\left|\langle f^0|\tilde{H}^1|I^0\rangle\right|^2 \delta\left(\hbar\left(\omega-\omega_{fi}\right)\right)$

where $\hbar\omega_{fi} \equiv E^0_f - E^0_I$

Treatment of the case when the initial state is bound and the final state is in the continuum spectrum --



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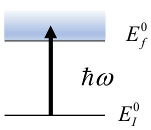
Absorption of radiation in the case of photoemission of a H-like atom



Initial state: $\left|I^0 = 1s\right\rangle = \left(\dfrac{Z^3}{a_0^3\pi}\right)^{1/2} e^{-Zr/a_0} \qquad E^0_I = -\dfrac{Z^2e^2}{8\pi\epsilon_0 a_0}$

It is convenient to approximate the final state as a plane wave (Born approximation)

$$\left|f^0\right\rangle \approx \mathcal{N}e^{i\mathbf{k}\cdot\mathbf{r}} \quad \text{where } k = \sqrt{(2mE^0_f/\hbar^2)}$$

Transition rate:

$$\mathcal{R}_{I\to f} \approx \frac{2\pi}{\hbar}\left|\langle f^0|\tilde{H}^1|I^0\rangle\right|^2 \delta\left(-\hbar\omega + E^0_f - E^0_I\right)$$

In this case, for a uniform electric field amplitude $\mathbf{F}$:

$\tilde{H}^1(\mathbf{r}) = e\mathbf{F}\cdot\mathbf{r}$ or $\tilde{H}'^1(\mathbf{r}) = \dfrac{e}{m\omega}\mathbf{F}\cdot\mathbf{p}$

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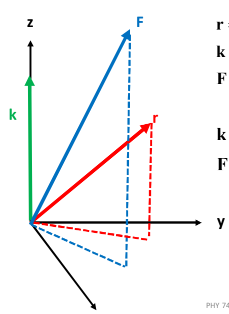
Convenient coordinate system --



$\mathbf{r} = r\left(\sin\theta\cos\phi\,\hat{\mathbf{x}} + \sin\theta\sin\phi\,\hat{\mathbf{y}} + \cos\theta\,\hat{\mathbf{z}}\right)$

$\mathbf{k} = k\hat{\mathbf{z}}$

$\mathbf{F} = F\left(\sin\psi\cos\chi\,\hat{\mathbf{x}} + \sin\psi\sin\chi\,\hat{\mathbf{y}} + \cos\psi\,\hat{\mathbf{z}}\right)$

$\mathbf{k}\cdot\mathbf{r} = kr\cos\theta$

$\mathbf{F}\cdot\mathbf{r} = Fr\left(\sin\psi\sin\theta\cos\left(\chi-\phi\right) + \cos\psi\cos\theta\right)$

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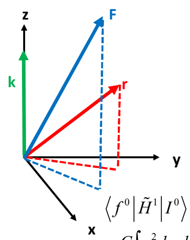
Approximate photoemission -- continued



$$\mathbf{r} = r\left(\sin\theta\cos\phi\hat{\mathbf{x}} + \sin\theta\sin\phi\hat{\mathbf{y}} + \cos\theta\hat{\mathbf{z}}\right)$$
$$\mathbf{k} = k\hat{\mathbf{z}}$$
$$\mathbf{F} = F\left(\sin\psi\cos\chi\hat{\mathbf{x}} + \sin\psi\sin\chi\hat{\mathbf{y}} + \cos\psi\hat{\mathbf{z}}\right)$$
$$\mathbf{k}\cdot\mathbf{r} = kr\cos\theta$$
$$\mathbf{F}\cdot\mathbf{r} = Fr\left(\sin\psi\sin\theta\cos\left(\chi-\phi\right) + \cos\psi\cos\theta\right)$$

$$\left\langle f^0\middle|\tilde{H}^1\middle|I^0\right\rangle = \left\langle f^0\middle|e\mathbf{F}\cdot\mathbf{r}\middle|I^0\right\rangle$$
$$= C\int r^2dr\ d\cos\theta\ d\phi\ e^{ikr\cos\theta}e^{-Zr/a_0}r\left(\sin\psi\sin\theta\cos\left(\chi-\phi\right)+\cos\psi\cos\theta\right)$$
$$\text{where } C \equiv \left(\frac{Z^3}{a_0^3\pi}\right)^{1/2}\mathcal{N}eF$$

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Approximate photoemission -- continued

Some details:

$$\int r^2dr\ d\cos\theta\ d\phi\ e^{ikr\cos\theta}e^{-Zr/a_0}r\left(\sin\psi\sin\theta\cos\left(\chi-\phi\right)+\cos\psi\cos\theta\right)$$
$$=2\pi\int r^2dr\ d\cos\theta\ e^{ikr\cos\theta}e^{-Zr/a_0}r\cos\psi\cos\theta$$
$$=\frac{4i\pi\cos\psi}{k^2}\int_0^\infty rdr\left(kr\cos(kr)-\sin(kr)\right)e^{-Zr/a_0}$$
$$=-32i\pi\cos\psi\frac{ka_0^5}{Z^5}\frac{1}{\left(1+k^2a_0^2/Z^2\right)^3}$$

$$\left\langle f^0\middle|e\mathbf{F}\cdot\mathbf{r}\middle|I^0\right\rangle = -32i\pi\left(\frac{Z^3}{a_0^3\pi}\right)^{1/2}\mathcal{N}eF\frac{ka_0^5}{Z^5}\frac{\cos\psi}{\left(1+k^2a_0^2/Z^2\right)^3}$$

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Approximate photoemission -- continued

$$\mathcal{R}_{I\to f} \approx \frac{2\pi}{\hbar}\left|\left\langle f^0\middle|\tilde{H}^1\middle|I^0\right\rangle\right|^2\delta\left(-\hbar\omega+E_f^0-E_I^0\right)$$
$$\left\langle f^0\middle|e\mathbf{F}\cdot\mathbf{r}\middle|I^0\right\rangle = -32i\pi\left(\frac{Z^3}{a_0^3\pi}\right)^{1/2}\mathcal{N}eF\frac{ka_0^5}{Z^5}\frac{\cos\psi}{\left(1+k^2a_0^2/Z^2\right)^3}$$

Digression – In general, the full transition rate is determined by averaging over all initial states and summing over all final states.

In our case, there is only one initial state, but a continuum of final states.

$$\mathcal{R}_I(\omega) = \sum_f \mathcal{R}_{I\to f} = \sum_f \frac{2\pi}{\hbar}\left|\left\langle f^0\middle|\tilde{H}^1\middle|I^0\right\rangle\right|^2\delta\left(-\hbar\omega+E_f^0-E_I^0\right)$$

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Approximate photoemission -- continued

$$\mathcal{R}_I(\omega) = \sum_f \mathcal{R}_{I\to f} \quad = \sum_f \frac{2\pi}{\hbar}\left|\left\langle f^0\middle|\tilde{H}^1\middle|I^0\right\rangle\right|^2 \delta\left(-\hbar\omega + E_f^0 - E_I^0\right)$$

Note that there are contributions when $E_f^0 = E_I^0 + \hbar\omega$

$$\left|f^0\right\rangle \approx \mathcal{N} e^{i\mathbf{k}\cdot\mathbf{r}} \qquad \text{where } k = \sqrt{(2mE_f^0/\hbar^2)}$$

Note that there are multiple values of k for each E_f^0

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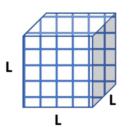
Digression – how can we count the number of plane waves?



Imagine that the plane waves associated with this box satisfy periodic boundary conditions. $\Psi(\mathbf{r}) = \Psi(\mathbf{r} + n_1 L\hat{\mathbf{x}} + n_2 L\hat{\mathbf{y}} + n_3 L\hat{\mathbf{z}}) = \mathcal{N} e^{i\mathbf{k}\cdot\mathbf{r}}$

This is only possible if $\mathbf{k} = \frac{2\pi}{L}\left(m_1\hat{\mathbf{x}} + m_2\hat{\mathbf{y}} + m_3\hat{\mathbf{z}}\right)$

Now we can count the number of final states --

$$\sum_f \rightarrow \sum_{\mathbf{k}} \rightarrow \left(\frac{L}{2\pi}\right)^3 \int d^3k = \frac{\mathcal{V}}{(2\pi)^3}\int d^3k$$

For consistency, we should normalize the plane waves within the box

$$\Rightarrow \mathcal{N} = \sqrt{\frac{1}{L^3}} = \sqrt{\frac{1}{\mathcal{V}}}$$

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Approximate photoemission -- continued

$$\mathcal{R}_I(\omega) = \sum_f \mathcal{R}_{I\to f} \quad = \sum_f \frac{2\pi}{\hbar}\left|\left\langle f^0\middle|\tilde{H}^1\middle|I^0\right\rangle\right|^2 \delta\left(-\hbar\omega + E_f^0 - E_I^0\right)$$

$$\left\langle f^0\middle|e\mathbf{F}\cdot\mathbf{r}\middle|I^0\right\rangle = -32i\pi\left(\frac{Z^3}{a_0^3\pi}\right)^{1/2}\left(\frac{1}{\mathcal{V}^{1/2}}\right)eF\frac{ka_0^5}{Z^5}\frac{\cos\psi}{\left(1+k^2a_0^2/Z^2\right)^3}$$

$$\mathcal{R}_I(\omega) = \frac{2\pi}{\hbar}\frac{\mathcal{V}}{(2\pi)^3}\int d^3k \left|32i\pi\left(\frac{Z^3}{a_0^3\pi}\right)^{1/2}\left(\frac{1}{\mathcal{V}^{1/2}}\right)eF\frac{ka_0^5}{Z^5}\frac{\cos\psi}{\left(1+k^2a_0^2/Z^2\right)^3}\right|^2 \delta\left(\frac{\hbar^2k^2}{2m} - E_I^0 - \hbar\omega\right)$$

Writing $d^3k = k^2dk\ d\Omega_k$

$$\frac{\mathcal{R}_I(\omega)}{d\Omega_k} = \frac{2\pi}{\hbar}\frac{\mathcal{V}}{(2\pi)^3}\int k^2dk \left|32i\pi\left(\frac{Z^3}{a_0^3\pi}\right)^{1/2}\left(\frac{1}{\mathcal{V}^{1/2}}\right)eF\frac{ka_0^5}{Z^5}\frac{\cos\psi}{\left(1+k^2a_0^2/Z^2\right)^3}\right|^2 \delta\left(\frac{\hbar^2k^2}{2m} - E_I^0 - \hbar\omega\right)$$

$$\frac{\mathcal{R}_I(\omega)}{d\Omega_k} = \frac{256mk^3e^2F^2a_0^7/Z^7}{\pi\hbar^3\left(1+k^2a_0^2/Z^2\right)^6}\cos^2\psi \qquad \text{where } \frac{\hbar^2k^2}{2m} = E_I^0 + \hbar\omega$$

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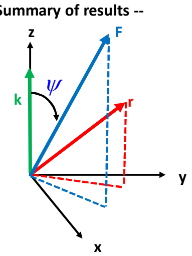
Summary of results --



$$\frac{\mathcal{R}_I(\omega)}{d\Omega_k} = \frac{256 m k^3 e^2 F^2 a_0^7 / Z^7}{\pi \hbar^3 \left(1 + k^2 a_0^2 / Z^2\right)^6} \cos^2 \psi$$

where $\frac{\hbar^2 k^2}{2m} = E_I^0 + \hbar\omega$

$$E_I^0 = -\frac{Z^2 e^2}{8\pi\epsilon_0 a_0} = -\frac{\hbar^2}{2 m a_0^2 / Z^2}$$

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m e^2}$$

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