

Introduction to Quantum Mechanics
Prof. Manoj Kumar Harbola
Department of Physics
Indian Institute of Technology, Kanpur

Lecture – 04

Application of the correspondence principle: Einstein's A Coefficient of the harmonic oscillator and the selection rules for atomic transitions

(Refer Slide Time: 00:15)

Calculate Einstein's A coefficient
for harmonic oscillator

Classical result for rate of
radiation from an oscillating charge

$e \rightarrow a$

$$\left(\frac{dE}{dt}\right) = \frac{2}{3} \left(\frac{e^2}{4\pi\epsilon_0}\right) \frac{a^2}{c^3} \quad a = \text{acceleration}$$

$x(t) = A \cos \omega t$
 $a(t) = -\omega^2 A \cos \omega t$

$$\left(\frac{dE}{dt}\right) = \frac{2}{3} \left(\frac{e^2}{4\pi\epsilon_0}\right) \frac{A^2 \omega^4}{c^3} \cos^2 \omega t$$

What you learned in this that in this harmonic oscillator when the jumps takes place, they take place at most by 1 delta n and not more than that. Let us now use correspondence principle to calculate the A coefficient for harmonic oscillator. So, I am going to calculate Einstein's A coefficient for harmonic oscillator, for this I will use a classical result and the classical result for rate of radiation from an oscillating charge and use that result and that says classically it is rate of radiation form a charge.

Let us say this charge is e and it is accelerating with the acceleration a, a is given by the formula 2 thirds which is known as (Refer Time: 01:37) formula e square over 4 pi epsilon 0 a square over C cubed where a is the acceleration. Now for a particle that is performing a simple harmonic motion. So, if x t is given as amplitude cosine of omega t, the acceleration we know is minus omega A square a cosine of omega t, And therefore d E d t, the rate of radiation would become 2 thirds e square over 4 pi epsilon 0, A square is

the amplitude square omega raise to 4 divide by C cubed where C is the speed of light cosine square omega t.

(Refer Slide Time: 02:37)

From an oscillating charge

$$x(t) = A \cos \omega t \quad \left(\frac{dE}{dt} \right) = \frac{2}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right) \frac{\omega^4 A^2 \cos^2 \omega t}{c^3}$$

time averaged $\left(\frac{dE}{dt} \right) = \frac{1}{T} \int_0^T$

$$\left(\frac{dE}{dt} \right)_{av} = \frac{1}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right) \frac{\omega^4 A^2}{c^3}$$

Calculation of A coefficient for a harmonic oscillator

So, we have from an oscillating charge $x(t) = A \cos \omega t$ dE/dt is equal to $\frac{2}{3} \frac{e^2}{4\pi\epsilon_0} \frac{\omega^4 A^2 \cos^2 \omega t}{c^3}$. So, time averaged dE/dt which is nothing but integrate this from 0 to time period and divided by T gives you a half for cosine square omega T. So, time average dE/dt an average comes out to be $\frac{1}{3} \frac{e^2}{4\pi\epsilon_0} \frac{\omega^4 A^2}{c^3}$. This is the average rate at which a charge particle radiates the charge particle is oscillating with frequency omega radiates.

(Refer Slide Time: 04:25)

$$x(t) = A \cos \omega t$$
$$\left(\frac{dE}{dt}\right) = \frac{1}{3} \left(\frac{e^2}{4\pi\epsilon_0}\right) \frac{\omega^4 A^2}{c^3}$$

Quantum Mechanically

$$\left(\frac{dE}{dt}\right) = \left(\frac{dN}{dt}\right) h\nu$$
$$= A_{n \rightarrow n-1} h\nu$$
$$A_{n, n-1} h\nu = \left(\frac{dE}{dt}\right)_{\text{average}}$$

Quantum Mechanical quantity

Now, let us see come to calculation of A coefficient for a harmonic oscillator. So, when a harmonic oscillator is performing motion $x(t)$ equals a cosine of ωt , I have the rate of average rate of radiation is equal to $\frac{1}{3} \frac{e^2}{4\pi\epsilon_0} \omega^4 A^2 / c^3$.

Now, quantum mechanically, the rate of radiation would be the number of photons coming out from an atom. So, number of photons coming out would be nothing but dN/dt per unit time times $h\nu$; that will be the rate and this I know is nothing but $A_{n \rightarrow n-1} h\nu$. So, $A_{n \rightarrow n-1} h\nu$ is equal to dE/dt average. This I should remind you is a quantum mechanical quantity A coefficient because $A_{n, n-1}$ gives you the probability through which the x state decays and with that multiplied by $h\nu$ gives you the rate in the large n limit by correspondence principle the 2 result should match.

(Refer Slide Time: 06:22)

In the large 'n' limit (by correspondence principle)

$$h\nu A_{n,n-1} = \frac{1}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right) \frac{\omega^4 A^2}{c^3}$$

For large n $\underline{n h \nu} = \frac{1}{2} k A^2$ Classical result

Q.Mech

$$A^2 = \frac{2 n h \nu}{k} = \frac{2 n h \nu}{m \omega^2}$$

$$= \frac{2 n h \omega}{2 \pi m \omega^2}$$

$$A^2 = \frac{n h \omega}{\pi m \omega^2} = \left(\frac{n h}{\pi m \omega} \right)$$

So, $h \nu A_{n, n-1}$ should be equal to $\frac{1}{3} \frac{e^2}{4 \pi \epsilon_0} \frac{\omega^4 A^2}{c^3}$ and then hopefully whatever a $n, n-1$, I calculate here that will be true in the lower limit also.

So, this is where I am using the correspondence principle. Now how do I calculate the amplitude? Now for large n or small n the energy is $n h \nu$ and if it is large n , I can write this as $\frac{1}{2} k A^2$ that is energy classically. So, on the left hand side, I am using a quantum mechanical result, on the right hand side, I am using the classical result. Similarly in the equation above, this is a quantum mechanical result and this is a classical result. So, I can write these arrows here also.

Because in the left hand side, the mechanism through probability on the right hand side; it is through an accelerating charge giving out radiation in any guess, I can now calculate the amplitude A^2 is equal to $\frac{2 n h \nu}{k}$ which is nothing but $\frac{2 n h \nu}{m \omega^2}$. It changes to ω against $\frac{2 n h \omega}{2 \pi m \omega^2}$ and therefore, I can write the amplitude square as $\frac{n h \omega}{\pi m \omega^2}$ which is $\frac{n h}{\pi m \omega}$ plus A^2 value and now I am going to substitute that A^2 value in the expression for $h \nu A_{n, n-1}$.

(Refer Slide Time: 08:55)

The image shows a handwritten derivation of the Einstein A coefficient for a dipole transition. The derivation starts with the expression for the energy flux from an oscillating dipole, $\hbar \nu A_{n, n-1} = \frac{1}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right) \frac{\omega^4 A^2}{c^3}$. This is then equated to the energy of the photon, $\hbar \nu$, multiplied by the transition rate $A_{n, n-1}$, which is $\frac{1}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right) \frac{\omega^4 \omega^3}{c^3} \cdot \frac{\hbar}{\pi m \omega}$. The \hbar terms cancel, and the ω terms are simplified to $\frac{1}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right) \frac{\omega^3}{c^3} \cdot \frac{n}{\pi m \omega}$. This is further simplified to $\left[\frac{2}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right) \frac{\omega^2}{m c^3} \right] n$. The final result is boxed: $A_{n, n-1} = \left[\frac{2}{3} \left(\frac{e^2}{4\pi\epsilon_0} \right) \frac{\omega^2}{m c^3} \right] n$.

So, if you do that I have $\hbar \nu A_{n, n-1}$ is equal to $\frac{1}{3} \frac{e^2}{4\pi\epsilon_0} \frac{\omega^4 A^2}{c^3}$.

A square over C cubed and which is equal to $\frac{1}{3} \frac{C^2}{4\pi\epsilon_0} \frac{\omega^4}{C^3}$ and I just calculated the value of a square which is nothing but $\frac{\hbar}{\pi m \omega}$. Now I can cancel terms on both 2 sides is \hbar cancels. So, notice how beautifully, I have actually converted a classical formula for amplitude to a quantum mechanical quantity $n \hbar$ cross energy.

So, I get $A_{n, n-1}$ is equal to and here, I can cancel this ω to ω^3 is equal to $\frac{1}{3} \frac{e^2}{4\pi\epsilon_0} \frac{\omega^3}{C^3} \frac{n}{\pi m \omega}$ again substitute ν for ω , I get $\frac{1}{3} \frac{e^2}{4\pi\epsilon_0} \frac{\omega^3}{C^3} \frac{n}{\pi m \omega}$ over C^3 times n over $\pi m \omega$ over 2π which gives me $\frac{2}{3} \frac{e^2}{4\pi\epsilon_0} \frac{\omega^2}{m C^3} n$.

So, the Einstein's A coefficient $A_{n, n-1}$ is this $\frac{2}{3} \frac{e^2}{4\pi\epsilon_0} \frac{\omega^2}{m C^3} n$. This is $\omega^2 \omega^2$. So, $A_{n, n-1}$ is $\frac{2}{3} \frac{e^2}{4\pi\epsilon_0} \frac{\omega^2}{m C^3} n$ and this is a formula which is given purely in terms of the frequency of the oscillator the n index for the level form is the transition is taking place.

So, this is the formula which is quantum mechanical, we have used correspondence principle, in this we have mix rates of we know transition in classical, the regime to what would happen in the quantum regime, where it is given by the Einstein's A coefficient and using that wave found the formula. Similarly, we can apply to other places also and one of those, I will give you as an assignment problem finally; I also like to tell you about selection rules.

(Refer Slide Time: 11:53)

Selection rule for transition in atoms

$$x = R \cos \phi$$

$$= \frac{R(e^{i\omega t} + e^{-i\omega t})}{2}$$

$$y(t) = R \sin \phi$$

$$= \frac{R(e^{i\omega t} - e^{-i\omega t})}{2i}$$

$\omega =$ frequency of revolution

Quantum mechanically $n \rightarrow n - \tau$ (large n limit) $(\tau \omega_n)$

For consistency with Correspondence principle $\tau = 1$

In fact, one selection rule for transition in atoms; in atoms I take the simplified version where the board orbits are there and particles are moving in circular orbits when the particles are moving in a circular orbits, x is the radius times cosine of ϕ which is $R \cos \phi$ and y is equal to $R \sin \phi$ which is equal to $R \frac{e^{i\omega t} + e^{-i\omega t}}{2}$ and y is equal to $R \frac{e^{i\omega t} - e^{-i\omega t}}{2i}$ where ω is the frequency revolution.

Notice again that there is only one frequency that exists quantum mechanically, when the transition takes place from n to $n - \tau$ in the large n limit, the frequency that can exist is $\tau \omega_n$, where as classically we see only one radiation frequency existing and that is the frequency of revolution and there for this implies for consistency which correspondence principle, I should have $\tau = 1$, it can be either from one up or one down, but the change can be maximum one.

(Refer Slide Time: 14:00)

n represent the angular momentum
 $mvr = n h$
 $= l h$

$\Delta l = \pm 1$

Selection rule

$n \rightarrow$ No restriction
 $l \rightarrow \pm 1$
 $m_l \rightarrow \pm 1$

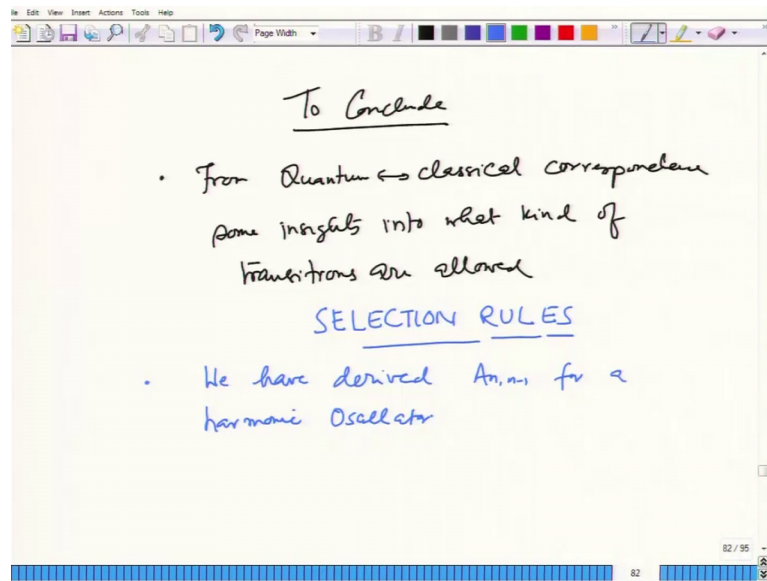
$y = R \sin \phi$
 $x = R \cos \phi$

$\Delta l = \pm 1$ transition will give circularly polarized light

And therefore now remember when we have Bohr orbits, what does n represent; n represents the angular momentum through the condition that mvr is equal to $n h$ and this implies that this n that quantum number that gives you the angular momentum which is Sommerfeld case, we called $l h$ and the change of l can be maximum Δl can be plus or minus 1, if higher l changes were allowed in the classical regime, I would not see the fundamental frequency out, see harmonics which are not seen what I see classically is the only one frequency of radiation and that is the frequency at which particle is rotating. And therefore, maximum Δl can be 1. So, this is another selection rule. Now remember from the old quantum theory I had n, l, m_l or m_z quantum numbers. So, what we found is l plus minus 1 is allowed. In fact, when you do the more recursive this is also comes out to be plus minus 1. However, there are more restrictions on n .

But the idea want to do give rather than just deriving these is that true correspondence principle, you can get some inside into what is allowed; what is not allowed; not only that you see one more thing when a particle is moving in a circle, in this manner that x is some radius cosine ϕ and y is some radius sin ϕ , then the radiation will be given out there will be given out will be circular polarized. So, we can say also by correspondence Δl equals plus minus 1 transition will give circularly polarized light.

(Refer Slide Time: 16:23)



So, to conclude this lecture what we have done is we found from quantum classical correspondence some insights into what kind of transitions are allowed enough given a term to this selection rules and the important particle in spectroscopy and to we have derived $A_{n, n-1}$ for a harmonic oscillator, you know ask why $A_{n, n-1}$ why not $A_{n, n-2}$ that is because $A_{n, n-2}$ represent transition from $n-2$ level and change of n by 2 is not allowed harmonic oscillators.

So, only nonzero points are $A_{n, n-1}$ or $A_{n, n+1}$ also recall from the lecture Einstein's A and B coefficients once you know the a coefficient, you can also calculate the B coefficient that is the coefficient for stimulated emission or absorption.

Thank you.