The Quantum Dynamics of Lasing

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Abstract

The quantum mechanics underlying the operation of the laser¹ are developed. An analysis of the atom - radiation interaction is presented in three ways: First, following Einstein's initial proto-quantum mechanical reasoning about a gas radiation system, the existence of stimulated emission is demonstrated, and key relations between transition rate coefficients are derived. Second, a semiclassical quantum mechanical derivation of Einstein's result is given, revealing interesting properties of the atom - radiation interaction. Finally, the second quantization of the atomic Hamiltonian is performed, giving a full quantum mechanical description of atomic transitions in a quantized radiation field. The final formulation of the system reveals the properties of stimulated emission that allow lasing as we know it.

1 Introduction

The laser is an amazing technological achievement of quantum mechanics. It is probably the flashiest direct macroscopic demonstration of a quantum mechanical process. Anyone can appreciate the remarkable physical characteristics that lasers can achieve: high emission coherence, monochromatic emission, miniscule beam divergence, extremely short pulses, tunable emission frequency, etc. Lasers have found their way into a multitude of scientific, industrial, and popular applications, including interferometry measurement, frequency calibration, ultrashort light pulse generation, fluorophore excitation, exertion of nano-scale force on nano-scale elements, precision etching and cutting, and even inertial fusion ignition! The special properties of the

¹laser = Light Amplification by Stimulated Emission of Radiation

laser are a result of the peculiar physics of stimulated emission, which is a very nonclassical phenomenon. I hope to make the basic quantum mechanics of stimulated emission (and therefore the laser) accessible at the undergraduate level of physics. My goal here is to present the development of the quantum theory of lasing and optical pumping, and demonstrate some of the elementary lasing applications of this theory.

This paper is loosely organized according to the historical development of the theory of lasing, because that development is a convenient and interesting way to present the quantum theory. The theory of the laser began with Einstein's mostly classical approach to atom-radiation interaction; after Schrödinger and Heisenberg, a quantum mechanical description for Einstein's processes became available. Eventually, with the advent of quantum electrodynamics, everything, including the radiation field, could be fully described by quantum mechanics. Only at this last step is the theory underlying the essential coherent amplification property of stimulated emission available.

2 The laser

I begin by briefly presenting the basic idea behind laser technology, so that the following physics is presented in the context of a real system. Refer to Figure 1 for a diagram. A simple laser consists of a cavity filled with a lasing medium and bounded by mirrors at opposite ends. One of these mirrors is completely reflective, the other is partially reflective. The lasing medium is chosen such that, at the energies of interest, there are only three excitable states, named the 'reservoir' state, state 0, and state 1, in order of increasing energy (lasers generally have more than three levels, but the concept is the same). Furthermore, a source of light with energy equal to $E_1 - E_{res}$ is applied to the lasing medium. The result is that the population of state 1 in the medium is artificially 'pumped' up above the thermal equilibrium population. The pumped atoms may then be stimulated to relax by radiation with energy $E_1 - E_0$.

As we will discuss, an amazing property of the resulting emitted radiation (from process 3 in Figure 1) is that it is emitted with exactly the same phase, frequency, and direction as the stimulating radiation! With sufficient pumping, this stimulated process will amplify in the laser cavity as the emitted radiation reflects back and forth between the mirrors. Since one of the mirrors is only partially silvered, the laser cavity emits a beam which is monochromatic, coherent, and directional - a laser beam is born.



Figure 1: The basic schematic of a laser is shown here. The callout box contains an energy diagram of five of the most important atomic transition processes within the laser cavity. Process 1 is spontaneous emission from 1 to 0. Process 2 is absorption moving from 0 to 1. Process 3 is stimulated emission from 1 to 0. Process 4 is spontaneous emission from 0 to the reservoir state. Process 5 is absorption of the pumping radiation moving atoms from the reservoir state to 1.

3 The proto-quantum theory of lasing

In 1917, Albert Einstein published a paper in Physika Zeitschrift, a leading European physical journal at the time, entitled 'Zur Quantentheorie der Strahlung', translated as 'On the Quantum Theory of Radiation' [1]. At the time of publication, the quantum mechanics of atomic spectra was yet in its infancy, and Einstein's own paper on the photoelectric effect had only recently provided evidence of the quantization of light. Quantum electrodynamics was not yet on the horizon. Einstein's paper approaches the interaction between an atomic gas and a radiation field by dealing mainly with the simplified situation in which the atoms in the gas have two relevant electronic levels; i.e. only two levels with significant thermal excitation. Einstein's goal was to determine the dynamics of the populations of the two levels under the influence of the atom-radiation interaction. He therefore sought to determine the transition rates between the energy levels in the gas. The determination of those rates goes something as follows (following Loudon [5]): Consider a gas of N atoms contained in a blackbody cavity. Throughout we will assume the gas is homogeneous and that the radiation field is isotropic and homogeneous. Let the energies of the two electronic levels in the atoms be E_0 and E_1 ($E_0 < E_1$), with corresponding degeneracy numbers d_0 and d_1 . Let the number of atoms with energy E_0 be N_0 , and the number in the excited state be N_1 . These two populations are of course governed by the conservation law

$$N_0 + N_1 = N \tag{1}$$

where we will assume the system is closed, and therefore N is constant. An electronic transition in one atom between the two levels must result in the absorption or emission of a photon with energy $E_{\gamma} = E_1 - E_0 = \hbar \omega$, where ω is the angular frequency of the absorbed or emitted radiation. I will denote the transition rate from state 0 to state 1, or the absorption rate, as R_{01} , and the rate from 1 to 0, or the emission rate, as R_{10} . It is simple to write the rate equation for the atomic level populations using these transition rates

$$\frac{dN_0}{dt} = -\frac{dN_1}{dt} = R_{10}N_1 - R_{01}N_0 \tag{2}$$

In general, we should assume that the transition rates may depend on the energy density of the radiation at the transition frequency ω , denoted $u(\omega)$. Indeed, the absorption transition can only occur via absorption of a photon of energy $\hbar\omega$; it is reasonable to expect that the transition rate would depend on $u(\omega)$. I will therefore decompose the rates into two sets of rate coefficients: spontaneous rate coefficients, a_{ij} , and stimulated rate coefficients b_{ij}^{ω} such that

$$R_{ij} = a_{ij} + b_{ij}^{\omega} u(\omega) \tag{3}$$

I use the superscript ω solely to remind the reader of the differing units of the coefficients. It is clear from energy conservation that $a_{01} = 0$, since in the absence of electromagnetic energy at the transition frequency $(u(\omega) = 0)$ there can be no absorption and no transition from 0 to 1. The coefficient b_{10}^{ω} will eventually be the most interesting quantity in this set, as it is not intuitively obvious that the radiation field should affect R_{10} , the transition rate from 1 to 0. The transition process represented by the rate coefficient b_{10}^{ω} is known as 'stimulated emission', since it represents emission that is triggered by incident radiation; perhaps the reader will not be shocked by this development given the contents of the acronym 'laser'.

The rate a_{10} is known as the 'spontaneous emission' rate, since it is the rate of transition down from 1 to 0 in the absence of radiative interaction. The *a* and *b* coefficients (commonly capitalized in literature) are known as the Einstein coefficients, as they were originally identified and determined in his 1917 paper. Substituting the coefficients defined in (3) into the rate equation (2)

$$\frac{dN_1}{dt} = a_{10}N_1 + b_{10}^{\omega}u(\omega)N_1 - b_{01}^{\omega}u(\omega)N_0$$
(4)

where we have again set $a_{01} = 0$. If our atomic level populations are in equilibrium the individual populations are constant

$$\frac{dN_1}{dt} = 0 = a_{10}N_1 + b_{10}^{\omega}u(\omega)N_1 - b_{01}^{\omega}u(\omega)N_0$$
(5)

This seemingly innocent equilibrium expression suddenly allows us to solve for the energy density as a function of our four (three) rate coefficients and two populations

$$u(\omega) = \frac{a_{10}N_1}{b_{01}^{\omega}N_0 - b_{10}^{\omega}N_1} \tag{6}$$

According to Maxwell-Boltzmann statistics, the ratio of populations is

$$\frac{N_0}{N_1} = \frac{d_0}{d_1} \frac{e^{\frac{-E_0}{k_B T}}}{e^{\frac{-E_1}{k_B T}}} = \frac{d_0}{d_1} e^{\frac{E_1 - E_0}{k_B T}} = \frac{d_0}{d_1} e^{\frac{\hbar\omega}{k_B T}}$$
(7)

where k_B is the Boltzmann constant and T is the gas temperature, and d_i is again the degeneracy of the i^{th} state. We can then rewrite (6) and substitute the Boltzmann relation in (7):

$$u(\omega) = \frac{a_{10}}{b_{10}^{\omega}} \frac{1}{\frac{d_0 b_{01}^{\omega}}{d_1 b_{10}^{\omega}}} e^{\frac{\hbar\omega}{k_B T}} - 1$$
(8)

If the reader recalls Planck's formula for the energy density of blackbody radiation $u(\omega)$, (8) may look extremely suggestive. Planck's formula is

$$u(\omega) = \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$
(9)

In fact, to preserve physical consistency these two expressions must be the same for all values of T and ω . If they are to be equal, it must be true that

$$\frac{a_{10}}{b_{10}^{\omega}} = \frac{\hbar\omega^3}{\pi^2 c^3}$$
(10)

and

$$\frac{b_{01}^{\omega}d_0}{b_{10}^{\omega}d_1} = 1 \tag{11}$$

We should pause for a moment and consider the extraordinary implications of these relations. Equations (10) and (11) in no uncertain terms demand that there be a transition process which is stimulated by radiation! Otherwise b_{10}^{ω} would be identically zero. Einstein discovered this process theoretically via the above reasoning without knowledge of the mechanism behind it. We will find that mechanism later by invoking a full quantum mechanical theory. We have derived these relations between the four rate coefficients based on Planck's blackbody law, Maxwell-Boltzmann statistics, and some reasoning based on energy and mass conservation in a closed system in equilibrium. Notice that except for a_{01} , all the coefficients must be non-zero, and that for the non-degenerate case ($d_0 = d_1 = 1$), $b_{10}^{\omega} = b_{01}^{\omega}$. Einstein recognized that the nature of stimulated emission evoked the idea of radiative amplification. However, because of the latter equality, there must be a population inversion - a situation in which $N_1 > N_0$ - for amplification to occur. That population inversion is achieved in lasers via the pumping technique described in Section 2.

Note that the linear dependence of the rate on $u(\omega)$ was weakly motivated in (3). However, in retrospect, based on the reasoning from (8) to (11), it is clear that a nonzero higher order dependence of R_{ij} on $u(\omega)$ would not allow the correspondence with Planck's formula. The linearity of the dependence will also be seen to arise naturally from the quantum mechanics of transition in Section 4. It is remarkable that we have advanced thus far into the physics of atom-radiation interaction with only the simplest invocation of quantum theory - the quantization of the atomic spectrum. In fact, the reader might feel, as I did, that the whole derivation was somewhat 'tricky'. In a way, it was a trick, albeit an extremely clever and successful one! The calculations above depend mostly on phenomenological relations; they are constructed to match experimental results, with little reference to an underlying mechanism. This is because, at the time, there was no known mechanism - it was a decade before Heisenberg and Schrödinger formulated quantum mechanics as we know it. The really fantastic property of stimulated emission which enables laser technology is the coherent directional property of stimulated emission radiation. The derivation of this property requires the quantum electrodynamics which will be presented in Section 5.

4 The semiclassical theory of lasing

I will now derive the quantum mechanical mechanism of atomic transition using the method of time dependent perturbation approximation. I thereby hope to confirm Einstein's determination of transition rates quantum mechanically, and perhaps gain more insight into the dynamics of the system. As the section title indicates, we still will not achieve a full quantum theory; I will employ a quantum mechanical description of the electronic levels, but an entirely classical one of the radiation fields. Given a system governed by a time dependent Hamiltonian, the transition probability for the system to begin in the state $|m\rangle$ and move to the state $|n\rangle$ at time t is given by

$$P_{mn}(t) = |c_n(t)|^2$$
(12)

where $c_n(t)$ is the complex probability amplitude of $|n\rangle$ in the atomic state $|\psi(t)\rangle$. In this derivation, I will start by considering a general system with k basis states, since lasing systems always involve at least three states. However, at important junctions, I will show how the special two-state case relates to Einstein's system.Following Griffiths [2] and Sakurai [3], in Dirac notation, the Schrödinger equation gives the time evolution of an unperturbed general state

$$|\psi(t)\rangle = \sum_{n=0}^{k} c_n e^{-iE_n t/\hbar} |n\rangle$$
(13)

The numbered states $|n\rangle$ are the energy eigenstates of \hat{H}^0 , the unperturbed Hamiltonian. We will consider the effect of a small perturbing Hamiltonian \hat{H}^1 . Eventually, we will analyze the problem for a perturbation of the form of a classical electromagnetic wave, but for now, \hat{H}^1 will be general. The full Hamiltonian is the sum

$$\hat{H} = \hat{H}^0 + \hat{H}^1 \tag{14}$$

We define $\frac{d}{dt}\hat{H}^0 = 0$ and $\frac{d}{dt}\hat{H}^1 \neq 0$. Unlike the unperturbed case, we will consider a set of $c_n(t)$ which are not necessarily constant. This variation will account for the perturbation of the system. The time dependent Schrödinger equation is

$$i\hbar \frac{d}{dt} |\psi\rangle = \hat{H} |\psi\rangle \tag{15}$$

We can substitute the eigenstate expansion in (13) with perturbed coefficients $c_n(t)$ into the Schrödinger equation from (15). Taking the inner product throughout with

 $\langle m |$, we have

$$\dot{c}_m = \sum_{n=0}^k -\frac{i}{\hbar} \langle m | \hat{H}^1 | n \rangle e^{-i(E_n - E_m)t/\hbar} c_n \tag{16}$$

This becomes more concise using matrix notation and with the transition energy expressed as $E_n - E_m = \hbar \omega_0$

$$\dot{c}_m = \sum_{n=0}^k -\frac{i}{\hbar} H_{mn}^1 e^{-i\omega_0 t} c_n$$
(17)

This is a very interesting result: (17) is a coupled linear differential set of equations in k+1 variables. To solve them we will use the initial values $c_n(0)$ in the differential equations (17) (this is the first order perturbation approximation), then integrate the equations. That will allow us to find the transition probability between two states $P_{mn}(t)$. That integration depends on the explicit form of the perturbation Hamiltonian \hat{H}^1 and the initial conditions. Therefore, we will pause to define the circumstances of interest.

I am interested again in Einstein's two state situation, specifically one in which the system is in the m^{th} eigenstate at t = 0; we therefore set $c_m(0) = 1$ and $c_n(0) = 0, n \neq m$. The time-dependent perturbation that we will apply is a classical electromagnetic wave. Considering a particular mode of the electromagnetic field, specified by frequency ω , wave vector \vec{k} ($\omega = c|\vec{k}|$), and polarization \vec{e} ($\vec{k} \cdot \vec{e} = 0$), with electric amplitude E_0 . The electric field is given by

$$\vec{E}(\omega, \vec{k}, \vec{e}, \vec{r}) = E_0 \cos\left(\omega t + \vec{k} \cdot \vec{r} + \phi\right) \vec{e}$$
(18)

To simplify calculations, we will assume the atom to be at $\vec{r} = 0$, and the phase $\phi = 0$:

$$\vec{E}(\omega, \vec{k}, \vec{e}) = E_0 \cos\left(\omega t\right) \vec{e} \tag{19}$$

We will also assume that the electric field does not vary significantly on the scale of the radius of the atom; $\frac{1}{|\vec{k}|} \ll a_0$ (where a_0 is the Bohr radius). This assumption is quite reasonable for the visible region of spectrum. Furthermore, we will asume that the dominant interaction is that between the electric dipole of the atom $\vec{p} = \sum_{e_i} e\vec{r}$ (a sum over the electrons in the atom) and the electric field. We can therefore ignore the magnetic component of the field, which the atom responds to much more weakly, as well as higher order electric interactions. Following Loudon [5], the Hamiltonian of that interaction, \hat{H}^{ED} , is given by

$$\hat{H}^{ED} = \vec{p} \cdot \vec{E} \tag{20}$$

For a two state system (k = 1), the equations (17) reduce to

$$\dot{c}_{0} = -\frac{i}{\hbar} H_{01}^{1} e^{-i\omega_{0}t} c_{1} - \frac{i}{\hbar} H_{00}^{1} c_{0}$$

$$\dot{c}_{1} = -\frac{i}{\hbar} H_{10}^{1} e^{i\omega_{0}t} c_{0} - \frac{i}{\hbar} H_{11}^{1} c_{1}$$
(21)

Consider that the dipole moment operator \vec{p} has an odd parity over r. Therefore, since the states $|n\rangle$ are eigenstates of parity, whatever the parity of $|n\rangle$ the quantity H_{nn}^1 must integrate to 0; this considerably simplifies our coupled equations (21) for c_0 and c_1

$$\dot{c}_{0} = -\frac{i}{\hbar} H_{01}^{1} e^{-i\omega_{0}t} c_{1}$$

$$\dot{c}_{1} = -\frac{i}{\hbar} H_{10}^{1} e^{i\omega_{0}t} c_{0}$$
(22)

Since the Hamiltonian \hat{H}^1 must be hermitian, $H_{01}^1 = (H_{10}^1)^{\dagger}$, there is really only one quantity left to calculate to fully determine the perturbation effect. It is interesting to observe that H_{01}^1 is nonzero only if the two states n and m have opposite parity in r. Finally,

$$H_{mn}^{1} = \langle m | \vec{p} \cdot \vec{e} | n \rangle E_{0} \cos(\omega t) = p_{mn}^{\vec{e}} E_{0} \cos(\omega t)$$
(23)

where $p_{mn}^{\vec{e}}$ is the component of the electric dipole between the two states in the direction of the electric field polarization vector; it represents the strength of the ability of the dipole interaction to couple between states m and n. Substituting into (22),

$$\dot{c}_{0} = -\frac{i}{\hbar} p_{01}^{\vec{e}} E_{0} \cos(\omega t) e^{-i\omega_{0}t} c_{1}$$

$$\dot{c}_{1} = -\frac{i}{\hbar} p_{10}^{\vec{e}} E_{0} \cos(\omega t) e^{i\omega_{0}t} c_{0}$$
(24)

As anticipated, we are now faced with a coupled pair of differential equations with no obvious method of exact solution. Following Griffiths [2], we will apply a first order perturbation approximation by setting $c_0(t) = c_0(0) = 1$ and $c_1(t) = c_1(0) = 0$ in (24)

$$\dot{c}_0 \approx 0$$

$$\dot{c}_1 \approx -\frac{i}{\hbar} p_{10}^{\vec{e}} E_0 \cos(\omega t) e^{i\omega_0 t}$$
(25)

We could solve these equations, then go back to (24) and substitute the solutions to obtain the second order perturbation, but we will stick with a first order analysis.

Expanding the cosine, simplifying, and integrating,

$$c_{0}(t) = 1$$

$$c_{1}(t) = -\frac{i}{2\hbar}p_{10}^{\vec{e}}E_{0}\int_{0}^{t}dt' \left(e^{i(\omega_{0}+\omega)t'} + e^{i(\omega_{0}-\omega)t'}\right)$$
(26)

The integral of (26) can easily be evaluated:

$$c_1(t) = -\frac{1}{2\hbar} p_{10}^{\vec{e}} E_0 \left(\frac{e^{i(\omega_0 + \omega)t} - 1}{\omega_0 + \omega} + \frac{e^{i(\omega_0 - \omega)t} - 1}{\omega_0 - \omega} \right)$$
(27)

Essentially, the work is now finished. We have determined $c_1(t)$ which will immediately yield P_{01} . However, if we make a few approximations, the answer will be much more intelligible and satisfying. The denominators of the two terms in (27) are astronomically different in most circumstances we will be interested in. Visible frequencies are on the order of $10^{15}Hz$. First, notice that at that frequency magnitude, unless $\omega \approx \omega_0$, $c_1(t)$ will approximately vanish. Secondly, if the two frequencies are indeed very close together the first denominator will be much larger than the second denominator, such that the first term can be neglected. Therefore, in the visible (and neighboring) regions of the transition spectrum, $c_1(t)$ is given by

$$c_1(t) = -\frac{1}{2\hbar} p_{10}^{\vec{e}} E_0 \frac{e^{i(\omega_0 - \omega)t} - 1}{\omega_0 - \omega}$$
(28)

$$P_{01}(t) = \left(\frac{1}{\hbar} p_{10}^{\vec{e}} E_0\right)^2 \frac{\sin^2\left((\omega_0 - \omega)t/2\right)}{(\omega_0 - \omega)^2} \tag{29}$$

The symmetry of equations (24) makes it a simple matter to find the reverse transition probability - it turns out they are the same [2];

$$P_{10}(t) = P_{01}(t) \tag{30}$$

which supports Einstein's relation between stimulated rate coefficients in (11). Finally, we have a mechanism for stimulated emission - the perturbation of the Hamiltonian has been shown to cause the probability of transition to rise above zero over time. The curious oscillation of that probability is sometimes known as 'Rabi flopping'. Now, if we are to model the same system of Einstein, we need to calculate these probabilities for light in thermal equilibrium with a blackbody cavity. That means the light is polychromatic, unpolarized, and directionally isotropic. Therefore we must average (29) over all incident directions, polarizations, and frequencies. First we will complete the frequency average. In order to represent a blackbody electromagnetic wave, we must replace the arbitrary amplitude E_0 with a spectrum of amplitudes appropriate for blackbody radiation $E_0(\omega)$. That can be easily accomplished by recognizing that E_0 is related to the energy density in the wave by $u(\omega) = \frac{\epsilon_0}{2} E_0^2(\omega)$, which automatically gives us the the form for the blackbody electromagnetic wave.

$$\langle P_{10}(t) \rangle_{\omega} = \int_{-\infty}^{\infty} d\omega P_{01}(\omega, t)$$

$$\langle P_{10}(t) \rangle_{\omega} = \frac{2}{\epsilon_0 \hbar^2} (p_{10}^{\vec{e}})^2 \int d\omega u(\omega) \frac{\sin^2 \left((\omega_0 - \omega) t/2 \right)}{(\omega_0 - \omega)^2}$$
(31)

As in the earlier discussion, the scale of ω is enormous, resulting in a very sharply peaked function multiplying $u(\omega)$ in the integral in (31). Since $u(\omega)$, Planck's blackbody energy density function, varies comparatively slowly, we can replace $u(\omega)$ with $u(\omega_0)$, the radiative energy density at the transition frequency.

$$\langle P_{10}(t) \rangle_{\omega} = \frac{2}{\epsilon_0 \hbar^2} (p_{10}^{\vec{e}})^2 u(\omega_0) \int d\omega \frac{\sin^2 \left((\omega_0 - \omega) t/2 \right)}{(\omega_0 - \omega)^2}$$
(32)

This is actually a very important and powerful statement - this indicates that the transition rates we are about to derive will be applicable to any radiation field with a slowly varying energy density function; essentially, our derivation will be valid for almost any radiation environment, including a a monochromatic beam of light with $u(\omega)$ some characteristic gaussian centered at ω_0 . Continuing, the frequency average results in

$$\langle P_{10}(t) \rangle_{\omega} = \frac{\pi}{\epsilon_0 \hbar^2} (p_{10}^{\vec{e}})^2 u(\omega_0) t \tag{33}$$

It can be shown [2, p. 354] that by averaging over all directions and polarizations of incident waves yields an additional factor of 1/3 in the transition probability. It makes sense that the probability would decrease, since the dipole interaction is maximized by an alignment between the electric field and the dipole, so averaging the energy over all directions would result in a weaker overall interaction. Finally, the transition rate, which for a statistical ensemble is the time derivative of the probability, is given by

$$b_{10}^{\omega} = b_{01}^{\omega} = \frac{dP_{10}(t)}{dt} = \frac{\pi}{\epsilon_0 \hbar^2} (p_{10}^{\vec{e}})^2 \tag{34}$$

Notice that this method is at a loss to explain the so-called spontaneous emission process, because in the absence of perturbation, the eigentstates are stationary and there are no transitions. The theory presented in the following section will not be limited in that manner.

5 The quantum mechanical theory of lasing

I will now present a considerably abbreviated introduction to the full quantization of the problem of the atom-radiation interaction. I will not be as thorough here as in other sections because a rigorous treatment of the subject spans the contents of entire textbooks. This is the beginning of 'quantum electrodynamics' (QED), the theory that describes particle interactions mediated by photons. It is a remarkable theory with a sublimely accurate record of experimental verification. However, I will only follow it as far as is necessary for an introduction to the quantum mechanics of lasing.

The following development does not introduce any principles unknown to a 3^{rd} year physics student. However, for those who are unfamiliar to the subject, it is made difficult by a disorienting trip from familiar electromagnetic fields to electromagnetic potential operators and their algebra. With perseverence, the familiar harmonic oscillator will emerge miraculously from the scrum. From there the well-known harmonic oscillator algebra will allow us to represent the field as a composition of modes each of which exist in a harmonic oscillator state. Our first aim will be to transform the classical electromagnetic field energy into a Hamiltonian formulation, which will allow us to apply quantum mechanical principles to electromagnetism. That classical quantity is

$$E = \frac{1}{2} \int d^3r \left(\mu_0^{-1} |\vec{B}|^2 + \epsilon_0 |\vec{E}_T|^2 \right)$$
(35)

I refer forward to (43) to explain the T subscript. The process starts with one of the most successful series of physical relations ever created - Maxwell's equations.

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{36}$$

$$\nabla \cdot \vec{E} = \frac{\sigma}{\epsilon_0} \tag{37}$$

$$\nabla \times \vec{B} = \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t} + \mu_0 \vec{J}$$
(38)

$$\nabla \cdot \vec{B} = 0 \tag{39}$$

Consider the potentials \vec{A} and ϕ that generate the electric and magnetic fields, defined by

$$\nabla \times \vec{A} = \vec{B}$$

$$-\nabla \phi - \frac{\partial \vec{A}}{\partial t} = \vec{E}$$
(40)

Following Loudon [5], substitution of (40) into Maxwell's equations, then the choice of the gauge defined by

$$\nabla \cdot \vec{A} = 0 \tag{41}$$

defines a set of equations which are essentially the potential formulation of Maxwell's equations. Those equations are

$$-\nabla^{2}\vec{A} + \frac{1}{c^{2}}\frac{\partial}{\partial t}\nabla\phi + \frac{1}{c^{2}}\frac{\partial^{2}}{\partial t^{2}}\vec{A} = \mu_{0}\vec{J} -\nabla^{2}\phi = \frac{\sigma}{\epsilon_{0}}$$
(42)

We now proceed to find a set of field equations in which the potentials are uncoupled. The Helmholtz theorem asserts that any vector field \vec{V} may be separated into two parts - one 'longitudinal' or 'irrotational', with zero curl, \vec{V}_L , and one 'transverse', with zero divergence, \vec{V}_T , such that

$$\vec{V} = \vec{V}_L + \vec{V}_T \tag{43}$$

We can decompose (42) in the same way by subsequently taking the curl and divergence over the equation.

$$-\nabla^{2}\vec{A}_{L} + \frac{1}{c^{2}}\frac{\partial}{\partial t}(\nabla\phi)_{L} + \frac{1}{c^{2}}\frac{\partial^{2}}{\partial t^{2}}\vec{A}_{L} = \mu_{0}\vec{J}_{L}$$
$$-\nabla^{2}\vec{A}_{T} + \frac{1}{c^{2}}\frac{\partial}{\partial t}(\nabla\phi)_{T} + \frac{1}{c^{2}}\frac{\partial^{2}}{\partial t^{2}}\vec{A}_{T} = \mu_{0}\vec{J}_{T}$$
(44)

From the chosen gauge (41), we know that $\vec{A}_L = 0$ and therefore $\vec{A}_T = \vec{A}$. Also, the identity $\nabla \times \nabla f = 0$ for a scalar field f indicates that $(\nabla \phi)_T = 0$. Now our equations simplify and uncouple. The three uncoupled field equations are

$$\frac{1}{c^2} \frac{\partial}{\partial t} \nabla \phi = \mu_0 \vec{J}_L$$
$$-\nabla^2 \vec{A} + \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \vec{A} = \mu_0 \vec{J}_T$$
$$-\nabla^2 \phi = \frac{\sigma}{\epsilon_0}$$
(45)

With these relationships governing the potentials, we are armed to approach the quantization of the free electromagnetic field, defined as a region where $\vec{J}_T = 0$ and $\sigma = 0$ [5]. In a free region, \vec{A} is governed by a wave equation:

$$-\nabla^2 \vec{A} + \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \vec{A} = 0$$
(46)

If we consider an arbitrary volume of space (for simplicity, a cube of side L), we can decompose \vec{A} into spatial modes $\vec{A}_{k,\vec{e}}(t)$. The solution of equation (46) yields the explicit time dependence of each mode. Therefore, the decomposition is

$$\vec{A} = \sum_{k,\vec{e}} A_{k,\vec{e}}(r,t) = \sum_{k,\vec{e}} \vec{e} (a_{k,\vec{e}} e^{(-i\omega_k t + ik \cdot r)} + a_{k,\vec{e}}^* e^{(i\omega_k t - ik \cdot r)})$$
(47)

where the sum is over the three discrete wavenumbers for the three dimensions, represented by k, and the two possible polarization vectors \vec{e} , constrained by $\vec{k} \cdot \vec{e} = 0$. The frequency ω_k is given by $\omega_k = |\vec{k}|c$. $\vec{A}_{k,\vec{e}}$ is accordingly the k^{th} mode in the \vec{e}^{th} polarization, and $a_{k,\vec{e}}$ and $a^*_{k,\vec{e}}$ represent its travelling wave vector potential components.

Based on this classical quantity \vec{A} , we will now define the corresponding quantum mechanical operator \hat{A} as

$$\hat{A} = \sum_{k,e} \hat{A}_{k,e} = \sum_{k,e} \left(\hat{a}_{k,e} e^{(-i\omega_k t + ik \cdot r)} + \hat{a}^{\dagger}_{k,e} e^{(i\omega_k t - ik \cdot r)} \right)$$
(48)

where k again represents the three quantized wavenumbers and e is now the polarization number in whatever polarization basis is chosen.

The next step is to use this expression for the quantized potential \hat{A} to find \hat{E}_T and \hat{B} , the quantum mechanical field operators ². We can then substitute the \hat{E} and \hat{B} operators into a quantum mechanical version of (35). Using the definitions in (40) with (48), we find

$$\hat{E}_{T} = \sum_{k,e} i\omega_{k}\vec{e}_{k} \left(\hat{a}_{k,e}e^{(-i\omega_{k}t+k\cdot r)} - \hat{a}_{k,e}^{\dagger}e^{(i\omega_{k}+k\cdot r)}\right)$$

$$\hat{B} = \sum_{k,e} i\omega_{k}\vec{k} \times \vec{e}_{k} \left(\hat{a}_{k,e}e^{(-i\omega_{k}t+k\cdot r)} - \hat{a}_{k,e}^{\dagger}e^{(i\omega_{k}+k\cdot r)}\right)$$
(49)

The quantum mechanical radiation Hamiltonian is obtained by analogy to (35), and the field operators (49) are substituted (with substantial simplification) to yield [5]

$$\hat{H}_{rad} = \frac{1}{2} \int_{V} d^{3}r \left(\mu_{0}^{-1} \hat{B}^{2} + \epsilon_{0} \hat{E}_{T}^{2} \right) = \sum_{k,e} \frac{\hbar^{2}}{4\epsilon_{0}V} \left(\hat{a}_{k,e} \hat{a}_{k,e}^{\dagger} + \hat{a}_{k,e}^{\dagger} \hat{a}_{k,e} \right)$$
(50)

²In the case of the free electromagnetic field, we are only interested in the transverse electric field \hat{E}_T , which solely depends on \hat{A} via (40). The longitudinal field, which we neglect, represents the electrostatic contribution from nonzero charge distribution σ [5, p. 132]

where $V = L^3$. If we define more convenient dimensionless operators

$$\hat{\alpha}_{k,e} = \sqrt{\frac{\hbar}{2\epsilon_0 \omega_k V}} \hat{a}_{k,e} \tag{51}$$

which can be shown to have the commutation relation $[\hat{\alpha}_{k,e}, \alpha_{k',e'}^{\dagger}] = \delta_{k,k'}\delta_{e,e'}$ then rearrange (50), we have

$$\hat{H}_{rad} = \sum_{k,e} \hbar \omega_k \left(\hat{\alpha}_{k,e}^{\dagger} \hat{\alpha}_{k,e} + \frac{1}{2} \right) = \sum_{k,e} \hbar \omega_k \left(n_{k,e} + \frac{1}{2} \right)$$
(52)

We have found something strange and wonderful. This is the Hamiltonian for a quantum mechanical harmonic oscillator, in fact the sum of an infinite number of independent ones! The raising and lowering operators $\hat{\alpha}$ and $\hat{\alpha}^{\dagger}$ are the dimensionless version of the travelling wave vector potential operators³. Our free electromagnetic system immediately inherits the whole battery of properties that physics undergraduate students study so exhaustively. The eigenstates of the radiation field are therefore given by an infinite set of harmonic oscillator number states

$$\hat{H}_{rad}|\{n_{k,e}\}\rangle = \hat{H}_{rad} \sum_{k,e} |n_{k_1,1}\rangle |n_{k_1,2}\rangle |n_{k_2,1}\rangle |n_{k_2,2}\rangle \dots \\
= \sum_{k,e} \hbar \omega_k \left(n_{k,e} + \frac{1}{2}\right)$$
(53)

The number of the state of a particular mode $n_{k,e}$ represents the number of 'photons' present in that mode, or the mode's 'occupation number'.

We have outlined the quantization of the free electromagnetic field. However, the system we wish to describe is the interaction of the free field with an atomic system; thus we have only completed half the derivation (and for a rigorous treatment, considerable less than half the work). I will now skip a large segment of intricate formalism involving the coupling of the nucleus-electron system to the quantized electromagnetic field. We arrive at a completed Hamiltonian formulation of the atomradiation system

$$\hat{H}_{atom-rad} = \hat{H}_0 + \hat{H}_{coupling} = \left(\hat{H}_{atom} + \hat{H}_{rad}\right) + \hat{H}_{ED}$$
(54)

³The intuitive explanation for this is that what we classically considered forward and backward travelling waves, we can equivalently consider positive and negative frequency waves; the operators representing these positive and negative frequency components therefore becomes the raising and lowering operators for the occupation of the quantum mechanical electromagnetic modes.

where \hat{H}_{atom} is the usual atomic Hamiltonian, and \hat{H}_{ED} is the electric-dipole Hamiltonian from (20). This is sometimes known as the 'second quantization' of the atomic Hamiltonian [5]. We have made one important approximation - we used only the first order term from the radiation-atom interaction Hamiltonian, which is \hat{H}_{ED} . Consider a basis of states which are a combination of the radiation field states from (53) and the atomic states, labeled with integers for convenience:

$$|\Psi\rangle = |\{n_{k,e}\}\rangle|n_{atom}\rangle = |\{n_{k,e}\}, n_{atom}\rangle$$
(55)

This basis is subject to the orthonormality relation $\langle n_{k,e}, n_{atom} | n_{k',e'}, n'_{atom} \rangle = \delta_{k,k'} \delta_{e,e'} \delta_{n,n'}$. Note that this basis is an eigenstate basis of $\hat{H}_0 = \hat{H}_{atom} + \hat{H}_{rad}$ from (54); the coupling Hamiltonian \hat{H}_{ED} is responsible for the dynamics of the system.

If we restrict our basis to two atomic states, $|0\rangle$ and $|1\rangle$ as in previous sections, then we can define atomic raising and lowering operators $\hat{\beta}^{\dagger} = |1\rangle\langle 0|$ and $\hat{\beta} = |0\rangle\langle 1|$. Thus,

$$\hat{\beta}|\{n_{k,e}\},1\rangle = |\{n_{k,e}\},0\rangle
\hat{\beta}^{\dagger}|\{n_{k,e}\},0\rangle = |\{n_{k,e}\},1\rangle$$
(56)

It can be shown that the electric dipole Hamiltonian in this restricted basis is given by

$$\hat{H}_{ED} = \sum_{k,e} i E_{k,e,01} \left(\hat{\beta}^{\dagger} \hat{\alpha}_{k,e} e^{(ik \cdot r)} - \hat{\beta} \hat{\alpha}_{k,e}^{\dagger} e^{(-ik \cdot r)} \right)$$
(57)

where $E_{k,e,01}$ is a quantity dependent on the radiation mode and p_{01} , with units of energy. It is now straightforward to determine that in the basis (55),

$$\hat{H}_{ED} = \sum_{k,e} \left(\gamma_{k,e,01} | n_{k,e} - 1, 1 \rangle \langle n_{k,e}, 0 | + \gamma_{k,e,10} | n_{k,e} + 1, 0 \rangle \langle n_{k,e}, 1 | \right)$$
(58)

where several presently distracting quantities have been hastily concealed in the $\gamma_{k,e,ij}$. Conservation of energy must be invoked as a selection rule, allowing only those transitions where the energy gained or lost from the radiation field equals the energy lost or gained by the atom.

We have now arrived at our last goal. According to (58), a system described by the state $|n_{k,e}, 1\rangle$ may transition via the dipole coupling to the state $|n_{k,e} + 1, 0\rangle$ (provided that $\hbar\omega_k = E_1 - E_0$ and no other selection rules are violated). This is stimulated emission! Pay very close attention to the fact that the mode which is populated by an extra photon after the transition is in the same mode as the one which stimulated the transition. Thus, stimulated emission results in the emission of a photon with the same frequency, direction, and polarization as the stimulating photon. *This is the cause of coherent amplification in a laser*. Einstein's mysterious spontaneous emission process is described here too - it is represented by the term

$$\hat{H}_{ED-spontaneous} = \gamma_{k,e,10} |1,0\rangle \langle 0,1| \tag{59}$$

This transition is one from the ground state of one of the radiation modes to its first excited state. Thus, even in the 'vacuum state' of the radiation field in which there are no photons present, the radiation field can still stimulate transitions via the electric dipole interaction! In the semiclassical picture, the vacuum electromagnetic field has nonzero energy, and nonzero field amplitude. This fascinating phenomenon, which gives rise to the Casimir effect, is sometimes described as 'vacuum fluctuations' of the field, however it is an inherently quantum mechanical property of the radiation - atom system.

The QED derivation of the absorption and emission rates are unfortunately a bit out of reach at the level of the formulism in this paper, but we are not far from finding those rates; the use of Fermi's golden rule is the main remaining operation required, and the results prove to be consistent with (10), (11), and (34) [5, p. 170].

6 Conclusions

It is my hope that this paper has given the reader a deeper understanding of the basic quantum mechanics of the atom-radiation system, as well as an appreciation for the remarkable diversity of analytical approaches to describing that system. From Einstein's pre-Schrödinger phenomenological approach we obtained the existence of stimulated emission, and several relations between transition rates, but gained little insight into the mechanisms. From semi-classical perturbation theory and the quantum theory of the atom, we determined an exact expression for the stimulated absorption and emission rates and identified a clear mechanism for those transitions, but spontaneous emission eluded us, hinting that the mechanism is incomplete or incorrect.

Finally, the second quantization of the atom provided a theory capable of encompassing all the observed phenomena. Spontaneous emission was found to be simply an electric dipole transition with initial radiation occupation number of 0, and the coherent directional properties of stimulated emission became evident. It is unusual and very satisfying in undergraduate quantum mechanics to find such a dramatic macroscopic quantum phenomenon that is within one's theoretical reach. As entrancing and amusing as a bright laser beam has always been, it is only more amazing with a sense of the physics of its creation.

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