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Notes for lecture 7, 2-12-2014, PHYS 522

These notes are intended to compliment the lecture slides. So not all information from the slides is reproduced here, but the notes here include discussion and comments in class that were not a part of the slides and expounds upon some of the topics discussed in class.

1st Quiz:

What is the order of magnitude of the longest wavelength produced by an electron transitioning between states in an infinite square well? The width of the well a = 10 nm.

From solving the time independent Schrödinger equation with the potential of the infinite square well, one derives that $E_n = \frac{n^2\pi^2h^2}{2ma^2}$ where h represents h-bar and n = 1,2,3,… . Since the separation between successive energy levels of the infinite square well increase with increasing energy, we want to look at the energy difference between the states corresponding to n = 1,2. $E_{photon} = E_{n=2} - E_{n=1} = 1.81 \times 10^{-21}J = h\omega$, so the frequency $f = 2.7 \times 10^{12}HZ$ and the wave length $\lambda = 1.1 \times 10^{-4}m$.

Classical view of radiation

Radiative transition in atoms, specifically looking at the 2-level system; if two energy levels of a system are isolated "enough" then the local system can be well approximated as a 2-level system.

Dipole Oscillators

In a classical picture of radiation one can consider a dipole composed of a negative particle connected to a positive particle. The forces between them are modeled with the same mathematics as if they were connected by a spring. In this case, the dipole emits radiation at the frequency that it is oscillating at. When the dipole is driven by an incident electric field, in the form of light, the dipole will reradiate at the driving frequency. That is, the dipole will oscillate at the driving frequency once enough time has passed for the system to settle into its steady state.

The spring dipole model produces expressions for the electric permittivity of a material. This is used to calculate the dielectric constant and the refractive index, both of which are complex numbers. As in the notes, the reflection coefficient $R = \left|\frac{n-1}{n+1}\right|^2$ for complex n, therefore, the transmission coefficient is $T = 1 - R$.

Semi-classical view of radiation

Einstein Coefficients

The Einstein coefficients characterize the processes of spontaneous emission, absorption and stimulated emission for a two level system.

Spontaneous Emission:

$$\frac{dN_2}{dt} = -A_{21N_2}$$

Absorption:

$$\frac{dN_1}{dt} = -B_{12}^{\omega} N_1 u(\omega)$$

Stimulated Emission:

$$\frac{dN_2}{dt} = -B_{21}^{\omega} N_2 u(\omega)$$

$u(\omega)$ is the energy density of the electromagnetic field that is incident on the 2-level system.

If a collection of atoms are considered to interact with blackbody radiation only (associated with temperature T) and not with each other, then an expression for their steady state is $B_{12}^{\omega} N_1 u(\omega) = A_{21N_2} + B_{21}^{\omega} N_2 u(\omega)$.

The relationships between the Einstein coefficients are as follows:

$$g_1 B_{12}^{\omega} = g_2 B_{21}^{\omega}$$

$$A_{21} = \frac{h\omega^3}{\pi^2 c^3} B_{21}^{\omega}$$

g represents the degeneracy of the level of its subscript. The above equations show that having a high rate for one of these processes correlates to a higher rate for the other two processes.

Radiative Transition Rates:

The transition rate between two states due to incident electromagnetic radiation on a system is given by Fermi's Golden Rule: $W_{1\rightarrow 2} = \frac{2\pi}{h} |M_{12}|^2 g(h\omega)$ where M_{12} is a matrix element of the transition and $g(h\omega)$ is the density of states.

This is a result of casting the problem of electron radiation in an atom in terms of perturbation theory. This is a semi classical approach as we consider the quantized states of electrons interacting with a classical electromagnetic field, not a single photon. The electric field of the electromagnetic wave interacting with the electrons is seen as a perturbation. The Perturbed Hamiltonian takes on the form

$H' = e(x\mathcal{E}_x + y\mathcal{E}_y + z\mathcal{E}_z)$. The matrix value for transitioning between two states is calculated by the following calculation:

$$M_{ij} = e\mathcal{E}_k \int \psi_j^* r_k \psi_i d^3\boldsymbol{r}$$

Where k is one of x,y,z and epsilon is the amplitude of the electric field responsible for the perturbation. Because we are looking at an integral over all space, if we multiply an even and an odd function together inside the integral, then the matrix element will evaluate to zero. Since r_k is odd, if the product of the two wave functions is even, then M_{ij} will equal zero. The product of the wave functions will be even if they are either both even or both odd. Whenever the matrix element evaluates to zero, it denotes a forbidden transition between the two states considered. This analysis points at the fact that the parity of a wave function with respect to r_k must change upon an energy level transition.

Determining such transitions becomes more complicated when considering solids, as their energy structure contains continuous bands.

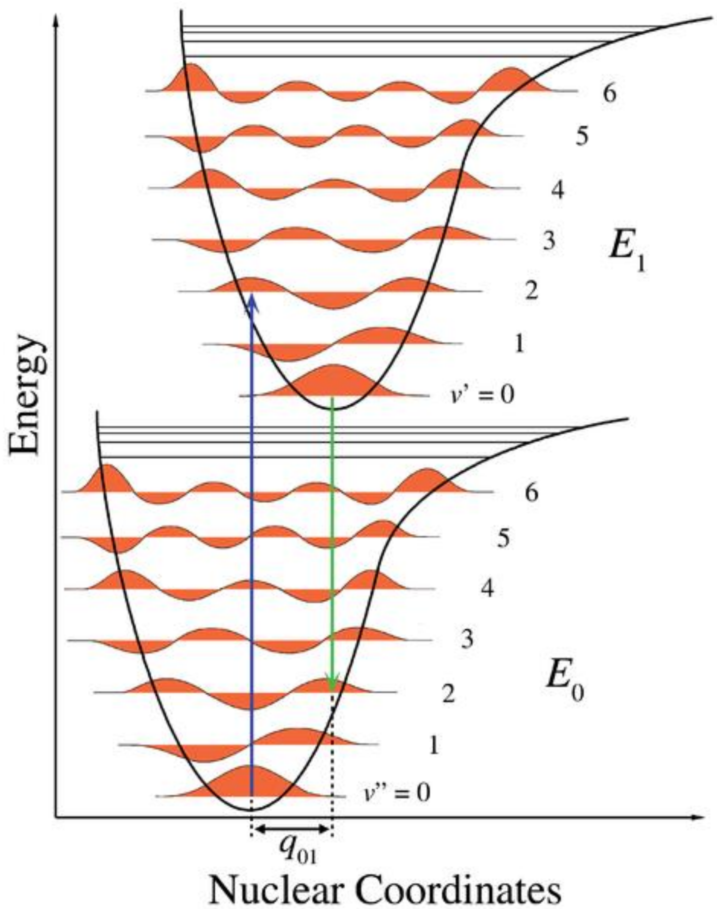
The matrix components considered above were calculated using a dipole to characterize the interaction between the driving electric field and the electrons in question. There are higher order terms that can be considered. Therefore there are pairs of states that are forbidden with respect to electron dipole transitions but can support a transition by a higher order transition.

Selection Rules

Selection rules are a set of rules that one can use to determine if a dipole transition is allowed in an atom. This allows one to determine which transitions are forbidden or allowed without calculating the transition matrix element. These rules are summarized on slide 13 and in the text book (FQ)

The term $g(h\omega)$ in Fermi's Golden Rule is the "malleable" term that can be manipulated in the lab to change the properties on a material.

Molecules and molecular solids



Consider the diagram above which depicts the energy levels of a molecule. Let the lower well be well 1 and the upper well be well 2.

Absorption:

When electrons absorb a photon and are promoted to well 2. These transitions usually start from the lowest energy level of well 1.

Fluorescence:

When electrons are in one of the energy levels in well 2, they typically transition to the lowest energy level of well 2 before transitioning down to well 1. The transition of electrons from the lowest energy of well 2 to the various states in well 1 is fluorescence.

Non-radiative transition: When an electron transitions to a lower energy level but a photon is not emitted. In such a case, the energy that would have gone into a photon goes into a different form of energy; a phonon for instance.

Jablonski Diagram

(Referring to the diagram on slide 17)

The arrows below represent the spins of the electrons in the energy levels on the Jablonski diagram.

Singlet: $\frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$

Triplet: $\uparrow\uparrow$ or $\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$ or $\downarrow\downarrow$

The triplet to singlet transition is carried out through a higher order process (it is forbidden by electric dipole transitions).

Laser Induced Fluorescence

The diagrams on slides 20-21 show the frequencies emitted during the fluorescence process. The diagrams show the intensity of the emitted light versus the quantum number of the state that the electron is transitioning to. In each diagram, the electrons are always transitioning from a given state but are transitioning to many states. On the diagram above, the electrons are transitioning from a single state in well 2 and transitioning to any of the states in well 1. As the diagram shows, there are forbidden transitions where the intensity profile goes to zero.