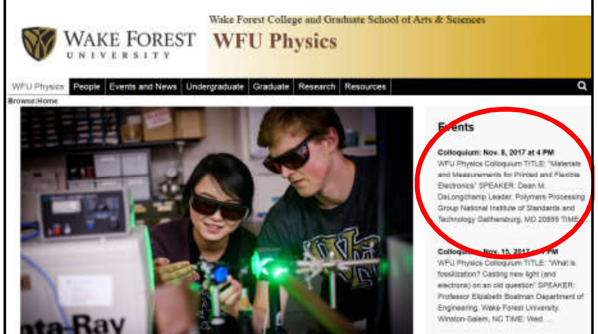
PHY 741 Quantum Mechanics
12-12:50 AM MWF Olin 103

Plan for Lecture 29:

Chap. 18 in Shankar: Time-dependent perturbation theory

1. Resonant phenomena
2. Sudden approximation
3. Adiabatic approximation



19	Mon, 10/16/2017		Discuss exam questions and topics for presentations	Topic	10/18/2017
20	Wed, 10/18/2017	Chap. 14	Intrinsic spin	#11	10/20/2017
21	Fri, 10/20/2017	Chap. 15	Addition of Angular Momentum	#12	10/23/2017
22	Mon, 10/23/2017	Chap. 15	Multi-electron atoms	#13	10/25/2017
23	Wed, 10/25/2017	Chap. 15	Multi-electron atoms	#14	10/30/2017
24	Fri, 10/27/2017		Effects of nuclear motion		
25	Mon, 10/30/2017	Chap. 17	Time-independent perturbation theory	#15	11/3/2017
26	Wed, 11/01/2017	Chap. 17	Time-independent perturbation theory		
27	Fri, 11/03/2017		Effects of a static magnetic field		
28	Mon, 11/06/2017	Chap. 18	Time-dependent perturbation theory	#16	11/10/2017
29	Wed, 11/08/2017	Chap. 18	Time-dependent perturbation theory		
30	Fri, 11/10/2017				
31	Mon, 11/13/2017				
32	Wed, 11/15/2017				
33	Fri, 11/17/2017				
34	Mon, 11/20/2017				
	Wed, 11/22/2017		*Thanksgiving Holiday -- No class*		
	Fri, 11/24/2017		*Thanksgiving Holiday -- No class*		
35	Mon, 11/27/2017				
36	Wed, 11/29/2017				

Summary of time-dependent perturbation expansions

$$i\hbar \frac{\partial}{\partial t}\left|\psi\right\rangle = H(t)\left|\psi\right\rangle$$

$$H(t) = H^0 + \epsilon H^1(t)$$

We approach the problem using the complete basis set of H^0 :

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

It is reasonable to assume that

$$\left|\psi(t)\right\rangle = \sum_n c_n(t)\left|n^0\right\rangle \equiv \sum_n k_n(t) e^{-iE_n^0 t/\hbar}\left|n^0\right\rangle$$

Summary of time-dependent perturbation treatment -- continued

1st-order equation, assuming that $k_n^0 = \delta_{nI}$

$$\frac{dk_m^1}{dt} = \frac{1}{i\hbar}\left\langle m^0\right| H^1(t)\left|I^0\right\rangle e^{i\left(E_m^0 - E_I^0\right)t/\hbar}$$

Example:

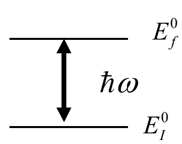
Suppose that $H^1(t) = \tilde{H}^1 h(t)$

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

Estimating the rate of transitions $I \rightarrow f$

$$\mathcal{R}_{I\rightarrow f} = \frac{\left|k^1_{I\rightarrow f}(t)\right|^2}{T} \approx \frac{2\pi}{\hbar}\left|\left\langle f^0\right|\tilde{H}^1\left|I^0\right\rangle\right|^2 \times \left(\delta\left(\hbar\omega + E_f^0 - E_I^0\right) + \delta\left(-\hbar\omega + E_f^0 - E_I^0\right)\right)$$

Fermi "Golden" rule



Example

H atom in presence of electric field

$$\tilde{H}^1 = -eFz \quad \text{representing field as scalar potential}$$
$$= -eFr\cos\theta$$

Some H^0 eigenstates for H-like ion:

$$\left|I^0 = 1s\right\rangle = \left(\frac{Z^3}{a_0^3\pi}\right)^{1/2} e^{-Zr/a_0} \qquad E_I^0 = -\frac{Z^2e^2}{2a_0}$$

$$\left|f^0 = 2p_0\right\rangle = \left(\frac{Z^3}{32a_0^3\pi}\right)^{1/2} \frac{Zr}{a_0} e^{-Zr/2a_0}\cos\theta \qquad E_f^0 = -\frac{Z^2e^2}{2a_0}\frac{1}{4}$$

$$\left\langle f^0\middle|\tilde{H}^1\middle|I^0\right\rangle = \left\langle f^0\middle|-eFr\cos\theta\middle|I^0\right\rangle$$

H^0 eigenstates for H-like ion: $\left|I^0 = 1s\right\rangle = \left(\frac{Z^3}{a_0^3\pi}\right)^{1/2} e^{-Zr/a_0}$

$$\left|f^0 = 2p_0\right\rangle = \left(\frac{Z^3}{32a_0^3\pi}\right)^{1/2} \frac{Zr}{a_0} e^{-Zr/2a_0}\cos\theta$$

$$\left\langle f^0\middle|\tilde{H}^1\middle|I^0\right\rangle = -eF\frac{Z^3}{a_0^3\pi}\left(\frac{1}{32}\right)^{1/2} 2\pi\frac{2}{3}\int_0^\infty r^3 dr\frac{Zr}{a_0}e^{-3Zr/2a_0}$$
$$= -eF\frac{Z^3}{a_0^3\pi}\left(\frac{1}{32}\right)^{1/2} 2\pi\frac{2}{3}\left(\frac{a_0}{Z}\right)^4\int_0^\infty x^4 dx\, e^{-\frac{3}{2}x}$$
$$= -\frac{eFa_0}{\sqrt{2}Z}\frac{256}{243}$$

Summary of results for resonant transitions for H-like ion

1s→2p₀

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

$$\left\langle f^0\middle|\tilde{H}^1\middle|I^0\right\rangle = -\frac{eFa_0}{\sqrt{2}Z}\frac{256}{243}$$

$$\hbar\omega = E_f^0 - E_I^0 = \frac{3}{4}\frac{Z^2e^2}{2a_0} = 10.204\, Z^2 \text{ eV}$$

Digression: Notion of oscillator strength for transition between states $l \rightarrow n$:

$$f_{nl} = \frac{2m}{\hbar^2}\left(E_n^0 - E_l^0\right)\left|\langle n^0|z|l^0\rangle\right|^2$$

$$\left[z,\left[z,H^0\right]\right] = z^2H^0 + H^0z^2 - 2zH^0z = \frac{i\hbar}{m}\left[z,p_z\right] = -\frac{\hbar^2}{m}$$

$$\langle l^0|\left[z,\left[z,H^0\right]\right]|l^0\rangle = 2E_l^0\langle l^0|z^2|l^0\rangle - 2\langle l^0|zH^0z|l^0\rangle = -\frac{\hbar^2}{m}$$

Inserting resolution of the identity: $1 = \sum_n |n^0\rangle\langle n^0|$

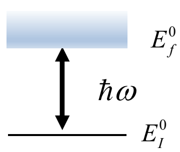
$$\sum_n\left(2E_l^0\langle l^0|z|n^0\rangle\langle n^0|z|l^0\rangle - 2\langle l^0|z|n^0\rangle E_n^0\langle n^0|z|l^0\rangle\right) = -\frac{\hbar^2}{m}$$

$$\frac{2m}{\hbar^2}\sum_n\left(E_n^0 - E_l^0\right)\langle l^0|z|n^0\rangle\langle n^0|z|l^0\rangle = \sum_n f_{nl} = 1$$

Absorption of radiation in the case of photo emission

$$|f^0\rangle = R_{El}(r)Y_{lm}(\hat{\mathbf{r}})$$

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + \frac{Ze^2}{r} + E\right)R_{El}(r) = 0$$



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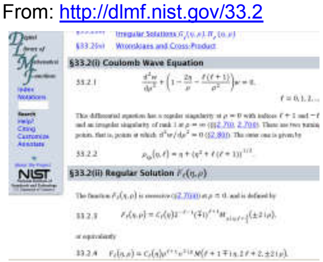

§33.2(iii) Irregular Solutions $G_\ell(\eta,\rho)$, $H_\ell^\pm(\eta,\rho)$

§33.2(iv) Wronskians and Cross-Product

§33.2(i) Coulomb Wave Equation

33.2.1 $\frac{d^2w}{d\rho^2} + \left(1 - \frac{2\eta}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right)w = 0$, $\ell = 0, 1, 2, \ldots$

This differential equation has a regular singularity at $\rho = 0$ with indices $\ell+1$ and $-\ell$, and an irregular singularity of rank 1 at $\rho = \infty$ (§§2.7(i), 2.7(ii)). There are two turning points, that is, points at which $d^2w/d\rho^2 = 0$ (§2.8(i)). The outer one is given by

33.2.2 $\rho_{tp}(\eta,\ell) = \eta + (\eta^2 + \ell(\ell+1))^{1/2}$.

§33.2(ii) Regular Solution $F_\ell(\eta,\rho)$

The function $F_\ell(\eta,\rho)$ is recessive (§2.7(iii)) at $\rho = 0$, and is defined by

33.2.3 $F_\ell(\eta,\rho) = C_\ell(\eta)2^{-\ell-1}(\mp i)^{\ell+1}M_{\pm i\eta,\ell+\frac{1}{2}}(\pm 2i\rho)$,

or equivalently

33.2.4 $F_\ell(\eta,\rho) = C_\ell(\eta)\rho^{\ell+1}e^{\mp i\rho}M(\ell+1\mp i\eta, 2\ell+2, \pm 2i\rho)$.

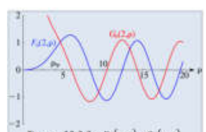


Figure 33.3.3: $F_\ell(\eta,\rho)$, $G_\ell(\eta,\rho)$ with $\ell = 0$, $\eta = 2$. The turning point is at $\rho_{tp}(2,0) = 4$.

Absorption of radiation in the case of photo emission approximating final state as a plane wave (Born approximation)

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

For initial state: $|I^0 = 1s\rangle = \left(\frac{Z^3}{a_0^3\pi}\right)^{1/2} e^{-Zr/a_0}$

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

$$\langle f^0|\tilde{H}^1|I^0\rangle = \langle f^0|-eFr\cos\theta|I^0\rangle$$

Note: In this case, it is necessary to modify the static electric field in order to account for electrodynamics …

For a H-like ion in a beam of photons with flux *S,* it is convenient to define a cross section:

$$\int d\omega \frac{d\sigma(\omega)}{d\Omega} = \int d\omega \frac{\mathcal{R}_{I\to f}(\omega)}{S(\omega)}$$

For a final state electron in the $\hat{\mathbf{k}}$ direction and a photon directed toward $\hat{\mathbf{z}}$:

$$\frac{d\sigma(\omega)}{d\Omega} = \frac{32e^2k^3\cos^2\theta}{mc\omega}\frac{Z^5}{a_0^5}\frac{1}{\left(\frac{Z^2}{a_0^2}+k^2+\frac{\omega^2}{c^2}-2k\frac{\omega}{c}\cos\theta\right)^4}$$

(Details: Merzbacher, Quantum Mechanics, third ed. (1998)

Sudden approximation

This method is useful when there is an abrupt change in the Hamiltonian of the system

$$\text{Suppose that for } t<0, \quad H = H^A$$
$$\text{for } t>0, \quad H = H^B$$

This can happen when we have a nuclear process occur which is "sudden" for the electronic states. It is also a reasonable approximation for some X-ray core absorption processes.

Sudden approximation -- continued

The most convenient method to analyze this system is to find the complete sets of eigenvalues of the two Hamiltonians:

$$H^A\left|\psi_n^A\right\rangle = E_n^A\left|\psi_n^A\right\rangle$$
$$H^B\left|\psi_\nu^B\right\rangle = E_\nu^B\left|\psi_\nu^B\right\rangle$$

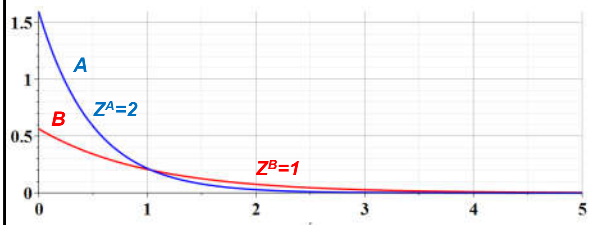
Suppose that at $t=0$, $\left|\Psi(t=0)\right\rangle = \left|\psi_0^A\right\rangle$

It is reasonable to assume that for $t>0$:

$$\left|\Psi(t>0)\right\rangle = \sum_\nu C_\nu \left|\psi_\nu^B\right\rangle e^{-iE_\nu^B t/\hbar}$$

where $C_\nu = \left\langle \psi_\nu^B \middle| \psi_0^A \right\rangle$

Example of a H-like ion initially with $Z^A=2$, transforming to one with $Z^B=1$.



In this case, $C_0 = \langle \psi_0^B | \psi_0^A \rangle = \frac{16}{27}\sqrt{2}$

Adiabatic approximation for treating Hamiltonians having a "slow" time-dependence --

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = H(t) |\Psi\rangle$$

Assume that at each t for each eigenstate n:

$$H(t)|\psi_n(t)\rangle = E_n(t)|\psi_n(t)\rangle$$

$$|\Psi\rangle = \sum_n a_n(t)|\psi_n(t)\rangle e^{-\frac{i}{\hbar}\int_0^t dt' E_n(t')}$$

If we assume that we can determine the functions $|\psi_n(t)\rangle$ and $E_n(t)$ for each t, we still need to determine the coefficients $a_n(t)$. These equations are ambiguous with respect to phase. For simplicity, we will choose $\left\langle \psi_n(t) \middle| \frac{\partial \psi_n(t)}{\partial t} \right\rangle = 0.$

$$\frac{da_m(t)}{dt} = \sum_n a_n(t) \left\langle \psi_m(t) \middle| \frac{\partial \psi_n(t)}{\partial t} \right\rangle e^{-\frac{i}{\hbar}\int_0^t (E_n(t') - E_m(t'))dt'}$$

Note that: $\left\langle \psi_m(t) \middle| \frac{\partial \psi_n(t)}{\partial t} \right\rangle (E_n(t) - E_m(t))$

$$= \langle \psi_m(t) | \frac{\partial H(t)}{\partial t} | \psi_n(t) \rangle$$