

Full Length Research Paper

Atom-field interaction, hydrogen atom and nature of detuningR. Bora Bordoloi^{1*}, R. Bordoloi² and G. D.Baruah²¹Department of Physics, Namrup College, Namrup – 786623, Assam, India.²Center for Laser and Optical Science, New Uchamati, Doom Dooma-786151 India.

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The nature of detuning in transition probabilities in atom field interaction has been investigated in the light of hydrogen atom problem. It has been shown that the detuning bears a striking similarity with the principal quantum number n in hydrogen atom.

Key words: Induced resonant transition, detuning, hydrogen atom.

INTRODUCTION

Hydrogen atom problem is a well known and simple example of a quantum mechanical system. The solution of the hydrogen atom problem, which gives rise to *principal quantum numbers* and from which we get the energy level diagrams are the basis of all atomic structures (Jenkins and White, 1981). The present investigation is related to the nature of time evolution of the transition probabilities of the interacting two level atoms with a coherent resonant radiation field (Sargent et al., 1974). We have shown that the detuning controlled transition probabilities exhibit a striking similarity with that of the principal quantum number controlled atomic energy level spacing.

HYDROGEN ATOM

In the absence of external forces the classical energy of an electron bound by its negative charge to the positively charged nucleus is given by:

$$H = \frac{p^2}{2m} - \frac{e^2}{r} \quad (1)$$

Where p , m , e and r have their usual meanings.

The time development of the wave function is determined by the Schrodinger equation.

$$i\hbar\psi(\vec{r}, t) = H(\vec{r}, \vec{p})\psi(\vec{r}, t) \quad (2)$$

The Hamiltonian is usually given by classical energy, in which the measurable quantities such as position and momentum are replaced by appropriate operators. The stationary solutions $\psi_n(\vec{r}, t)$ of the Schrodinger equation are those for which the time dependence can be separated from the space dependence, that, is for which

$$\psi_n(\vec{r}, t) = u_n(\vec{r}) \exp(-i\omega_n t) \quad (3)$$

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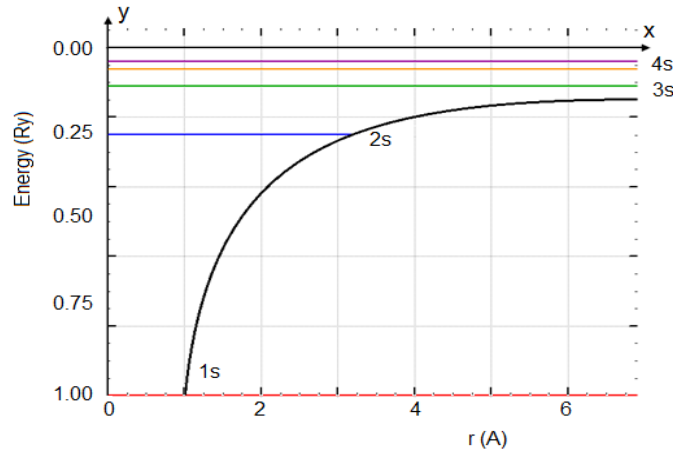


Figure 1. Energy level diagram for hydrogen atom. Horizontal lines indicate energy levels given by Equation (10).

Here ω_n is a circular frequency. Substituting Equation (3) into (2) we find the time-dependent equation

$$H(\vec{r}, \vec{p})u_n(\vec{r}) = \hbar\omega_n u_n(\vec{r}) \tag{4}$$

This is an eigen value equation for the Hamiltonian $H(\vec{r}, \vec{p})$ with eigen functions $u_n(\vec{r})$ and eigen value $\hbar\omega_n$. The eigen value Equation (4) must be solved for hydrogen atom and then we have

$$\left(\frac{\hbar^2 \nabla^2}{2m} - \frac{e^2}{r} \right) u(r) = \hbar\omega u(r) \tag{5}$$

Here it is advantageous to express ∇^2 in spherical coordinates, r , and ϕ , because of the spherical symmetry of the potential energy $\left(-\frac{e^2}{r} \right)$. The Equation (4) can be

separated into three equations, each containing a single spherical coordinate. The solutions of the equations correspond to discrete energies, as for the bound problems and have the values

$$u_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{lm}(\theta, \phi) \tag{6}$$

Here the $R_{nl}(r)$ are the Laguerre polynomials multiplied by the exponential factor $\exp(-r/na_0)$, $a_0 = 0.53 \text{ \AA}$ is the Bohr radius, and $Y_{lm}(\theta, \phi)$ are spherical harmonics. In particular first few $u_{nlm}(r, \theta, \phi)$ are as follows:

$$u_{100}(r, \theta, \phi) = (\pi a_0^3)^{-1/2} \exp(-r/a_0) \tag{7}$$

$$u_{200}(r, \theta, \phi) = (32\pi a_0^3)^{-1/2} (2 - r/a_0) \exp(-r/2a_0) \tag{8}$$

$$u_{210}(r, \theta, \phi) = (32\pi a_0^3)^{-1/2} (r/a_0) \cos \theta \exp(-r/2a_0) \tag{9}$$

The corresponding energies are given by

$$\hbar\omega_{nlm} = \hbar\omega_n = \frac{e^2}{2a_0 n^2} \tag{10}$$

Which are discrete, Figure 1 shows the energy level diagram for hydrogen atom worked out with the help of Equation (10).

INDUCED RESONANT TRANSITIONS

Let us now consider our important problem of induced resonant transitions. Specifically consider the hydrogen atom initially in the ground state u_{100} . At time $t=0$ we apply an oscillating electric field (Sargent et al., 1974).

$$E(t) = \hat{x} E_0 \cos vt \tag{11}$$

Where

$$v \cong (E_2 - E_1) / \hbar \tag{12}$$

Here \mathcal{V} is in radian/sec (not Hertz). The oscillating electric field is nearly resonant with the transitions from $n=1$ to $n=2$. From Figure 2 one can infer that the states u_{nlm} with

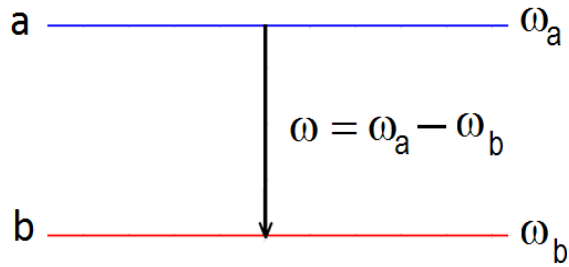


Figure 2. Diagram depicting two energy levels a and b of the unperturbed Hamiltonian.

$n > 2$ are way off resonance with the field incident and therefore can be neglected. Hence we can describe the atom by two level wave function given by:

$$\psi(\vec{r}, t) = C_a u_a(\vec{r}) \exp(-i\omega_a t) + C_b u_b(\vec{r}) \exp(-i\omega_b t) \quad (13)$$

And take the eigen functions

$$u_a = u_{210}$$

$$u_b = u_{100}$$

The coefficients in Equation (13) satisfy the normalization condition

$$|C_a|^2 + |C_b|^2 = 1 \quad (14)$$

The equations of motion for C_a and C_b are given by

$$\dot{C}_a = \frac{1}{2} i \wp \frac{E_0}{\hbar} \{ \exp[i(\omega - \nu)t] + \exp[i(\omega + \nu)t] \} C_b \quad (15)$$

$$\dot{C}_b = \frac{1}{2} i \wp \frac{E_0}{\hbar} \{ \exp[-i(\omega - \nu)t] + \exp[-i(\omega + \nu)t] \} C_a \quad (16)$$

Where the frequency

$$\omega = \omega_a - \omega_b \quad (17)$$

As shown in Figure 2.

Let us now suppose that the system is in the ground state at time $t=0$, that is, $C_a(0) = 0$ and $C_b(0) = 1$, the equation of motion become

$$\dot{C}_b = 0 \quad (18)$$

and

$$\dot{C}_a(0) = \frac{1}{2} i \wp \frac{E_0}{\hbar} \{ \exp[i(\omega - \nu)t] + \exp[i(\omega + \nu)t] \} \quad (19)$$

This yield

$$C_a^{(n)}(t) = \frac{1}{2} \wp \frac{E_0}{\hbar} \left[\frac{\exp\{i(\omega - \nu)t\} - 1}{\omega - \nu} + \frac{\exp\{i(\omega + \nu)t\} - 1}{\omega + \nu} \right] \quad (20)$$

For optical frequencies the denominator $\omega + \nu$ is very large ($\omega \gg 1$) and therefore the second term in R.H.S. is neglected with respect to the first since at resonance $\omega \cong \nu$. This is called Rotating Wave Approximation (RWA). Thus neglecting the perturbing matrix element is given by:

$$\begin{aligned} V_{ab} &= -\wp E_0 \cos \nu t = -\wp E_0 \frac{\exp(i\nu t) + \exp(-i\nu t)}{2} \quad (21) \\ &= -\frac{1}{2} \wp E_0 \exp(-i\nu t) = V_{ba} \end{aligned}$$

Therefore the equations of motion for C_a and C_b under rotating wave approximation become

$$\dot{C}_a = \frac{1}{2} i \wp \frac{E_0}{\hbar} \exp[i(\omega - \nu)t] C_b \quad (22)$$

$$\dot{C}_b = \frac{1}{2} i \wp \frac{E_0}{\hbar} \exp[-i(\omega - \nu)t] C_a \quad (23)$$

thus

$$C_a(t) = \frac{1}{2} \frac{\wp E_0}{\hbar} \frac{1}{\omega - \nu} \exp \frac{i(\omega - \nu)t}{2} 2i \sin \frac{(\omega - \nu)t}{2} \quad (24)$$

Thus the probability (Allen and Eberly, 1975) of finding the atom in the upper state is given by

$$|C_a(t)|^2 = C_a(t) C_a(t)^* = \left(\frac{\wp E_0}{2\hbar} \right)^2 \frac{\sin^2 [(\omega - \nu)t / 2]}{[(\omega - \nu)t / 2]^2} \quad (25)$$

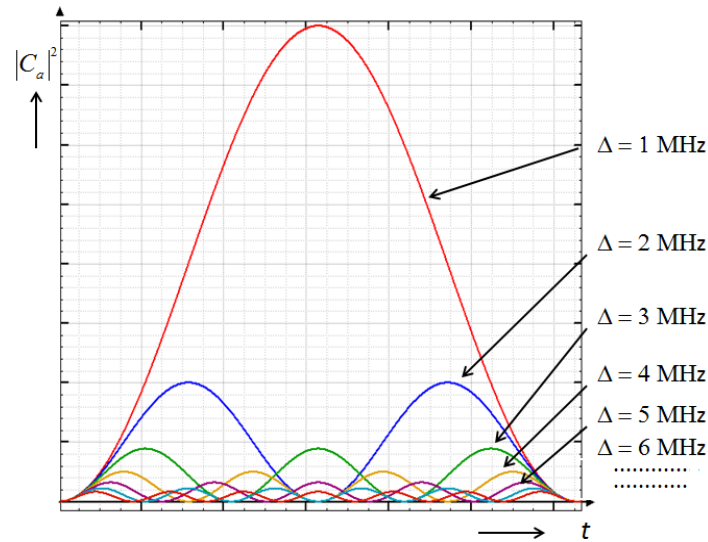


Figure 3. The probability of a transition to an upper level under the influence of an applied electric field.

This is known as stimulated absorption. We could have chosen $C_a(0) = 1$ and $C_b(0) = 0$, which shows that the atom is initially in the upper state and calculate the probability of stimulated emission. We find in this also the same formula as given by Equation (25). The probability is plotted in Figure 3.

NATURE OF DETUNING

From what has been discussed in the earlier sections it is now appropriate to describe the nature of detuning, $\Delta\omega = \omega - \nu$. Here ω is the atomic line center frequency and ν is the laser oscillation frequency in radian/sec. As ν increases (or decreases) from the atomic line center frequency ω , the atomic system goes away from resonance. In Figure 3 we have depicted the transition probabilities versus time at different values of detuning. The salient feature of this figure is that if we draw horizontal lines joining the maxima of the transition probabilities for detunings corresponding to integral values of $\Delta\omega$ we obtain a series of horizontal lines with relative separations, the reverse of which shows striking similarity with the Energy level diagram of the Hydrogen atom.

Figure 4a indicates the horizontal lines thus generated in a reverse way. Figure 4b shows the corresponding energy levels for hydrogen atom as illustrated in Figure 1. The energy level separation of hydrogen atom goes on decreasing as principal quantum number n increases up to ionization limit. This is also observed in Figure 4a, where it is seen that as detuning increases the relative separation decreases. At higher values of detuning the

separation of the horizontal lines become extremely small, this is quite similar to the energy levels of hydrogen atom near ionization limit. It is reasonable to explore the physical consequences of the similarity as describe above. The energy level diagram in hydrogen atom is drawn according to energy in Rydberg (Ry). Likewise the horizontal lines in Figure 4a are arranged according to frequency (in Mz). We must note here that the transition probability $|C_a(t)|^2$ or $|C_b(t)|^2$ was worked out on the basis of a two body problem or a two level atom. At time $t = 0$ we applied an electric field which is resonant (or nearly resonant) with the transition from $n = 1$ to $n = 2$. Our work is based on the idea that the detuning has a range of values corresponding to 1, 2, 3...etc (in Mz). It is a matter of common experience that the spectral lines (cm^{-1}) corresponding to a particular series (say Balmer series) is precisely obtained by manipulating the principal quantum number n . Thus the transition probabilities at different values of detuning are the manifestation of an atomic structure in general. This observation is expected to draw light in laser physics particularly in atom field interaction. In this connection it is appropriate to recall the statements by Jenkins and White (1981) who indicates the importance of the horizontal lines as energy levels. According to them the importance of this type of diagram is two fold: (1) regardless of the atomic model presented, whether it is an orbital model or any other yet to be proposed in the future, like a quantum mechanical wave model, it represents with high degree of precession the stationary energy states of atom; and (2) it represents the well established law of conservation of energy as applied through Bohr's third postulate. We thus reasonably conclude that our work concerning the

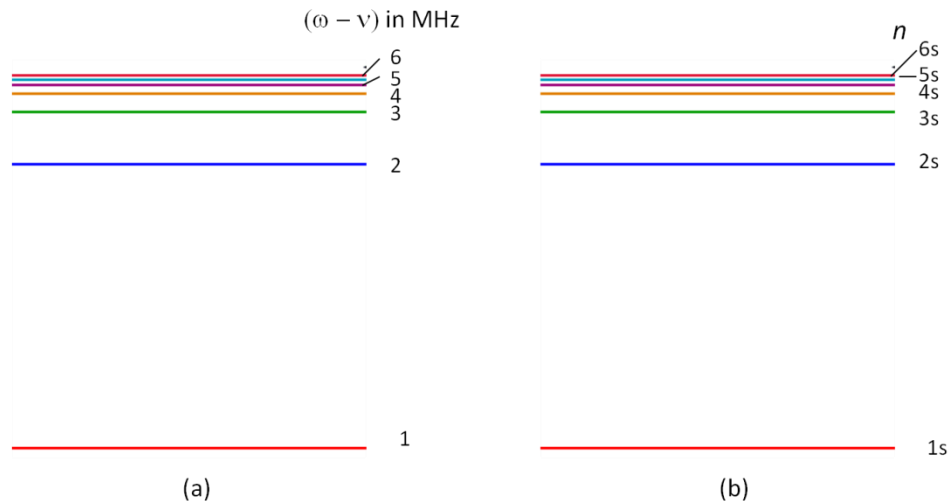


Figure 4. (a) Relative separations of the horizontal lines generated by joining the maxima of the transition probabilities at different detuning (b) Energy levels of hydrogen atom showing relative separations of the principal quantum numbers.

horizontal lines drawn by joining the maxima of the transition probabilities at different values of detuning ($\omega - \nu = 1, 2, 3, \dots$) only justifies the energy level diagram scheme being introduced more than hundred years ago.

CONCLUSION

In the present work it has been shown that the so called detuning ($(\omega - \nu)$) bear a striking similarity with the principal quantum number “ n ” and hydrogen atom. We reasonably conclude that in the present work concerning the horizontal lines joining the maxima of transition probabilities at different values of detuning ($(\omega - \nu = 1, 2, 3, \dots)$) only justifies the energy level diagram scheme being introduced more than hundred years ago.

Conflict of Interest

The authors have not declared any conflict of interest.

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