To the Graduate Council:

I am submitting herewith a dissertation written by John T. F. Barwick II entitled "Classical Theory of Radiative Transitions." I recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Physics.

Harry C. Jacobson, Major Professor

We have read this dissertation
and recommend its acceptance:

Don B Hinton

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Vice Chancellor
Graduate Studies and Research

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CLASSICAL THEORY OF RADIATIVE TRANSITIONS

A Dissertation

Presented for the

Doctor of Philosophy

Degree

The University of Tennessee, Knoxville

John T. F. Barwick II

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DEDICATION

To my father and mother and my wife Jean

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ABSTRACT

Shrödinger's original conception of the connection between the electric field and the wave function ψ is reinterpreted and extended. The new semiclassical approach to radiative transitions is based on the exact (not perturbative) description of a particle undergoing a transition between two energy eigenstates $\psi_1(\vec{r},t)$ and $\psi_2(\vec{r},t)$ as

$$\psi = c_1(t)\psi_1 + c_2(t)\psi_2 \ .$$

The physical existence of such a wave function during a transition allows for a simple classical explanation of the origin of radiation from quantum mechanical systems, both in the usual bound state cases and in some new free particle transitions for which there have been no previous semiclassical accounts. The Compton effect, perhaps the phenomenon most frequently cited as evidence of the quantum nature of radiation, is thus given a classical explanation which yields the Klein-Nishina cross section and demonstrates the classical origin of photon-like behavior of the incident and scattered radiation.

Further confirmation of the classical nature of the electromagnetic field at the quantum mechanical level is presented in a new derivation of the Lamb shift, another famous phenomenon whose only acceptable explanation has been quantum electrodynamical. The calculated value of the $2P_{\frac{1}{2}} \Leftrightarrow 2S_{\frac{1}{2}}$ shift in hydrogen is

$$\nu_L = 1110 \text{ MHz} \ ,$$

in good agreement with experiment (1057 MHz).

A more complete discussion of the $c_1(t)$ and $c_2(t)$ transition coefficients is also carried out, leading finally to new semiclassical treatments of spontaneous emission and the blackbody spectrum. These two subjects have again long been believed to be explainable only by quantum electrodynamics.

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I. INTRODUCTION

A. CLASSICAL AND QUANTUM CONCEPTS OF RADIATION

Modern theories concerning the problem of the connection between a simple quantum mechanical system and radiation can be broadly classified as either semiclassical or quantum electrodynamical, depending on the treatment of the electromagnetic field.[1,2] The semiclassical approaches are based in general on the idea that the classical wave nature of this field constitutes the essence of radiation, and that its large scale behavior, as expressed in Maxwell's equations, can in principle be extrapolated to arbitrarily small spatial scales. Quantum electrodynamics, on the other hand, is more in accord with a quantum theoretical viewpoint of the electromagnetic field and its physical manifestation in terms of a particle or "photon" concept of radiation. These two fundamentally different ways of conceiving of light today are characteristic of a long historical division along similar lines in the attitudes and experiments on this subject. Newton, who espoused a materialistic particle idea of light, and Young, whose interference experiments provided a foundation for the wave theory, are representative of the historical figures who can be marshalled on the two sides of the question. Maxwell's derivation of the wave equation for the electromagnetic field in 1865 and subsequent discoveries in the late nineteenth century provided precise theoretical and experimental verification of a wave theory of radiation which has been and is, so

attractive that it provides the complete description of the electromagnetic field in all semiclassical theories. The apparent inability of a simple classical wave theory to account for all radiative phenomena and the first hints of new particle-like properties of light first began to manifest themselves in 1900 when Planck obtained the black-body radiation formula by the introduction of quantized frequencies for the oscillators in the source, and in 1905, when Einstein specifically suggested the extension of this quantization concept to light itself in order to explain the photoelectric effect. The concept of light photons was also inherent in Einstein's important 1917 paper in which the Planck formula was obtained from a consideration of a rate equation involving the "A" and "B" coefficients.[3] All of this, along with several newly investigated phenomena, such as the Compton effect, and the classically inconsistent form of the continuous x-ray spectrum, led by 1926 to a natural impetus to extend the new quantum theory of matter to radiation, a step which was taken by Dirac in 1927.[4]

From the time of the advent of the new quantum mechanics in 1926 until the present, the two views of the nature of radiation have coexisted uneasily, partly under the compromise provided by Bohr known as "complementarity," according to which macroscopic space-time (λ, ν) or causality ($\vec{p}$, E) concepts can be applied exactly on a quantum mechanical scale only one at a time. Wave or particle attributes detected (or even only conceived of) preclude exact detection (or conception) of the "conjugate" attributes. Since 1926 many calculations involving the interaction of matter and radiation have therefore been carried out in

terms of either an unquantized or quantized field, or both. Some of the earliest discussions, such as those on the photoelectric effect,[5] the Compton effect (Klein-Nishina formula),[6] and stimulated emission and absorption by an atom,[7] were done semiclassically, in the spirit of Schrödinger's original and important interpretation of quantum mechanics.[8] At the same time, however, the usefulness of the general idea of quantization and its mathematical formalism, as perhaps first suggested in Heisenberg's alternative formulation of quantum mechanics,[9] led to a rapid development of a quantum electrodynamic viewpoint of radiative processes which was highly successful. Dirac's initial paper on field quantization was followed by papers on second quantization in 1927[10] and 1928,[11] general procedures for the quantization of wave fields in 1929[12] and 1930,[13] spontaneous emission in 1930,[14] and discussions of general methods along lines of perturbation theory for the treatment of any matter-radiation phenomena.[15,16]

The calculational success of this perturbation theory formalism for the interaction of quantum states and electromagnetic fields, quantum electrodynamics, with or without the quantization of the eigenfunction expansion of the states involved,[17] and including any of its various other interpretations such as the S matrix approach[18] or Feynman's path integral formulation,[19] led to its increasing preeminence over the next several decades, the effects of which in most respects still continue today. The simplicity of semiclassical explanations of certain processes, however, has helped to stimulate a recent revival of interest in its use in certain cases, of which some of the

phenomena connected with the advent of the laser, either directly[20] or indirectly,[21] are prime examples. The "neoclassical" theory of Jaynes and his associates has recently extended the application of semiclassical methods to some effects which have been generally considered to be properly explainable only by quantum electrodynamics, such as the Lamb shift, spontaneous emission, and black body radiation.[22,23]

There are two reasons why semiclassical theories should be pursued and extended as far as possible. One which has been pointed out by Jaynes is that the present theory of quantum electrodynamics contains many mathematical and logical difficulties. Divergent and infinite expressions which occur frequently and require various amounts of ingenuity to avoid suggest a need for a continued reevaluation of the mathematical structure of QED and/or a search for a more acceptable formulation. The other reason is more fundamental and is connected in a way with the previously mentioned uneasiness with which the concept of the limited applicability of classical concepts on a quantum scale is generally received. Just as Schrödinger's interpretation of the wave function provides a physical picture of quantum concepts in addition to its purely computational aspects, a model to which classical ideas of space and time can be extended and which is entirely lacking for the more formal manipulations of matrix mechanics, semiclassical theories allow a similar microscopic space-time conception of the origin of radiation from the wave function. Since the radiation is classically familiar and since the semiclassical explanations of many phenomena are so intriguingly simple and natural mathematically, an

intuitively attractive and satisfying theory is possible, in which no appeal need be made to a limitation of classical ideas of time and space. This would seem to be a critically important motivation for any efforts in this direction.

B. THE VIEWPOINT OF THE PRESENT THEORY

The interpretation of semiclassical ideas which is presented in the next section is based on a synthesis of more modern ideas with Schrödinger's original conception of the wave function and its connection with the electromagnetic field. At the time of the third communication of the four which composed his historic 1926 paper on wave mechanics,[8] Schrödinger sought to attach some physical meaning to the function ψ, the "mechanical field scalar" which was defined only formally as the solution of his wave equation. He attempted to provide an electromagnetic interpretation by postulating initially that the electric charge density was given by

$$\rho = e\mathrm{Re}\ \psi \frac{\partial \psi^*}{\partial t} \ .$$

By expanding ψ in terms of discrete energy eigenfunctions

$$\psi = \sum_i c_i u_i(\vec{r}) e^{-\frac{i}{\hbar} E_i t} \ ,$$

he could easily show that the use of this expression for ρ in the calculation of the dipole moment of an atom provided terms which

oscillated at exactly those frequencies known to be radiated and had coefficients of the form

$$p_{ij}^{(x)} = \iiint u_i(\vec{r}) x\, u_j(\vec{r}) d^3r \ ,$$

which accounted correctly for the various intensities and polarizations of the emitted radiation. In the last section of the fourth communication of his paper, Schrödinger removed some problems with his initial definition of ρ by replacing it with

$$\rho = e\psi\psi^* \ .$$

He could then use the continuity equation $\partial_t \rho = -\nabla \cdot \vec{j}$ to obtain an expression for the current density $\vec{j}$, just as is done in Section IIC, and also calculate correctly the intensity relationships among various component lines in the Zeeman and Stark effects (from dipole moment components $p_{ij}^{(x)}$ as above). In this same paper he used his time dependent perturbation theory to show that a combined (two level) system oscillates between the two states at a rate proportional to the perturbing coupling energy. He had thus by 1926 established all of the important features of all semiclassical radiation theories since.

The particular interpretation of such semiclassical ideas developed in Section II seems to be capable of providing a simple classical description of the origin of radiation in most quantum mechanical transitions involving a single electron, including bound state to free state and free state to free state transitions in addition to the commonly considered interatomic bound state cases. The photoelectric

effect and Compton effect are the specific examples which are discussed in the two sections following. Brehmsstrahlung, although not treated in the present work, should be, and does seem to be, another free to free type of transition that can be handled in exactly the same manner as the Compton effect. The starting point for the present interpretation consists of the standard expressions for quantum states and Hamiltonian terms, but a means of extending the method to new free particle cases is suggested by the adoption of a viewpoint which has not been considered explicitly in recent work on the subject, with the result that it has never been carried to its limits. In essence, attention is focused on the direct effects of the sort of charge and current densities considered by Schrödinger, rather than on equations describing the time development of an atomic dipole moment, for example, which is the usual frame of reference for modern semiclassical discussions. The transitions treated in the following sections really have no dipole moments. The new (or old) point of view, which in essence simply attaches a new meaning to the c_i in $\psi = \sum_i c_i \psi_{E_i}$, is developed in general in Section II and then applied in Section III to a detailed analysis of the Compton effect, a phenomenon in which the photon nature of x-rays has always seemed most evident, both in its mathematical explanation and in the experimentally observed particle-like nature of the radiation emitted in each event.[24] The most important part of the discussion of this effect in Section IIIA, therefore, is probably the natural classical appearance of a photon-like behavior of the radiation. A similar sort of behavior might be hypothesized to occur in other similar types of transitions in which a quantized character of the emitted radiation seems to be apparent. Further discussion of the

physical mechanism of the Compton effect is to be found in Section VD, where the necessary treatment of the appropriate form of the equations describing the time development of the transition (the "$\dot{c}_i$ equations") is carried out.

The applicability of the present or any other interpretation of semiclassical ideas should also be tested in other directions. All of the ramifications of the use of a classical electromagnetic field should be explored. The analysis of the Lamb shift given in Section IV provides just such an evaluation of certain classical field properties on an atomic scale, and, in addition, addresses a problem which has had as yet no clearly acceptable semiclassical explanation. Section IV therefore represents a shift in subject matter but not in philosophy. It is really more closely related to Sections II and III than might be apparent, since it provides direct evidence for the reality of classical fields on an atomic level. The calculations which are carried out deal classically with the same contributions to the energy of an electron state as were used by Bethe in the original quantum electrodynamical derivation of the shift. Bethe considered the change in the kinetic energy of the bound electron in state $|\psi_E\rangle$ by interactions with the electromagnetic field represented by the diagram in Figure 1. The (second order) shift due to this diagram can be broken up into two identifiable parts, one of which is infinite and represents the correction to the kinetic energy due to the (renormalized) electromagnetic mass, while the other can be plausibly shown to represent a small energy shift, ΔE. Bethe's calculated value of ΔE agreed well

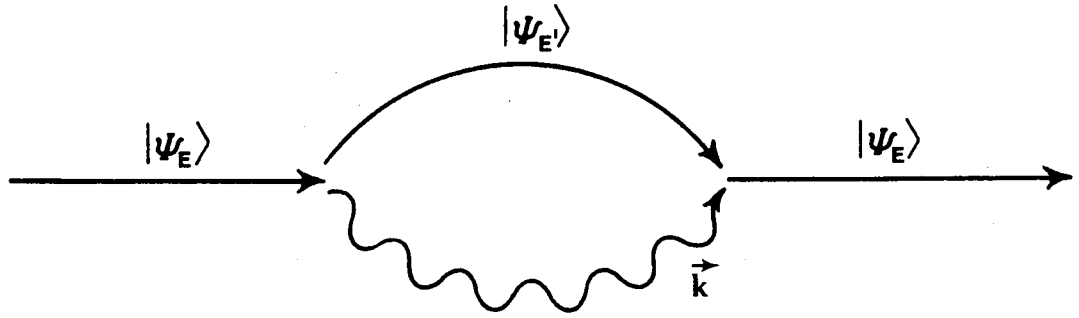

Figure 1. Feynman diagram representing the second order correction to the energy of the bound electron state $|\psi_E\rangle$. The correction is

$$E_n^{(2)} = E^{(2)}_{\substack{\text{electromag-}\\\text{netic mass}}} + \Delta E^{(2)}_{\text{Lamb}} ,$$

where the observable Lamb shift $\Delta E^{(2)}_{\text{Lamb}}$ is, according to Bethe's original expression,

$$\Delta E_n^{(2)} = \frac{4}{3} Z \frac{k_e^2 e^4 \hbar}{m^2 c^3} |\psi_n(0)|^2 \log \left| \frac{mc^2}{(E_{n'} - E_n)_{av}} \right| ,$$

with $|\psi_{n,\ell=0}(0)|^2 = \frac{1}{\pi} \left(\frac{Z}{na_0} \right)^3$.

with the famous hydrogen $2s \leftrightarrow 2p$ shift measured by Lamb. Classically, however, one can calculate in a straightforward way both the static field energy due to $\rho = e\langle \psi_E | \psi_E \rangle$ and also the shift in kinetic and atomic interaction energies due to the "velocity" of ρ,

$$\langle \vec{v} \rangle = \langle \psi_E | \frac{\hbar}{im} \nabla | \psi_E \rangle \ .$$

These classical energies can be considered to be the analogues of the quantum electrodynamic energies represented by the Feynman diagram, the self field energy corresponding to the infinite renormalization energy, and the velocity dependent energies corresponding to the quantum electrodynamic kinetic energy shift. As will be seen in Section IV (B and C), these small classical energies yield in a logical way a very good value for the hydrogen Lamb shift.

The major part of the research on the basic aspects of semiclassical theory since 1926 has been concerned with the solution of the equations for the $c_i(t)$ coefficients which result when the eigenfunction expansion above is used in the time dependent Schrödinger equation along with various types of perturbing energy terms. These equations are

$$i\hbar \dot{c}_i = \sum_j c_j \langle u_i | \hat{H}_1 | u_j \rangle \, e^{-\frac{i}{\hbar}(E_j - E_i)t} \ ,$$

where $\hat{H}_1$ is the perturbation Hamiltonian, which in most cases is taken to be a result of an incident electromagnetic wave consisting of one or more frequencies. These equations are discussed briefly in Section II in the case of a two level transition and an incident monochromatic plane wave. Section V, however, is devoted almost exclusively to a

complete analysis of the equations and their solutions, both for the case of an external electromagnetic field and for the slightly more complicated case of the self fields emitted by the system itself. The former case provides the context for the introduction of a new method of solution in part VB which makes previous approximations unnecessary ("rotating wave" approximation) and which shows how the angular momentum of the incident field is coupled with that of the transition. The latter self field case leads to discussion in part VC of two other phenomena which have long presented difficulties for semiclassical theories, spontaneous emission and the blackbody radiation spectrum. The more recent phenomenon of photon antibunching,[25] which is defined in Section VB, can also be given a possible explanation. The self field case has been advanced to a great extent by the work of Jaynes, who has recently discovered a method by which the $\dot{c}_i$ equations may be used to explain the Lamb shift and spontaneous emission.[22] Instead of employing an external field to "cause" a transition, he introduces in $\hat{H}_1$ the field produced by the charge and current densities of the wave function itself. Thus for the eigenfunction expansion of ψ given above, the appropriate characterization of the self field for use in $\hat{H}_1$, the vector potential $\vec{A}$, can be obtained from

$$\vec{j} = \sum_{i,j} \frac{e\hbar}{2im} (c_i c_j^* \psi_j^* \nabla \psi_i - c_i^* c_j \psi_j \nabla \psi_i^*)$$

and

$$\vec{A}_{self} = \frac{(k_e k_m)^{1/2}}{c} \iiint \frac{\vec{j}'_{retarded}}{|\vec{r} - \vec{r}'|} d^3r'$$

where k_e and k_m are constants introduced for use with electromagnetic units and $\vec{j}'_{retarded} = \vec{j}(\vec{r}', t - \frac{1}{c}|\vec{r} - \vec{r}'|)$. Since $\vec{A}_{self}$ will involve the c_i coefficients, the $\dot{c}_i$ equations become more complicated. The solution requires a phase shift of the c_i values which can be related to a frequency shift in $\vec{j}_{ij}$ (Lamb shift). In addition the variation of the real parts of c_i provides a simple description of spontaneous emission. This form of the $\dot{c}_i$ equations is solved in Section VC by a method which is similar to that of Jaynes but which differs from it in several important ways. The equations are written and analyzed directly in terms of the coefficients c_i themselves rather than in Jaynes' form, which uses the "density matrix" elements $\sigma_{ij} = c_i c_j^*$. Also, nonresonant frequency terms are not ignored, as they are in Jaynes' (and others') solutions. The results of this analysis are then applied to a discussion of the form of the blackbody spectrum and finally, in part VD, to a possible mechanism for the time development of a single event of the specific type treated in Section III, a Compton scattering event.

A final word is in order on the wide range of material covered in the present work. The common thread which joins the apparently disparate subject matter of Sections II-V is the consistent attempt to focus on a classical treatment of the electromagnetic fields for all problems. The specific choice of subjects is determined by a desire to touch on most of the major phenomena which have in the past been used as evidence

against semiclassical theories. These would include the discrete nature of Compton radiation (Section III), the Lamb shift (Section IV), spontaneous emission (Section V), and the blackbody spectrum (Section V).

II. CONNECTION BETWEEN THE QUANTUM MECHANICAL WAVE FUNCTION AND THE ELECTROMAGNETIC FIELD

A. BASIC HYPOTHESIS

A straightforward classical description is sought for the radiative transitions between stationary states of a simple quantum mechanical system. Therefore, a nonrelativistic spinless electron in an atom, as it undergoes a transition from atomic state $\psi_1 = u_1(\vec{r})e^{-i/\hbar\, E_1 t}$ to $\psi_2 = u_2(\vec{r})e^{-i/\hbar\, E_2 t}$, is considered. Many of the results obtained can easily be generalized to states of the Dirac equation. The transition of the electron from ψ_1 to ψ_2 is accompanied by the emission of radiation of frequency $\omega = \frac{E_1 - E_2}{\hbar}$. That is, ω is proportional to the <u>difference</u> of the wave function frequencies. So if one is to provide a classical mechanism for the emission, it should involve both ψ_1 and ψ_2 for the entire time of the transition, since the photon has a "memory" of both states. The product $\psi_1\psi_2^*$ of the two complex wave functions, of course, satisfies these conditions,[26] and in addition, it can be fit into a consistent picture of the wave function-electromagnetic field connection by the usual semiclassical assumption of the existence of superposition states. That is, during the transition,[27] a <u>single</u> electron wave function is given by:

$$\psi = c_1\psi_1 + c_2\psi_2 \tag{1}$$

where c_1 and c_2 are coefficients which may depend on time but not on spatial coordinates. Here they represent the actual state of a

particular electron and have no statistical connotation. Then the usual formula for the charge density associated with ψ gives:

$$\rho = e\psi\psi^* = e(|c_1|^2\psi_1^2 + |c_2|^2\psi_2^2 + c_1^*c_2\psi_1^*\psi_2 + c_1c_2^*\psi_1\psi_2^*) \ . \qquad (2)$$

The first two terms give the static[28] charge densities of the fractions of the electron in the 1 and 2 states, and the second two, which are complex conjugates, give a real, time dependent, radiation charge density. If c_1 and c_2 are of the form $c_1 = c_1' e^{i\phi_i(t)}$, $c_2 = c_2' e^{i\phi_2(t)}$, and

$$e\psi_1(\vec{r},t)\psi_2^*(\vec{r},\ t) = \rho_r + i\rho_i$$

then $$\rho_{rad.} = 2c_1'c_2' [\rho_r \cos(\omega_2 - \omega_1)t] \ ,$$

if $\phi_1(t) = \phi_2(t)$. The imaginary parts of $\psi_1\psi_2^*$ and $\psi_1^*\psi_2$ then cancel in expressions such as (2). If $\phi_1(t) \neq \phi_2(t)$, imaginary parts of $c_1^*c_2\psi_1^*\psi_2$ and $c_1c_2^*\psi_1\psi_2^*$ still cancel and there is introduced a phase shift in the cosine factor. The various terms in (2) are formally equivalent to "matrix elements" of the charge, which establishes a connection between this view and some of the recent expressions used by various authors, in which it is usually the dipole moment matrix elements between states whose physical existence is explicitly investigated.[22,29]

Superposition states present some problems, which can in part be traced to the fact that they are not energy eigenstates in general.[30] Einstein's objection to them in anything but a statistical sense[31] is illustrated by the Franck-Hertz experiment. If the individual atomic electron involved in the transition $\psi_1 \rightarrow \psi_2$ ($E_1 \rightarrow E_2$) can occupy

$\psi = c_1\psi_1 + c_2\psi_2$, there would be no discrete energy absorption. Actually, the case cannot be argued one way or the other until the mechanics of the excitation process is examined in detail. The relative opacity of the atom to transfer of electron kinetic energy until the electron wave function reaches a certain wavelength and frequency may be due to the way in which the electromagnetic fields of this wave function interact with the radiation fields of the superposition wave function. A suggestion of such an effect can be seen in the discussion of the photoelectric effect and in the next section. One other effect of superposition states is the introduction of the question of correlations in the radiation produced when more than two states are involved in a transition, since the wave function (1) could include any number of these states in general. In addition the charge and current densities for many particle wave functions must be handled in a slightly different way than is indicated by Eq. (2).[23] These problems are not considered, however, in the following discussion.

A well-known example[32] demonstrates the appropriateness and simplicity of thinking of $c_1^* c_2 \psi_1^* \psi_2 + c_1 c_2^* \psi_1 \psi_2^*$ as a radiation charge density in the classical sense. For an electron in a central potential, the states will be of the form

$$\psi_{n\ell m}(\vec{r},t) = A_{n\ell m} R_{n\ell}(r) P_\ell^m(\cos\,\theta) e^{\pm im\phi} e^{-i\frac{E_n}{\hbar}t} .$$

Therefore the radiation charge density in this case will be

$$\rho_{rad.} = c_1 c_2^* e \psi_1 \psi_2^* + (c.c.) = c_1 c_2^* e^{-i\Delta\omega t} A_{n'\ell'm'} A^*_{n\ell m} R_{n'\ell'} R^*_{n\ell} Y_{\ell'm'} Y^*_{\ell m}$$

$$+ (c.c.) \ .$$

Since the classical multipole moments of a charge density are defined by

$$q_{\ell m} = \iiint Y^*_{\ell m} r^{\ell} \rho d^3x \quad ,$$

the radiation charge density would consist of the following multipoles:

$$q_{LM} = A_{n'\ell'm'} A^*_{n\ell m} \iiint r^L R_{n'\ell'} R^*_{n\ell} Y_{LM} Y_{\ell'm'} Y^*_{\ell m} d^3x$$

$$+ A^*_{n'\ell'm'} A_{n\ell m} \iiint r^L R^*_{n'\ell'} R_{n\ell} Y_{LM} Y^*_{\ell'm'} Y_{\ell m} d^3x \ .$$

The recurrence relations for the Legendre polynomials then show, for example, that the transition $\psi \rightarrow \psi'$ with $m = m'$ and $\ell = \ell' \pm 1$ involves only the dipole moment $q_{1,0}$, and $m = m' \pm 1$ and $\ell = \ell' \pm 1$ involves only $q_{1,\pm 1}$. Thus, the electric dipole selection rules, which themselves follow from similar arguments, actually create classical dipole radiation charge densities and, of course, give pure dipole radiation.

A number of papers attest to the success of semiclassical explanations of emission processes and mechanisms for their occurrence in atomic and molecular electronic states.[20,22] At least as far as the charge and current densities produced in these cases is concerned, the above simple classical picture is completely sufficient. Many processes, however, which must then

also be given a classical explanation, involve the absorption or transformation (in frequency) of an incident electromagnetic wave. For the purpose of treating these cases, a method of including such radiations in the previous mechanism is necessary. Therefore, let the single transition be assumed here to be occurring in the presence of an incident plane wave described by the vector potential (Coulomb gauge)

$$\vec{A} = \vec{A}_c + \vec{A}_c^* \tag{3}$$

with $$\vec{A}_c = A\hat{\epsilon}_1 e^{i(\vec{k}\cdot\vec{r} - \omega t)} .$$

It is known from experiment (absorption line frequencies = emission line frequencies, etc.) that ψ_1 and ψ_2 must obey

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{x})\psi = -\frac{\hbar}{i}\partial_t\psi \tag{4}$$

and not

$$\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\sqrt{\frac{k_e}{k_m}}\vec{A}\right)^2\psi + V(\vec{x})\psi = -\frac{\hbar}{i}\partial_t\psi . \tag{5}$$

They must be the "unaffected" wave functions.[33] However, the actual wave function of the electron during the transition, supposedly given by equation (1), should really be a solution of (5), which should then describe the progress of the transition. This, of course, is just the argument on which time dependent perturbation theory is based, but here there is no constraint on the magnitude of $\vec{A}$, and there is no statistical or probabilistic

interpretation of the amplitude coefficients c_1 and c_2. Eq. (1) is not an approximate or expectation solution of (5) for small $\vec{A}$, but an exact solution for arbitrary $\vec{A}$. Just as in time dependent perturbation theory

$$\hat{H}\psi \equiv \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) + \frac{ie\hbar}{mc}\sqrt{\frac{k_e}{k_m}}\,\vec{A}\cdot\nabla + \frac{e^2 k_e}{2mc^2 k_m}\vec{A}^2 \right)\psi$$

$$\hat{H}_1\psi \equiv \left(\frac{ie\hbar}{mc}\sqrt{\frac{k_e}{k_m}}\,\vec{A}\cdot\nabla + \frac{e^2 k_e}{2mc^2 k_m}\vec{A}^2 \right)(c_1\psi_1 + c_2\psi_2)$$

$$= i\hbar\dot{c}_1\psi_1 + i\hbar\dot{c}_2\psi_2 \quad .$$

So, with normalized $\psi_j = u_j(\vec{x})e^{-\frac{i}{\hbar}E_j t}$,

$$\begin{aligned} i\hbar\dot{c}_1 &= c_1\langle u_1|\hat{H}_1|u_1\rangle + c_2\langle u_1|\hat{H}_1|u_2\rangle e^{-\frac{i}{\hbar}(E_2-E_1)t} \\ i\hbar\dot{c}_2 &= c_1\langle u_2|\hat{H}_1|u_1\rangle e^{-\frac{i}{\hbar}(E_1-E_2)t} + c_2\langle u_2|\hat{H}_1|u_2\rangle . \end{aligned} \tag{6}$$

These equations, which are equivalent to the usual Heisenberg (type) equations of motion for the "density matrix" elements $\sigma_{ji} = c_j c_i^*$, in the present application should yield a detailed physical description of the transition process, but a complete and correct solution for all radiative problems would require $\hat{H}$ to include the electromagnetic fields produced by the radiating charge density itself,[22] along with various other terms such as those resulting from atomic collisions.

B. PHOTOELECTRIC EFFECT

The adherence to the form of time dependent perturbation theory even for arbitrary fields should insure that all results involving relatively weak or perturbative fields remain valid. For then one can proceed through successive orders of approximation in the usual way, using

$$c_i = \sum_k c_i^{(k)} \lambda^k \quad , \quad H = H_0 + \lambda H_1 \ .$$

Since here the amplitude coefficients c_1 and c_2 are not statistical and do not represent probabilities but are the actual amplitudes of a single electron wave function during a (two level) transition, it is enlightening to verify that such an interpretation can follow the same perturbative argument in a representative case. For a harmonic $H_1(t) = H_1 \cos \omega t$, the first order (in λ) equation, from (6), is

$$c_2^{(1)}(t) = \frac{\langle 2|H_1|1\rangle}{-2h} \left[\frac{e^{i(\omega_{21}+\omega)t_0} - 1}{\omega_{21} + \omega} + \frac{e^{i(\omega_{12}-\omega)t_0} - 1}{\omega_{21} - \omega} \right]$$

where H_1 is applied until t_0 and $t \geq t_0$. If one is considering a process where $\omega_2 > \omega_1$, such as the photoelectric effect in the K- shell of an atom, where the wave functions are given by

$$\psi_1 = (\pi)^{-1/2} \left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{Zr}{a_0}} e^{-i\omega_1 t}$$

$$\psi_2 = (L)^{-3/2} e^{i(\vec{q}\cdot\vec{r}-\omega_2 t)}$$

then the second term of the above equation for c_2 implies an appreciable magnitude only if $\omega_{21} \equiv \omega_2 - \omega_1 = \omega$. Equations (6) then give

$$i\hbar\dot{c}_1 = c_2 \langle u_1|H_1|u_2\rangle \frac{1}{2} e^{i(\omega-\omega_{21})t}$$

$$i\hbar\dot{c}_2 = -c_1 \langle u_1|H_1|u_2\rangle \frac{1}{2} e^{i(\omega_{21}-\omega)t}$$

where $H_{11} = H_{22} = 0$, only the important time dependent term involving $\omega - \omega_{21}$ has been included,[34] and partial integration has been used.

$$H_{12} = \langle u_1|H_1|u_2\rangle = \frac{ie\hbar}{mc}\left(\frac{k}{k_m}\right)^{1/2}\left(\frac{Z}{a_0 L}\right)^{3/2}\pi^{-1/2}\iiint e^{-\frac{Zr}{a_0}} Ae^{-i\vec{k}\cdot\vec{r}}\vec{\epsilon}_1\cdot\nabla e^{i\vec{q}\cdot\vec{r}}\, d^3r \,.$$

Since $\omega - \omega_{21} \simeq 0$, a solution for these equations is:

$$c_1 = \cos H'_{12}t, \quad c_2 = -\sin H'_{12}t, \quad H'_{12} = \frac{1}{2i\hbar} H_{12} \,.$$

Thus the transition (amplitude) proceeds with a speed proportional to H_{12} according to these equations. The differential cross section in a case like this should be proportional to the initial transition probability per unit time to a physical state described by $c_2^2\psi_2^2$; therefore the usual formula[35] follows on evaluation of H_{12}:

$$\frac{d\sigma}{d\Omega} \propto \frac{H_{12}^2}{A^2} \propto \frac{(\vec{\epsilon}_1 \cdot \vec{q})^2}{\left[1 + \left(\frac{a_o}{Z}\right)^2 (\vec{k}-\vec{q})^2\right]^4} .$$

C. USE OF $\vec{j}$

One thus appears to have, in Eq. (2), a connection between the electromagnetic field and the Schrödinger wave function which gives correct results for those stationary and time dependent cases where one can work in terms of charge densities. In order to apply the same ideas to states for which the form of ρ is unknown, as in free electron transitions, it is more convenient to express the equations in terms of a current density $\vec{j}$. This also yields a form which is somewhat simpler for radiation calculations. Therefore, from (2), (5), and the continuity equation,

$$\partial_t \rho = -\nabla \cdot \vec{j} ,$$

the expression for the transition current density must be

$$\vec{j} = \frac{e\hbar}{2im} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{e^2}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \psi \psi^* \vec{A} . \qquad (7)$$

Since ψ here is the superposition wave function (1) (or its generalization), this expression will consist of a number of terms which describe various kinds of current densities. All of the major radiative effects of any two level transition appear to be obtainable by using the terms of (7) as classical sources of electromagnetic radiation. Except for the

inclusion of the last term, this is a typical expression of semiclassical radiation theory.[22] For the two state wave functions considered here Eq. (7) is ($c_i^2 \equiv c_i c_i^*$)

$$\vec{j} = c_1^2 \vec{j}_1 + c_2^2 \vec{j}_2 + c_1 c_2^* \vec{j}_{12^*} + c_1^* c_2 \vec{j}_{1^*2} \tag{8}$$

$$- \frac{e}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} (c_1^2 \rho_1 + c_2^2 \rho_2 + c_1 c_2^* \rho_{12^*} + c_1^* c_2 \rho_{1^*2}) \vec{A} , \tag{8}$$

where $\vec{j}_1$ and $\vec{j}_2$ are the usual quantum mechanical current density expressions corresponding to ρ_1 and ρ_2, and $\vec{j}_{12^*}$ and $\vec{j}_{1^*2}$ are the corresponding expressions for the radiation charge densities $\rho_{12^*} = e\psi_1\psi_2^*$ and $\rho_{1^*2} = e\psi_1^*\psi_2$. These transition current densities, $\vec{j}_{12^*}$ and $\vec{j}_{1^*2} = (\vec{j}_{12^*})^*$ can fully account for the emission of radiation during a transition, from bound states in an atom (emission spectra), or from free states (Brehmsstrahlung). The last term in Eq. (7) gives current densities which are in the same direction as is the incident electromagnetic field and which account for, among other things, the Compton effect (Section III).

The problem of the interaction of radiation and matter according to the present argument then is essentially reduced to the classical evaluation of the radiation patterns produced by the current densities in (8). The usual procedure[6,36] for doing this in this type of problem is based on the retarded wave solution of the inhomogeneous wave equation (Lorentz gauge):

$$\nabla^2\vec{A} - \frac{1}{c^2}\partial_t^2\vec{A} = -\frac{4\pi}{c}\sqrt{k_e k_m}\,\vec{j}_{rad}.$$

$$\therefore \quad A(\vec{r},t) = \iiint\int \frac{\delta(t' - (t - \frac{1}{c}|\vec{r}-\vec{r}'|))}{-4\pi|\vec{r}-\vec{r}'|}\,\frac{4\pi}{c}\sqrt{k_e k_m}\,\vec{j}_{rad}(\vec{r}',t')d^3x'dt'$$

$$= -\iiint \frac{\sqrt{k_e k_m}}{c}\,\frac{\vec{j}_{rad}(\vec{r}',t - \frac{1}{c}|\vec{r}-\vec{r}'|)}{|\vec{r}-\vec{r}'|}\,d^3x'. \qquad (9)$$

This equation is used in Section III with certain of the current densities mentioned above as sources in order to describe the radiation emitted in the Compton effect.

III. THE COMPTON EFFECT

A. SCATTERED RADIATION

The calculation of the cross section for the Compton effect provides a good test of the use of the model discussed above. An important new physical phenomenon appears in the characteristic "photon" type behavior of the radiation pattern produced by a single electron event. The transition considered is shown in Figure 2. The initial and final states are assumed to be free particle states of momenta $\hbar q_i \equiv 0$ and $\hbar q$. For a single electron assumed to be in a pure plane wave state, however, there is an added complication which does not appear with the use of the spatially limited wave functions of the previous section. The plane wave function is an incomplete description of the electron; it provides only a description of its translational motion. There must actually be some underlying spatial structure of relatively small dimensions upon which this translational wave function can be assumed to be superimposed. This is entirely analogous to the separation of the coordinates describing motion of the center of mass and the coordinates describing motion with respect to the center of mass in the solution of the Schrödinger equation for the hydrogen atom. The wave function describing motion of the entire atom must be thought of as superimposed over, and limited to, the structure provided by the usual hydrogen atom relative motion wave function. Therefore the Compton problem is treated here roughly as it is shown in Figure 2 under the

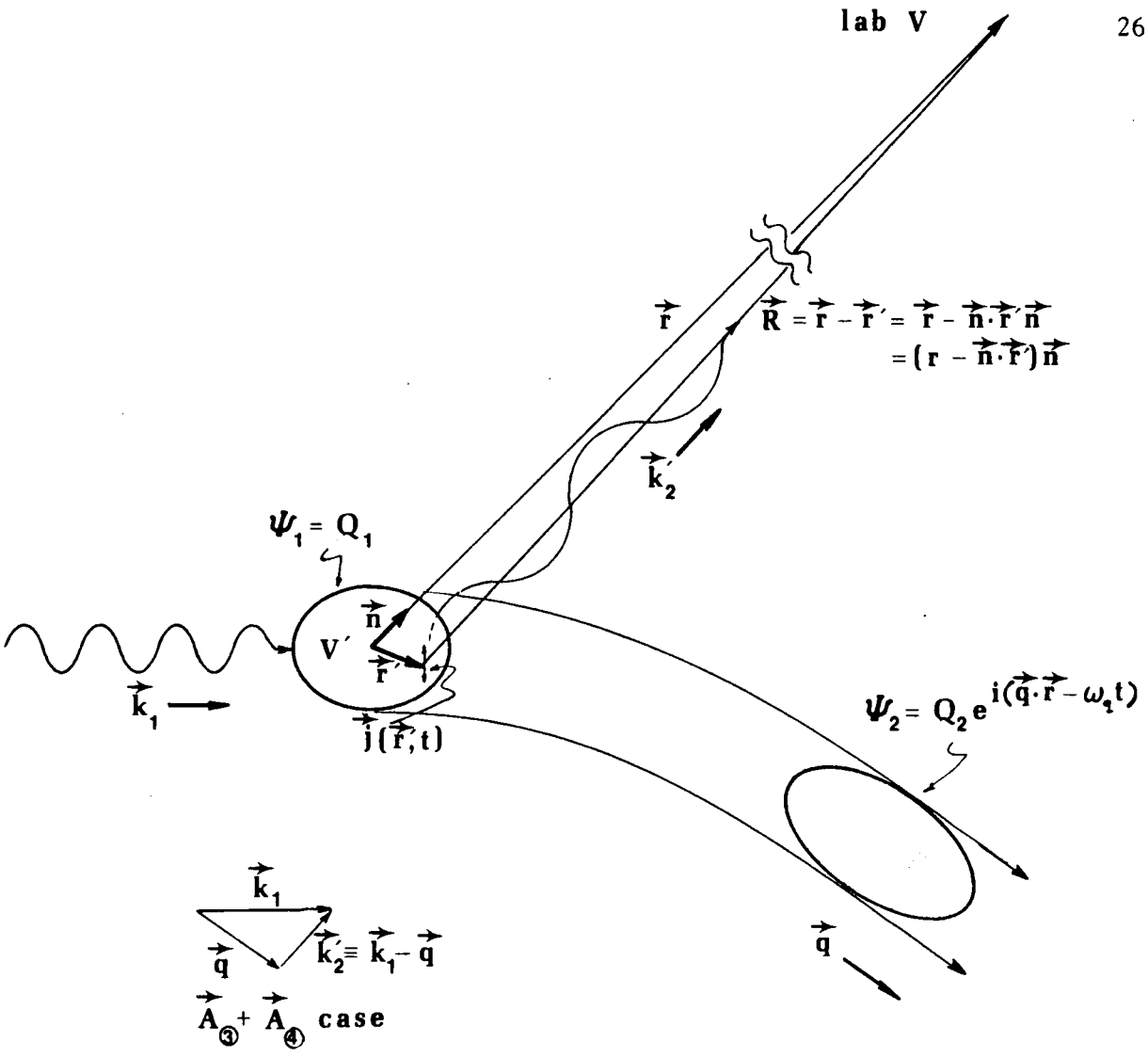

Figure 2. A Compton transition. The initially stationary ($\psi_1 = Q_1 =$ constant) electron charge density is assumed to occupy some small finite volume V' which justifies use of Eq. (9). The transition gives the electron a momentum $\hbar q$. Thus

$$\psi_2 = Q_2 \, e^{i(\vec{q}\cdot\vec{r} - \omega_q t)} \quad .$$

The scattered radiation has wave vector $\vec{k}_2 \equiv \vec{k}_1 - \vec{q}$.

assumption that the various wave functions are limited to some unknown, though small, "interaction" volume V'. The actual size and shape of V' is irrelevant as long as $V' \ll V$ which insures the validity of the approximations used in (9).

The incident radiation is described by:

$$\vec{E}_1 = \frac{1}{2i} E_1 \hat{\epsilon}_1 e^{i(\vec{k}_1 \cdot \vec{r} - \omega_1 t)} + (c.c.) = -\frac{1}{2} \left(\frac{k_e}{k_m}\right)^{1/2} \partial_t \vec{A}$$

$$\vec{A}_1 = -\left(\frac{k_m}{k_e}\right)^{1/2} \frac{cE_1 \vec{\epsilon}_1}{2\omega_1} e^{i(\vec{k}_1 \cdot \vec{r} - \omega_1 t)} + (c.c.) .$$

The amplitude parameters c_1 and c_2 in the transition wave function $c_1\psi_1 + c_2\psi_2$ must first be evaluated from Eqs. (6). The matrix elements to a first approximation (assuming $\vec{A} = \vec{A}_{inc.}$ and plane wave states) are

$$H_{11} \equiv \langle Q_1^* \left| \frac{k_e e^2}{2ik_m \hbar mc^2} \vec{A}^2 + \frac{e}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A} \cdot \nabla \right| Q_1 \rangle$$

$$= \langle Q_1^* | GA^2 \cos^2 (\vec{k}_1 \cdot \vec{r} - \omega_1 t) | Q_1 \rangle = Q_1^2 GA^2 \frac{V'}{2} \qquad (10)$$

where $G = \dfrac{k_e e^2}{2ik_m \hbar mc^2}$, $A = |\vec{A}_1|$, $\nabla \cdot \vec{A} = 0$, Q_i = constant, and the second part of $\hat{H}_1$ gives 0. Also

$$H_{12} \equiv \langle u_1 | H_1 | u_2 \rangle = 0, \quad H_{21} = 0 ,$$

$$H_{22} = \langle Q_2^* e^{-i\vec{q} \cdot \vec{r}} | \hat{H}_1 | Q_2 e^{i\vec{q} \cdot \vec{r}} \rangle = Q_2^2 GA^2 \frac{V'}{2} .$$

If the wave functions are normalized in the volume V', then $H_{11} = H_{22} = \frac{1}{2} GA^2$. Therefore

$$c_1 = B_1 e^{\frac{1}{2} GA^2 t} \quad , \quad c_2 = B_2 e^{\frac{1}{2} GA^2 t} \quad . \tag{11}$$

Since B_1 and B_2 are constants in this approximation, this does not give any useful information on the mechanics of the transition, indicating the need for a more complete evaluation of H_{11}, H_{12}, H_{21}, and H_{22}. Such an evaluation, including the effects of the emitted radiation, is carried out in Section V and a possible form for $B_i(t)$ obtained. However, since G is imaginary, this first order time variation of the c's does not affect the charge or current densities.

The last term of Eq. (7) contains the current density terms which are responsible for the modified radiation component, the Compton radiation. With the use of the transition wave function,

$$\psi = c_1 Q_1 + c_2 Q_2 e^{i(\vec{q}\cdot\vec{r}-\omega_q t)} \quad ,$$

this term becomes

$$\vec{j}_{rad} = -\frac{e^2}{mc}\left(\frac{k_e}{k_m}\right)^{1/2} (c_1 Q_1 + c_2 Q_2 e^{i(\vec{q}\cdot\vec{r}-\omega_q t)}) \times$$

$$(c_1^* Q_1^* + c_2^* Q_2^* e^{-i(\vec{q}\cdot\vec{r}-\omega_q t)}) \frac{A\vec{\varepsilon}_1}{2} (e^{i(\vec{k}_1\cdot\vec{r}-\omega_1 t)} + (c.c.))$$

$$= -\frac{e^2}{2mc}\left(\frac{k_e}{k_m}\right)^{1/2} A\vec{\varepsilon}_1 \{2(c_1^2 Q_1^2 + c_2^2 Q_2^2)\cos(\vec{k}_1\cdot\vec{r}-\omega_1 t)$$

$$+ c_1^* Q_1^* c_2 Q_2 e^{i[(\vec{q}+\vec{k}_1)\cdot\vec{r}-(\omega_q+\omega_1)t]} + c_1 Q_1 c_2^* Q_2^* e^{-i[(\vec{q}+\vec{k}_1)\cdot\vec{r}-(\omega_q+\omega_1)t]}$$

$$+ c_1^* Q_1^* c_2 Q_2 e^{i[(\vec{q}-\vec{k}_1)\cdot\vec{r}-(\omega_q-\omega_1)t]} + c_1 Q_1 c_2^* Q_2^* e^{-i[(\vec{q}-\vec{k}_1)\cdot\vec{r}-(\omega_q-\omega_1)t]}\}$$

$$= \vec{\varepsilon}_1 \frac{e E_1}{2m\omega_1}\{2(c_1^2 Q_1^2 + c_2^2 Q_2^2)\cos(\vec{k}_1\cdot\vec{r}-\omega_1 t) + \textcircled{1} + \textcircled{2}$$

$$+ \textcircled{3} + \textcircled{4} \quad ,$$

since

$$A_1 = -\left(\frac{k_m}{k_e}\right)^{1/2} \frac{cE_1\vec{\varepsilon}_1}{\omega_1}$$

The scattered (modified) radiation is given by the terms (1), (2), (3), and (4) and equation (9):

$$\vec{A}_{2\textcircled{1}} = \frac{-1}{c}\sqrt{k_e k_m}\iiint \frac{[\vec{j}_{rad.\textcircled{1}}]_{ret.}}{|\vec{r}-\vec{r}'|} d^3x'$$

$$= \frac{1}{c}\sqrt{k_e k_m}\iiint \left(\vec{\varepsilon}_1 \frac{e^2 E_1}{2m\omega_1}\right) Q_1 Q_2 B_1 B_2 \frac{1}{R} e^{i\left[(\vec{q}+\vec{k}_1)\cdot\vec{r}' - (\omega_q+\omega_1)(t-\frac{R}{c})\right]} d^3x'$$

$$= \frac{1}{c}\sqrt{k_e k_m}\left(\vec{\varepsilon}_1 \frac{e^2 E_1}{2m\omega_1} Q_1 Q_2 B_1 B_2\right)\frac{1}{r} e^{i(\frac{\omega_2}{c} r-\omega_2 t)} \iiint e^{i(\vec{k}_2 - \frac{\omega_2}{c}\vec{n})\cdot\vec{r}'} d^3x' \quad ,$$

where $R = |\vec{r}-\vec{r}'| = \vec{r}-\vec{n}\cdot\vec{r}'$ with $\vec{r} = r\vec{n}$, $\vec{k}_2 \equiv \vec{q}+\vec{k}_1$, and $\omega_2 \equiv \omega_q+\omega_1$. The last integral can be approximated by $(2\pi)^3\delta^3(\vec{k}_2 - \frac{\omega_2}{c}\vec{n})$. $A_{2\textcircled{2}}$ is evaluated in the same way and, if Q_1, Q_2, B_1, and B_2 are real

$$\vec{A}_{2\textcircled{1}} + \vec{A}_{2\textcircled{2}} = \frac{(2\pi)^3}{c}\sqrt{k_e k_m}\left(\vec{\varepsilon}_1 \frac{e^2 E_1}{m\omega_1} Q_1 Q_2 B_1 B_2\right)\frac{\cos(\vec{k}_2\cdot\vec{r}-\omega_2 t)}{r}\delta^3(\vec{k}_2 - \frac{\omega_2}{c}\vec{n}) \quad . \tag{12}$$

Similarly

$$A_2\textcircled{3} + A_2\textcircled{4} = \frac{(2\pi)^3}{c}\sqrt{k_e k_m}\left(\vec{\epsilon}_1 \frac{e^2 E_1}{m\omega_1} Q_1 Q_2 B_1 B_2\right)\frac{\cos(\vec{k}_2'\cdot\vec{r}-\omega_2' t)}{r}\,\delta\,(\vec{k}_2' - \frac{\omega_2'}{c}\vec{n}) , \tag{13}$$

where $\vec{k}'_2 \equiv \vec{k}_1 - \vec{q}$ and $\omega_2' \equiv \omega_1 - \omega_q$. These equations give typical spherical wave propagation, but the radiation pattern is a sharply defined narrow beam in a direction given by the δ-function. The δ-function thus has a much more physical realization than it may have been supposed. Equation (12), however, allows radiation only in the direction defined by:

$$\vec{q} + \vec{k}_1 = \frac{1}{c}(\omega_q + \omega_1)\vec{n} .$$

But since $\omega_1 = ck_1$ and $\hbar\omega_q = \sqrt{q^2h^2c^2 + m^2c^4}$, $\omega_q + \omega_1 > cq + ck_1$, and the above equation cannot be satisfied. So Eq. (12) gives nothing and the Compton radiation is wholly described by (13).

B. INTERPRETATION AS A CROSS SECTION

Although it is already more or less apparent that Eq. (13) correctly describes the Compton radiation,[17,37] it is a straightforward matter to put it in the usual form of a differential cross section. Thus, if the cosine in Eq. (13) is replaced by a complex exponential (subsequently accounted for in the $\langle\vec{S}\rangle_t$ expression), and primes are dropped, then

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

and

$$\nabla \times \vec{B} = \frac{1}{c}\left(\frac{k_m}{k_e}\right)^{1/2} \partial_t \vec{E}$$

give, in the radiation zone,

$$\vec{E} = \frac{k_2}{k_1}(2\pi)^3 E_1 Q_1 Q_2 B_1 B_2 r_0 \delta^3(\vec{k}_2 - k_2\vec{n})\frac{1}{r}\, e^{i(\vec{k}_2\cdot\vec{r}-\omega_2 t)}\vec{n}\times(\vec{n}\times\vec{\varepsilon}_1) \ ,$$

$$\vec{B} = -\frac{k_2}{k_1}(2\pi)^3 E_1 Q_1 Q_2 B_1 B_2 r_0 \left(\frac{k_m}{k_e}\right)^{1/2} \delta^3(\vec{k}_2 - k_2\vec{n})\frac{1}{r}\, e^{i(\vec{k}_2\cdot\vec{r}-\omega_2 t)}\vec{n}\times\vec{\varepsilon}_1 \ ,$$

where $r_0 = \dfrac{k_e e^2}{mc^2}$ is the classical electron radius. To complete the picture, one must consider the angle which the incident polarization vector makes with the q, k_2 plane. The necessary polarization vectors and angles are shown in Figure 3.

For case (1)

$$-\vec{n}\times\vec{\varepsilon}_1 = \cos\theta\ \vec{\beta}_2 = (-\vec{\varepsilon}_1^{(1)}\cdot\vec{\varepsilon}_2^{(1)})\vec{\beta}_2$$

and for case (2)

$$-\vec{n}\times\vec{\varepsilon}_1 = \vec{\beta}_2 = (-\vec{\varepsilon}_1^{(2)}\cdot\vec{\varepsilon}_2^{(2)})\vec{\beta}_2 \ .$$

Poynting's vector,

$$\langle\vec{S}\rangle_{\text{time}} = \frac{c}{4\pi\sqrt{k_e k_m}}\frac{1}{2}(\vec{E}\times\vec{B}^*) \ ,$$

then gives the radiated power for cases (1) and (2):

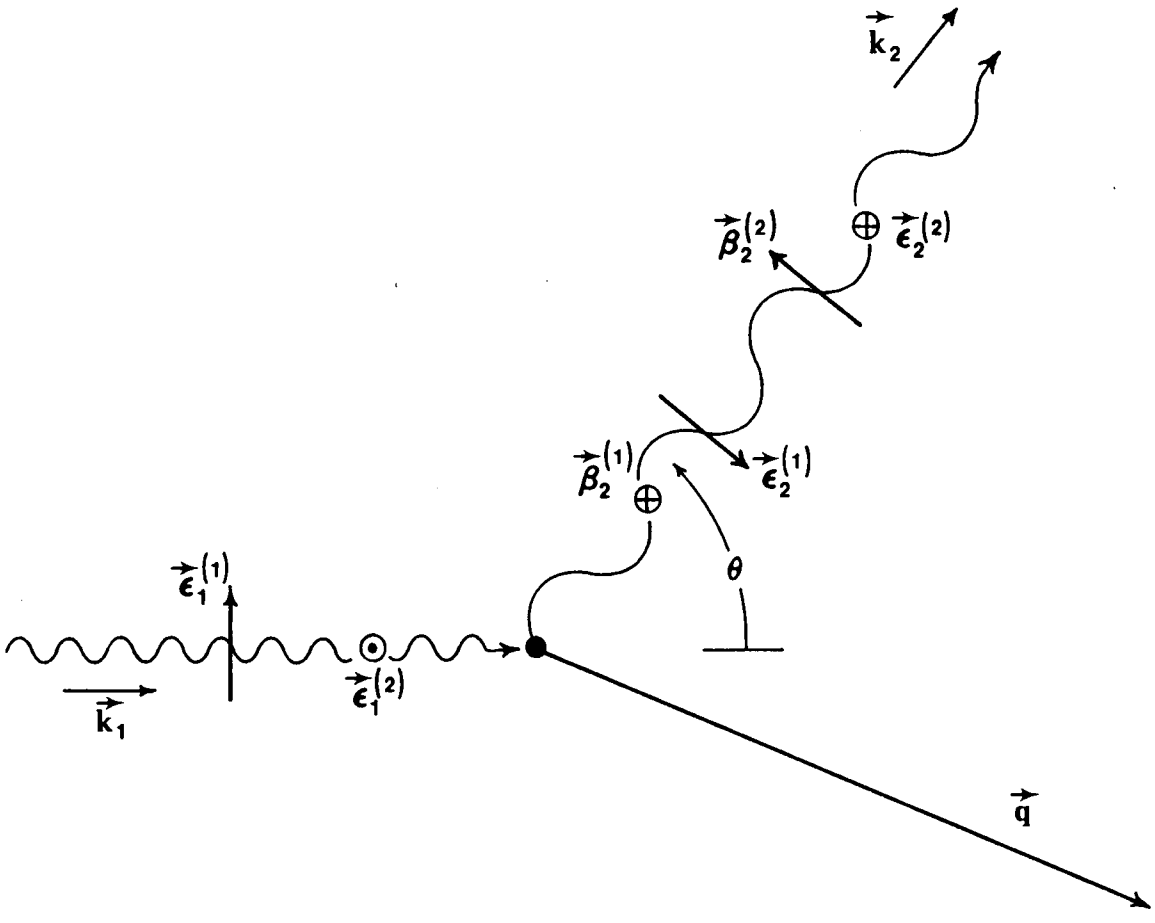

Figure 3. Polarization vectors for cases (1) and (2) of the Compton transition. In case (1) the incident electric field ($\vec{\epsilon}_1^{(1)}$) is in the scattering plane ($\vec{q}$, $\vec{k}_2$ plane); in case (2), the field ($\vec{\epsilon}_1^{(2)}$) is perpendicular to this plane.

$$\langle \vec{S}_1 \rangle_t = \frac{c(2\pi)^6}{8\pi k_e} \left(\frac{k_2}{k_1}\right)^2 (E_1 Q_1 Q_2 B_1 B_2 r_0)^2 \delta^3(\vec{k}_2 - k_2\vec{n}) \frac{\cos^2\Theta}{r^2} \vec{n}$$

$$\langle \vec{S}_2 \rangle_t = \frac{c(2\pi)^6}{8\pi k_e} \left(\frac{k_2}{k_1}\right)^2 (E_1 Q_1 Q_2 B_1 B_2 r_0)^2 \delta^3(\vec{k}_2 - k_2\vec{n}) \frac{\vec{n}}{r^2} .$$

Now $\langle \vec{S} \rangle_t$ is power per unit area; therefore, multiplication by r^2 gives power per unit steradian, $\Pi(\Theta,\phi)$. The incident intensity is

$$\langle \vec{S}_{inc.} \rangle_t = \frac{c}{8\pi k_e} E_1^2 \vec{n}_1 .$$

These formulas for scattered and incident powers per unit area, or intensities, are sufficient to derive the Compton effect cross section. The general definition of a differential cross section is

$$\frac{\Delta I}{I} = \left(\frac{d\sigma}{d\Omega} \Delta\Omega\right) Nx ,$$

in which I is the incident intensity, ΔI is the intensity scattered into the element of solid angle $\Delta\Omega$, and N is the number of targets per unit of target volume of thickness x. This relation may be used with the above expressions for I and $\frac{\Delta I}{\Delta\Omega}$, it being noted that the Nx factor implies that $\frac{d\sigma}{d\Omega}$ must always apply to exactly one particle. However, it is meaningless to try to use these $\langle \vec{S} \rangle_t$ formulas directly in the form in which they are given, since they contain the detailed information on a single event and therefore include a δ-function describing the sharply defined spatial radiation pattern of the individual event and the necessary unknown time dependence, which

regardless of other considerations must be such that $|B_1|^2 = 1$, $|B_2|^2 = 0$ at the beginning of the event and $|B_1|^2 = 0$, $|B_2|^2 = 1$ at the end. Both of these effects, a spatial and a temporal variation, can be eliminated, and are eliminated experimentally, by taking an average over many events per unit volume and over many events per unit time and then referring everything to an amount of matter equal to one particle, which here will not be equivalent to one scattering event. When this is done in the present case, the physical picture resembles that of a large number of pieces of charge density each of which is changing rapidly ($B_i(t)$) in size from zero to maximum and back to zero. When a Compton transition is occurring there is a charge density giving a contribution to the resultant cross section, but when there is no transition there is no Compton effect charge density observed, no electron. One can avoid this rapid time variation problem by working with matter and charge densities entirely, in terms of which the above power formulas are already expressed ($\rho(t) = eQ_1Q_2B_1(t)B_2(t)$) and in terms of which the cross section formula is expressed ($\rho(t) = eN(t)$ = electron charge x number per unit volume). The important thing is to insure that in the above cross section formula there is an exact correspondence between what cross section $\frac{d\sigma}{d\Omega}$ is being measured and what charge density $eN(t)$ is referred to.

In order to apply these ideas in the present case the δ-functions can be expressed in a better form. The volume integral which gives the δ-functions in Eqs. (12) and (13) is actually only over the finite region V' which emits radiation. Therefore

$$(2\pi)^3\delta^3(\vec{k}_2 - \frac{\omega_2}{c}\vec{n}) \langle\equiv\rangle V'\delta_{\vec{k}_2 k_2 \vec{n}} .$$

If this is substituted in the Poynting vector formula for $\langle \vec{S}_1 \rangle_t$ and $\langle S_2 \rangle_t$ and the ratio of $\Pi_1(\Theta)$ and $\Pi_2(\Theta)$ to $\langle \vec{S}_{inc.} \rangle_t$ obtained, the resulting expressions,

$$\frac{\Pi_1(\Theta)}{\langle S_{inc.} \rangle_t} = K^2 r_0^2 \left(\frac{k_2}{k_1}\right)^2 \cos^2\Theta \, \delta_{\vec{k}_2 k_2 \vec{n}} ,$$

$$\frac{\Pi_2(\Theta)}{\langle S_{inc.} \rangle_t} = K^2 r_0^2 \left(\frac{k_2}{k_1}\right)^2 \delta_{\vec{k}_2 k_2 \vec{n}} ,$$

where $K^2 = (Q_1 Q_2 B_1(t) B_2(t) V')^2$, give the fractional scattering per unit steradian for a single Compton event. Now it can be assumed that the transition wave function of a particular event is normalized to one particle in the interaction volume V',

$$\iiint_{V'} \psi\psi^* d^3r = 1 ,$$

which implies that $V'|B_1 Q_1|^2 + V'|B_2 Q_2|^2 = 1$, or $Q_1 = Q_2 = \frac{1}{\sqrt{V'}}$ and $|B_1|^2 + |B_2|^2 = 1$. The oscillating charge density proportional to $eB_1 B_2 Q_1 Q_2$ which is responsible for the emission of the radiation during the transition gives no net contribution to the above integral, however, although it is the radiation charge density for which the Compton cross section must be expressed. Thus, in keeping with the ideas discussed above, $\frac{d\sigma}{d\Omega}$ must be put in terms of the matter or charge density which causes it and it must refer to one particle. Therefore

the radiation charge density must be divided by the radiation particle density, which essentially normalizes (instantaneously) the radiating charge to that associated with one particle:

$$\frac{eQ_1Q_2B_1(t)B_2(t)}{Q_1Q_2B_1(t)B_2(t)} = e \ .$$

That is, from a fraction $V'Q_1Q_2B_1B_2$ of a particle, effects depending on a charge $eV'Q_1Q_2B_1B_2$ are obtained; therefore from one particle (which defines $\frac{d\sigma}{d\Omega}$) the effects will be due to a charge e. The Kronecker delta causes no problem, since, just as for the time dependent $B_i(t)$, it is actually a result of looking in detail at a single event. It will not appear in an average cross section.

Another way of arriving at the same conclusions follows from consideration of a spatial average over a large number of events as shown in Figure 4. The total radiation charge density contributing to Π_T is

$$\rho_T = \frac{q}{V} = \sum_i e\, B_1^{(i)}B_2^{(i)}Q_1^{(i)}Q_2^{(i)} \equiv \sum_i eK^{(i)} \ .$$

Therefore,

$$\frac{\Pi_T}{\langle S_{inc.}\rangle_t} + \left(\sum_i K_i\right)^2 r_0^2 \left(\frac{k_2}{k_1}\right)^2 \begin{bmatrix} \cos^2\Theta \\ 1 \end{bmatrix} .$$

But to determine the single electron cross section one must divide ρ_T by the number per unit volume of observable particles, which is

$$n_T = \frac{N_T}{V} = \sum_i B_1^{(i)}B_2^{(i)}Q_1^{(i)}Q_2^{(i)} = \sum_i K^{(i)} \ .$$

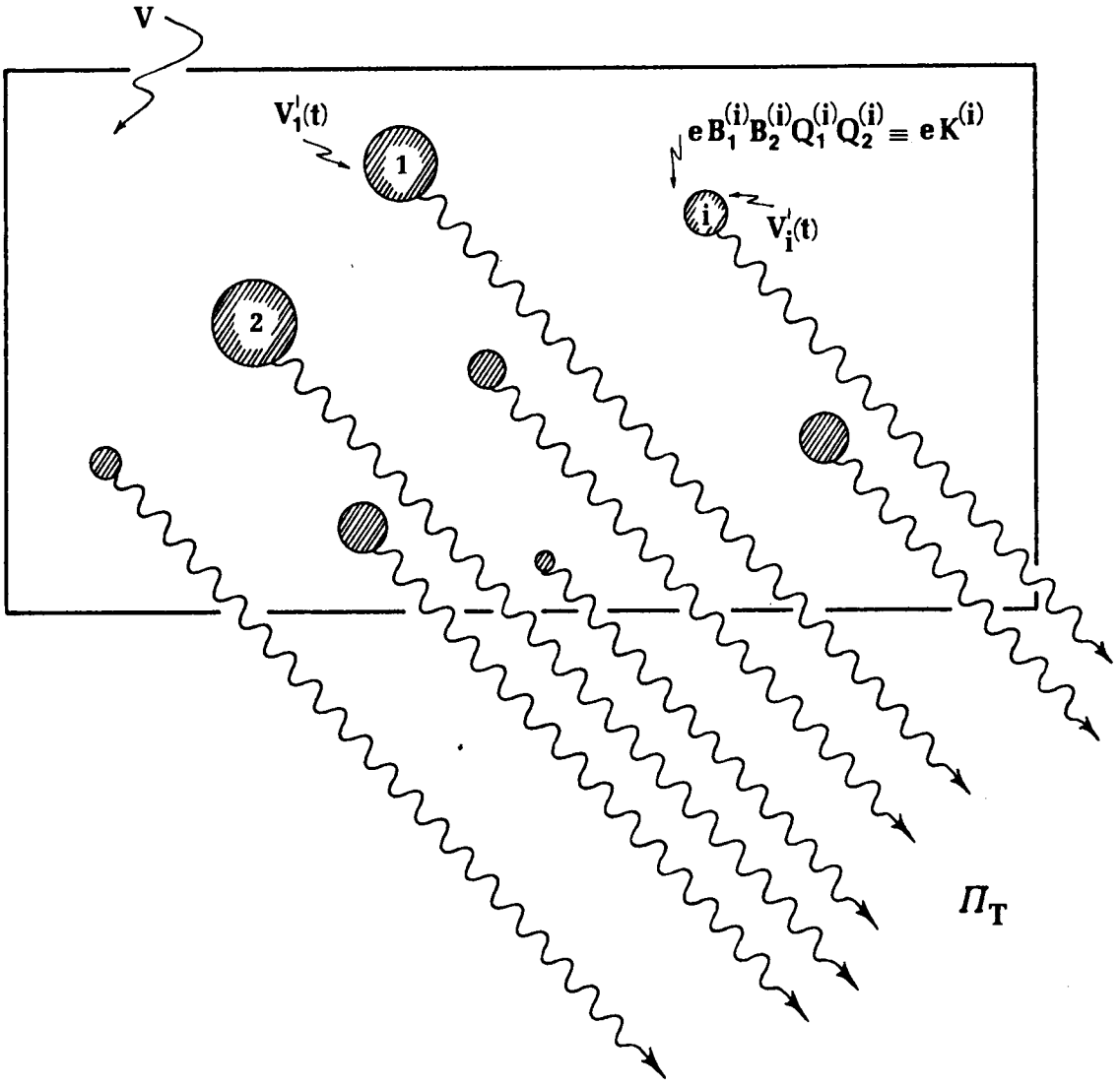

Figure 4. Space and time average for the Compton effect. An average over many Compton events in the determination of the cross section eliminates both the $B_i(t)$ time dependence and the δ-function spatial dependence of an individual event. In a similar way, the fractional charge density $eB_1^{(i)}B_2^{(i)}Q_1^{(i)}Q_2^{(i)}$ does not appear in the cross section.

Finally then, the correct cross section will be obtained from

$$\frac{d\sigma}{d\Omega} = \frac{1}{n_T^2} \frac{\Pi_T}{\langle \vec{S}_{inc.} \rangle_t}$$

and, for unpolarized incident radiation will be

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} r_0^2 \left(\frac{k_2}{k_1}\right)^2 (1 + \cos^2\theta) \ , \tag{14}$$

which may be compared with the Klein-Nishina cross section for the Compton effect. Dirac wave functions might be expected to give an exact correspondence, although the derivation could not follow the present nonrelativistic one since there exists no separate term involving $\vec{A}$ in the current density for the Dirac equation. In addition, the present analysis in terms of a constant incident intensity is not directly applicable to modern experiments in which γ-rays are used.[38] In that case the intensities can be interpreted as photons/time (photons in the nature of the above discussion) and the cross section as the probability of a certain event, as usual.

The final result here is, of course, nothing new, and even Klein and Nishina's original argument was semiclassical.[6] They considered the Dirac equation for an electron in an incident radiation field $\vec{A}$,

$$c\vec{\alpha} \cdot \left(\frac{h}{i} \nabla - \frac{e}{c} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}\right)\Phi + \beta \ mc^2\Phi = - \frac{h}{i} \partial_t \Phi \ ,$$

where the vector potential is given by,

$$\vec{A} = \vec{\varepsilon}_1 (Ae^{i(\vec{k}\cdot\vec{r}-\omega t)} + Ae^{-i(\vec{k}\cdot\vec{r}-\omega t)}) ,$$

and assumed solutions of the form

$$\Phi = ue^{-\frac{i}{\hbar}(\vec{p}\cdot\vec{r}-Et)}\left(1 + f(\vec{p})e^{-i(\vec{k}\cdot\vec{r}-\omega t)} + \bar{f}(\vec{p})e^{i(\vec{k}\cdot\vec{r}-\omega t)}\right) ,$$

where u is a four component spinor for a free electron of momentum $\vec{p}$ and energy E, and $f(\vec{p})$ and $\bar{f}(\vec{p})$ are constant four dimensional matrices. They then determined the f, $\bar{f}$ matrices by substituting Φ in the Dirac equation. The current density, $\vec{j}$, from

$$\vec{j} = ec\Phi^{+}\vec{\alpha}\Phi ,$$

could then be used to obtain the scattered radiation vector potential $\vec{A}'$ in much the same manner as was used above (Eq. (9)). Calculating $\vec{B}$ from $\vec{B}' = \nabla \times \vec{A}'$, Klein and Nishina obtained,

$$\vec{B}'^2 = k_m \frac{r_0^2}{r^2} \left(\frac{\nu'}{\nu}\right)^3 \left[\left(\frac{\nu}{\nu'} + \frac{\nu'}{\nu}\right)\vec{\varepsilon}^2 - 2(\vec{n}' \cdot \vec{\varepsilon})^2\right] .$$

from which the usual formula follows:

$$I = I_0 \frac{r_0^2}{r^2} \frac{\sin^2\phi}{(1 + \alpha(1 - \cos\Theta))^3} \left[1 + \alpha^2 \frac{(1 - \cos\Theta)^2}{2\sin^2\phi[1 + \alpha(1 - \cos\Theta)]}\right]$$

with $\vec{n} \cdot \vec{\varepsilon} = \cos\phi$, $\vec{n}' \cdot \vec{k} = \cos\Theta$, and $\alpha = \frac{h\nu}{mc^2}$. This can be put in a form for comparison with Eq. (10) by writing it in terms of a cross section for photon scattering rather than energy scattering. This removes one factor of $\frac{h\nu'}{h\nu} = \frac{1}{(1 + \alpha(1 - \cos\Theta))}$ from the right hand side

of the above equation. For unpolarized radiation an average of

$$\sin^2\phi \equiv 1 - \sin^2\theta \cos^2\psi$$

over the angle ψ between the scattering plane and polarization plane yields a factor $\frac{1}{2}(1 + \cos^2\theta)$. Thus,

$$\frac{d\sigma}{d\Omega} = \frac{(4\pi r^2)I}{(4\pi)I_0}\left(\frac{h\nu}{h\nu'}\right) = \frac{1}{2}r_0\left(\frac{h\nu'}{h\nu}\right)^2(1+\cos^2\theta)\left[1+\alpha^2\frac{(1-\cos\theta)^2}{(1+\cos^2\theta)(1+\alpha(1-\cos\theta))}\right].$$

For the nonrelativistic case the assumption that α is small reduces this to Eq. (14). Without the $\frac{k_2}{k_1}$ factor, this is just the Thomson scattering cross section. There is, however, no appearance in this derivation of the experimentally verified discrete nature of the scattered radiation. The method used in the present work is notable in this regard since it is a natural and completely classical extension of present day semi-classical ideas and, in addition, appears to reveal a classical origin of the "photon" behavior of electromagnetic radiation.

IV. A CLASSICAL EXPLANATION OF THE LAMB SHIFT

The success of a classical treatment of quantum mechanical transitions involving radiation leads one to consider the application of similar methods to certain phenomena which seem to have their best and simplest explanations in terms of quantum electrodynamics. A prime example is the Lamb shift,[39] which seems to have a clear cut (if not really physically plausible) interpretation according to QED,[40,41] but whose semiclassical explanation involves some unusual effects.[22] A different argument, based in a fundamental way on a classical view of the electromagnetic field, is presented here, yielding a result for the well-known hydrogen shift which is in good agreement with experiment.

A. FIELD ENERGY CALCULATIONS

The $2^2P_{1/2}$ $2^2S_{1/2}$ transition in hydrogen is considered for which the best experimental value of the frequency of the emitted radiation is

$$\nu = 1057.893 \text{ MHz}$$

while according to the Schrödinger and Dirac equations the two levels should be degenerate. In accord with classical ideas, this energy shift is ascribed to the effects of the energies contained in the electric and magnetic fields of the two spatial wave functions involved. These fields are calculated from $\rho = e\psi\psi^*$ and $\vec{j} = \frac{eh}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*)$, and their

successful use indicates that there is no need here to hypothesize a point electron. For the present purposes, $e\psi\psi^*$ is the electron.

The wave functions involved are:

$$\psi_{200} = \sqrt{\frac{1}{32\pi a_o^3}}\left(2 - \frac{r}{a_o}\right) e^{-\frac{r}{2a_o}}$$

$$\psi_{21\pm1} = \sqrt{\frac{1}{64\pi a_o^3}}\frac{r}{a_o} e^{-\frac{r}{2a_o}} \sin\Theta\, e^{\pm i\phi} .$$

The potential due to $\rho_{211} = e\psi_{211}\psi_{211}^*$ can be calculated from a spherical coordinate expansion of the appropriate Green's function:

$$V = \iiint \frac{k_e \rho'_{211}}{|\vec{r}-\vec{r}'|} d^3r'$$

$$= \iiint (-4\pi k_e \rho'_{211})\, G(\vec{r},\vec{r}')\, d^3r'$$

$$V = \iiint 4\pi k_e K^2 \left(\frac{r'}{a_o}\right)^2 e^{-\frac{r'}{a_o}} \sum_{\ell=0}^{\infty} \sum_{m=\ell}^{\ell} \frac{1}{2\ell+1} \frac{r_<^{\ell}}{r_>^{\ell+1}} Y_{\ell m}^*(\Theta',\phi') Y_{\ell m}(\Theta,\phi) \sin^2\Theta' d^3r'.$$

This yields

$$V = \frac{A}{a_o x}\left[24 - e^{-x}(x^3 + 6x^2 + 18x + 24)\right] +$$

$$\frac{AP_2(\cos\Theta)}{a_o x^3}\left[e^{-x}(x^5 + 6x^4 + 24x^3 + 72x^2 + 144x + 144) - 144\right]$$

where $A = \frac{8}{3}\pi k_e e K^2 a_o^3$, $K = \sqrt{\frac{1}{64\pi a_o}}$, and $x = \frac{r}{a_o}$. Therefore the electric field components are:

$$E_r = -\frac{1}{a_o}\frac{\partial V}{\partial x} = \frac{A}{a_o}\left[\frac{24}{x^2} - e^{-x}(x^2 + 4x + 12 + \frac{24}{x} + \frac{24}{x^2})\right.$$

$$+ e^{-x} P_2(\cos\Theta)(x^2 + 4x + 18 + \frac{72}{x} + \frac{216}{x^2} + \frac{432}{x^3} + \frac{432}{x^4})$$

$$\left. - 432\frac{P_2(\cos\Theta)}{x^4}\right] \qquad (15)$$

$$E_\Theta = -\frac{1}{a_o x}\frac{\partial V}{\partial \Theta} = \frac{A}{a_o^2 x^4}\left[e^{-x}(x^5 + 6x^4 + 24x^3 + 72x^2 + 144x + 144)\right.$$

$$\left. - 144\right] (3\cos\Theta\sin\Theta) .$$

The magnetic field of the ψ_{211} wave function is calculated by a method[42] which involves expressing a current density which has only a ϕ component on a spherical shell of radius r' in the form

$$j_\phi = -\sum_{n=1}^{\infty}\frac{C_n}{r'} P_n^1(\cos\Theta) .$$

The vector potential due to the shell is then given by

$$\vec{A} = \frac{4\pi}{c}\sqrt{k_e k_m}\,\vec{e}_\phi \sum_{n=1}^{\infty}\frac{-C_n}{2n+1}\left(\frac{r}{r'}\right)^n P_n^1(\cos\Theta),\ r<r'$$

$$\vec{A} = \frac{4\pi}{c}\sqrt{k_e k_m}\,\vec{e}_\phi \sum_{n=1}^{\infty}\frac{-C_n}{2n+1}\left(\frac{r'}{r}\right)^{n+1} P_n^1(\cos\Theta),\ r>r' .$$

In the present case, for the shell r = r'

$$\vec{j}'_{211} = \frac{e\hbar K^2}{ma_o^2} r' e^{\frac{r'}{-a_o}} \sin\Theta'\,\vec{e}_\phi$$

and

$$C_1' = - \frac{e\hbar K^2}{ma_o^2} r' 2e^{\frac{r'}{-a_o}}$$

$$C_i = 0 \quad , \quad i \neq 1 \ .$$

The B_Θ and B_r components for this shell are then:

$$B_r = - \frac{4\pi}{c} \sqrt{k_e k_m} \frac{2C_1'}{3r^1} \cos \Theta, \ r < r'$$

$$B_r = - \frac{4\pi}{c} \sqrt{k_e k_m} \frac{2C_1'}{3} \left(\frac{r^1}{r}\right)^3 \cos \Theta, \ r > r'$$

$$B_\Theta = \frac{4\pi}{c} \sqrt{k_e k_m} \frac{2C_1'}{3r'} \sin \Theta, \ r < r'$$

$$B_\Theta = - \frac{4\pi}{c} \sqrt{k_e k_m} \frac{C'}{3r'} \left(\frac{r'}{r}\right)^3 \sin \Theta, \ r > r' \ .$$

Integration over shells from r' = 0 to ∞ then gives the total fields:

$$B_r = \frac{2}{3} D \cos \Theta \left(\frac{24}{x^3} - \frac{e^{-x}}{x^3} (x^4 + 4x^3 + 12x^2 + 24x + 24) \right.$$

$$\left. + e^{-x} (x + 1) \right) \ ,$$

$$B_\Theta = \frac{1}{3} D \sin \Theta \left(\frac{24}{x^3} - \frac{e^{-x}}{x^3} (x^4 + 4x^3 + 12x^2 + 24x + 24) - 2e^{-x}(x + 1) \right). \tag{16}$$

where $D = \frac{4\pi}{c} \sqrt{k_e k_m} \frac{e\hbar K^2}{m}$, $x = \frac{r}{a_o}$.

The classical energies in the fields are then calculated from (15), (16), and the expressions

$$U_E = \iiint \frac{E_r^2 + E_\Theta^2}{8\pi k_e} d^3r$$

$$U_B = \iiint \frac{B_r^2 + B_\Theta^2}{8\pi k_m} d^3r \ .$$

An exact analytical evaluation of these integrals in the ψ_{211} case gives:

$$U_{E_{211}} = U_{E_r} + U_{E_\Theta} = \frac{A^2}{a_o k_e} (51.0191 + .8339)$$

$$= 2.44966 \text{ eV} \quad ,$$

$$U_{B_{211}} = U_{B_r} + U_{B_\Theta} = 2.31502 \times 10^{-6} \text{ eV} + .98693 \times 10^{-6} \text{ eV}$$

$$= 3.30195 \times 10^{-6} \text{ eV} \ .$$

A similar calculation for the ψ_{200} wave function gives the following:

$$V = \frac{C}{x} \left\{ 8 - e^{-x}(x^3 + 2x^2 + 6x + 8) \right\} \ ,$$

with $C = 4\pi k_e \ e \ K_1^2 \ a_o^2$, $K_1 = \sqrt{\frac{1}{32 \ a_o^3}}$, $x = \frac{r}{a_o}$,

$$E_r = \frac{C}{a_o x^2} \left\{ 8 - e^{-x} \ (x^4 + 4x^2 + 8x + 8) \right\} \ ,$$

and

$$U_{E_{200}} = (9.625) \frac{a_o C}{k_e} = 4.0924 \text{ eV}$$

$$U_{B_{200}} = 0 \ .$$

B. VELOCITY EFFECTS

It must now be determined in what way these field energies alter the quantum mechanical energy levels. The energies expressed by the Schrödinger equation, which the frequencies of the wave function solutions represent, reflect states of translational motion.[43] One could thus look for effects which would shift the kinetic energy of one state with respect to the other. As will be seen below, there are such classical energies which, if interpreted in a certain way, would provide a very good value for the hydrogen $2S_{\frac{1}{2}}$-$2P_{\frac{1}{2}}$ shift. Further consideration in Section IVC will show that these energies cannot account directly for the Lamb shift but that in general it must actually be the result of a different, though intimately related, effect of the field energies. However, since this analysis of the kinetic energy changes is essential to the subsequent more general discussion, it is presented first. To begin with then, the large difference in electric field energies, which is of the order of $\sim$2 eV in the present case, would not show up as a frequency difference between the wave functions. Rather, one can easily show that it is exactly equivalent to the self potential energy change of the charge density distribution for the transition under consideration.[36] If one ignores the field due to the positive nucleus and works only with the charge density $\rho = e\psi_{n\ell m}\psi^*_{n\ell m}$ of the electron, its electrostatic self potential energy can be written

$$W = \frac{k_e}{2} \iint \frac{\rho(\vec{r})\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} \, d^3r \, d^3r' \ .$$

One of the volume integrals in this expression is just the potential V of $\rho(\vec{r})$, therefore

$$W = \frac{1}{2} \int \rho(\vec{r}) V(\vec{r}) d^3r \ .$$

One can then use Poisson's equation and integration by parts to give

$$W = \frac{-1}{8\pi k_e} \int V \nabla^2 V d^3r$$

$$= \frac{1}{8\pi k_e} \int |\nabla V|^2 d^3r$$

$$= \frac{1}{8\pi k_e} \int |\vec{E}|^2 d^3r$$

$$= U_E \ .$$

The change in U_E is therefore another way of expressing part of the change in the total potential energy of ρ as it proceeds in its transformation from one energy eigenstate to another. That is, $U_{E_{211}}$ and $U_{E_{200}}$ are already included as unobservable self energies in the ψ_{211} and ψ_{200} states; and if these states are degenerate according to the Schrödinger equation, the degeneracy is entirely independent of the values of $U_{E_{211}}$ and $U_{E_{200}}$. They can really be identified with part of the infinite mass renormalization energy in quantum electrodynamics. On the other hand, the magnetic field energy of the ψ_{211} state is created by the electron motion associated with the state and could possibly show up in the wave function frequency. This electron velocity effect would also change the electric field energy slightly. Both of these effects

can be seen if the electron with its static electric field is assumed to be moving with velocity $\vec{v}$ (Figure 5). Fields due to the electron charge density, $\vec{E}'$ and $\vec{B}'$ in the electron rest frame, become in the atomic frame $(\vec{E}, \vec{B})$:

$$\vec{E} = \gamma(\vec{E}' + \frac{1}{c}\left(\frac{k_e}{k_m}\right)^{1/2} \vec{v} \times \vec{B}')$$

$$\vec{B} = \gamma(\vec{B}' - \frac{1}{c}\left(\frac{k_m}{k_e}\right)^{1/2} \vec{v} \times \vec{E}')$$

where $\gamma = (1 - \frac{v^2}{c^2})^{-1/2}$. $\vec{v}$ represents the assumed motion of $\vec{E}'$ and $\vec{B}'$ with respect to the atomic frame and need not be further specified except to hypothesize that it has the direction of $\langle \frac{\hbar}{im} \nabla \rangle_{n\ell m}$ for state $\psi_{n\ell m}$. For $\psi_{21\pm1}$ this will be the ϕ direction, $\hat{e}_\phi$. So the $\vec{B}$ field of the orbit is essentially due to $\gamma \frac{1}{c}\left(\frac{k_m}{k_e}\right)^{1/2} \vec{v} \times \vec{E}'$ since the orbital $B' = 0$ in the electron frame. The electric field $\vec{E}$ in the atomic frame is given by

$$\vec{E} = \gamma \vec{E} = (1 - \beta^2)^{-1/2} \vec{E}'$$

$$\cong \vec{E}' + \frac{1}{2}\beta^2 \vec{E}'$$

$$8\pi k_e u_{E_{211}} = (\vec{E}' + \frac{1}{2}\beta^2 \vec{E}_1')^2 \cong E'^2 + \beta^2 E'^2 .$$

The extra energy density due to motion is then

$$\Delta u_{E_{211}} = \beta^2 u_{E_{211}\text{original}} ,$$

under the assumption that $\vec{E}'$ can be replaced by $\vec{E}$ on the right-hand side of the above equations.

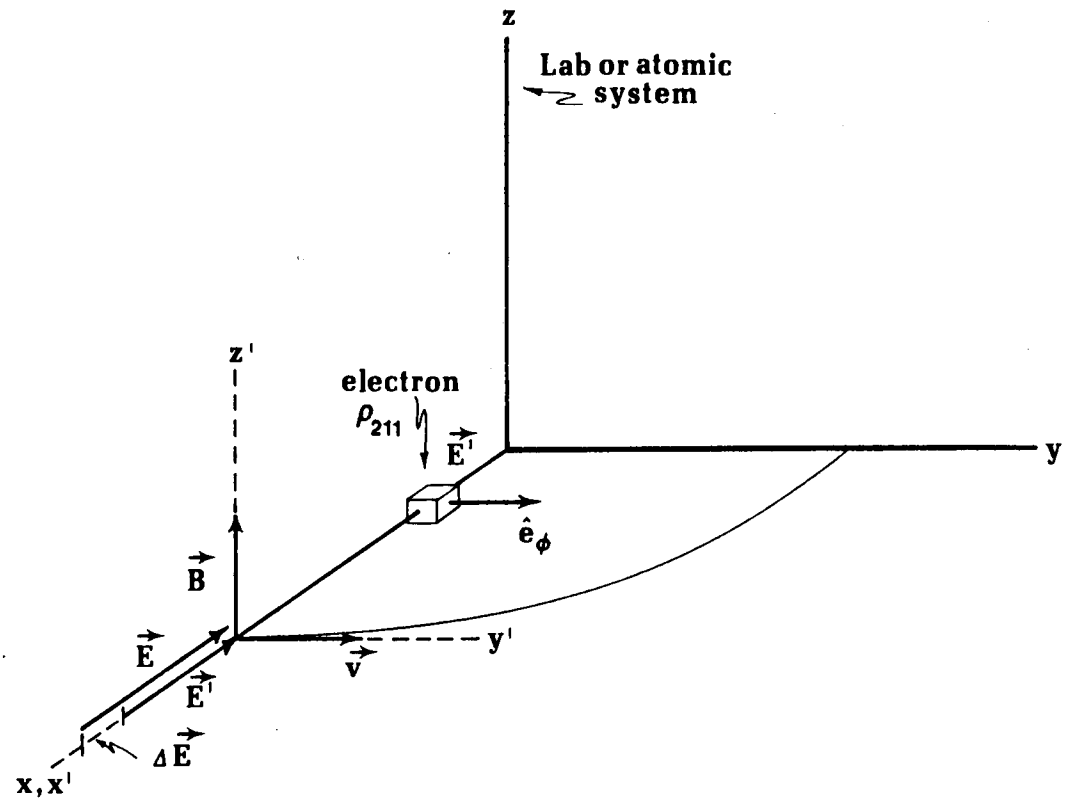

Figure 5. Field transformations. The essentially undeterminable velocity of the ρ_{211} charge density causes small differences between $\vec{E}'$ "attached" to the electron and the fields $\vec{E}$ and $\vec{B}$ observed in the lab.

This can be evaluated simply, without attempting to find v by noting that

$$\vec{B} = \gamma \frac{1}{c} \left(\frac{k_m}{k_e}\right)^{1/2} \vec{v} \times \vec{E}' = -\vec{e}_B \gamma \frac{1}{c} \left(\frac{k_m}{k_e}\right)^{1/2} |\vec{v}||\vec{E}'| \ .$$

Therefore $\vec{B}^2 \tilde{=} \frac{k_m}{k_e} \beta^2 E^2$.

The extra energy due to motion of the $\vec{E}'$ field is then

$$\Delta U_{E_{211}} = \frac{1}{8\pi k_e} \iiint \beta^2 E^2 d^3r = \frac{1}{8\pi k_m} \iiint B^2 d^3r = U_{B_{211}}$$

as one would perhaps suspect.

The total change in energy of the ψ_{211} state due to the creation of electric and magnetic fields by the velocity $\vec{v}_{211}$ is

$$U_{B_{211}} + \Delta U_E = 2(3.30195 \times 10^{-6} \text{ eV})$$

$$= 6.6039 \times 10^{-6} \text{ eV} \ .$$

The transition involved is from the $^2P_{1/2}$ state, which can be written as $\sqrt{\frac{1}{3}} (\sqrt{2}\, Y_{11}(\downarrow) - Y_{10}(\uparrow))$ for $m_j = \frac{1}{2}$ and $\sqrt{\frac{1}{3}} (-\sqrt{2}\, Y_{1,-1}(\uparrow) + Y_{10}(\downarrow))$ for $m_j = -\frac{1}{2}$, to the $^2S_{1/2}$ state, which can be $Y_{00}(\uparrow)$ or $Y_{00}(\downarrow)$. Thus the $^2P_{1/2}$ state is a mixture whose charge and current densities are $\frac{2}{3}$ due to $\psi_{21\pm1}$ if the effects of spin can be ignored. The $^2P_{1/2}$ level would then be shifted with respect to $^2S_{1/2}$ by

$$U_{Lamb} = \frac{2}{3} (6.6039 \times 10^{-6} \text{ eV})$$

$$= 4.4026 \times 10^{-6} \text{ eV} .$$

Then

$$\Delta\nu_{Lamb} = 1064.57 \text{ MHz} = .0355102 \text{ cm}^{-1}$$

which is very close to the experimental value[45,46] given previously, 1057.7 MHz.

C. INCLUSION OF ALL FIELD ENERGY EFFECTS

As good as this result is for the famous hydrogen shift, however, other experimental results indicate that the energies in such "velocity created" fields must be included with the electrostatic self energies as unobservable "renormalization" contributions to the electron mass and thus cannot be the cause of the Lamb shift. If it were correct, the preceding analysis should be applicable with almost no change to certain other atoms and ions in addition to some other states in hydrogen itself. For example, s levels in hydrogen should not be shifted at all by these velocity induced changes in the electromagnetic fields. In 1956, however, Herzberg carried out a difficult measurement of the $1S \leftrightarrow 2P$ absorption line in deuterium, looking for a wavelength shift of about .004 Å in the ultraviolet line at 1215 Å. A major problem was the lack of reference lines in this wavelength region against which the shift could be detected. He reported a shift of the 1S level of about .262 cm^{-1}, which was in good agreement with the theoretical QED value of

.273 cm^{-1}.[47] This result appears to be in marked disagreement with the present discussion, but there are other effects for this case which leave the issue in doubt. For example, Jaynes' neoclassical theory of the Lamb shift, which, as will be seen in Section IV, can be combined with the foregoing analysis for certain experimental conditions predicts .278 cm^{-1} for this shift. Recent laser measurements of the $1S_{1/2}$-$2S_{1/2}$ transition in hydrogen by "two photon" absorption[48] indicate a similar shift, in agreement with the QED value; however, Jaynes type of procedure may also be applicable in this case. On the other hand, there have been some recent experiments on hydrogen-like atoms and ions (one electron) in which the $2^2S_{1/2} \rightarrow 2^2P_{1/2}$ transition has been measured[49] and for which the above derivation should be applicable with only a change in atomic number Z and/or a_o. The Z and a_o dependence of the energies ΔU_E and U_B can be determined by replacing $\frac{1}{a_o}$ in the wave functions by $\frac{Z}{a_o'}$ and by carrying this through the analysis. This gives

$$U_E \quad (\frac{Z}{a_o'})^3 ,$$

$$U_B \quad (\frac{Z}{a_o'})^3 ,$$

where $a_o' = a_o(1 + \frac{m}{M})$, $a_o = \frac{\hbar}{k_e m e^2} = 5.2917706 \times 10^{-11}$ m, m = electron mass, and M = nuclear mass. Then for any one electron atom or ion the $2^2S_{1/2} \rightarrow 2^2P_{1/2}$ Lamb shift should be given by

$$\frac{\nu_{Z,M}}{\nu_H} = \frac{U_{Z,M}}{U_H} = (\frac{Z}{a'_{oM}})^3 \div (\frac{1}{a'_{oH}})^3 = (\frac{Za'_{oH}}{a'_{oM}})^3 .$$

For deuterium, for example, M = 1875.628 MeV, m = .5110034 MeV, and Z = 1. Therefore:

$$\frac{\nu_D}{\nu_H} = \left(\frac{a'_{oD}}{a'_{oH}}\right)^3 = \left(\frac{1.0005446}{1.0002724}\right)^3 = 1.0008165 \ .$$

Using the H shift obtained above, one obtains

$$\nu_D = 1065.439 \text{ MHz} \ ,$$

which corresponds with the measured value (1059.24 MHz) as closely as does the value for hydrogen. Neglecting the small change in a'_o for higher M and Z ions, one can also easily check the Z dependence predicted above, under the assumption that the entire shift for these ions is due to the energy changes discussed above for hydrogen. Therefore, the frequencies should obey

$$\nu_Z \simeq Z^3 \nu_H \ ,$$

giving 8516.56 MHz for $^4_2He^+$ (the experimental value is 14,040 MHz) and 28,743.39 MHz for $^6Li^{+2}$ (the experimental value is 63,031 MHz).[49] The comparisons for $^{12}C^{+5}$ and $^{16}O^{+7}$ show similar disagreement. The experimental values in fact show roughly a Z^4 dependence, and apparently fit the quantum electrodynamic calculations (including vacuum polarization, nuclear size effects, higher order corrections, etc.) very well. The Z^3 variation therefore represents a serious disagreement with experiment for any ion with $Z > 1$ and indicates that something is wrong with this "velocity effect" calculation. However,

it also provides an important hint towards a resolution of the problem. The factor of Z by which Z^3 and Z^4 differ is just the factor which appears in the nuclear charge, Coulomb potential, and electric field of an ion of atomic number Z. One must then ask what effects the nuclear electric field might have on the fields of the electron which supposedly move through it and how all of the fields, which are in relative motion, might interact. The nuclear electric field would contribute a factor Z in any of its interactions.

So it is necessary to begin with a complete expression for the fields in the vicinity of the ion. In addition to the previously calculated electric field E_- of the electric charge density there will be the nuclear Coulomb field just mentioned,

$$\vec{E}_+ = \frac{k_e Z e}{r^2} \vec{n} \ .$$

For most of space this field essentially cancels $\vec{E}_-$ (actually only for Z = 1) and so will certainly have significant effects on the field energies. The energy which has apparently disappeared, due to the fact that $\vec{E}_+ \cdot \vec{E}_- \cong 0$ for a large part of the space around the atom, is easily shown to be equivalent to the ordinary potential energy of the positive nucleus negative electron combination.[36] The argument is similar to that used in the previous discussion of the equivalence of the electron charge distribution self potential energy and the energy in its electric field. The total electric field around the atom or ion will thus be the vector sum of the positive and negative contributions:

$$\vec{E}_T = \vec{E}_+ + \vec{E}_- \ .$$

If it is again assumed that a nonzero expectation value of $\vec{v}$ (or $\vec{L}$) for a hydrogenic state actually implies some sort of movement of the charge density $\rho = e\psi_{n\ell m}\psi^*_{n\ell m}$ and that classical electrodynamics applies to the resultant fields, then an orbital magnetic field will be created,

$$\vec{B} = \gamma \frac{1}{c} \left(\frac{k_m}{k_e}\right)^{1/2} \vec{v} \times \vec{E}'$$

and the electric field ($\perp$) will be increased by a small amount,

$$\vec{E} = \vec{E}' + \frac{1}{2} \beta^2 \vec{E}' \ ,$$

as discussed previously. These changes then affect the energies contained in the total fields, energies which should reflect various potential and interaction energies of the system. The total electric field energy density is

$$U_E = \frac{1}{8\pi k_e} (\vec{E}_+ + \vec{E}_- + \frac{1}{2} \beta^2 \vec{E}_-)^2$$

$$= \frac{1}{8\pi k_e} (\vec{E}_+^2 + \vec{E}_-^2 + 2\vec{E}_+ \cdot \vec{E}_- + \beta^2 \vec{E}_-^2 + \beta^2 E_+ \cdot \vec{E}_-) \ ,$$

since $\vec{E}_-$ is perpendicular to $\vec{v}$ for the cases under consideration. Also,

$$U_B = \frac{1}{8\pi k_m} \vec{B}_-^2 \Leftrightarrow \frac{1}{8\pi k_e} \beta^2 \vec{E}_-^2 \ .$$

The various terms in these expressions can now be related to mechanical energies of the system as follows:

$\vec{E}_+^2 \Leftrightarrow$ self potential energy of nuclear ρ due to its own field.

$\vec{E}_-^2 \Leftrightarrow$ self potential energy of electron ρ.

$2\vec{E}_+ \cdot \vec{E}_- \Leftrightarrow$ usual interaction potential energy between nucleus and electron.

$\frac{2}{8\pi k_e} \beta^2 \vec{E}_-^2 \Leftrightarrow$ magnetic and electric field energy corrections to electron kinetic energy.

$\beta^2 \vec{E}_+ \cdot \vec{E}_- \Leftrightarrow$ correction to the interaction energy of nucleus and electron.

The fourth term in this list yields the hydrogen Lamb shift value previously obtained. It now appears that this term should be grouped with the first two as energies which do not affect the solution of the Schrödinger equation and which are unobservable. The third and last terms are related to the potential energy term which appears in the Schrödinger equation and the third at least must affect the wave function frequencies since it is the usual potential energy of an eigenstate. One can check this identification by a direct calculation, using $\vec{E}_- = \vec{E}_{211}$, for example, and $\vec{E}_+ = k_e Z e r^{-2} \vec{n}$. Thus,

$$\frac{1}{8\pi k_e} \iiint 2\vec{E}_+ \cdot \vec{E}_{211} r^2 \sin\Theta dr d\Theta d\phi = \frac{k_e Z^2 e^2}{4a_o} = \langle V \rangle_{211} ,$$

where $a_o = \frac{h^2}{k_e m e^2}$, and a minus sign is omitted ($\langle V \rangle_{211} = -Z^2$ (6.8) eV).

The last energy density listed above,

$$\Delta U_{E_+E_-} = \frac{1}{8\pi k_e} \beta^2 \vec{E}_+ \cdot \vec{E}_- ,$$

should then also affect the wave function frequencies since it is a part of this same potential energy V. The energy value calculated from this term,

$$\Delta U_{E_+E_-} = \frac{1}{8\pi k_e} \iiint \beta^2 \vec{E}_+ \cdot \vec{E}_- d^3r ,$$

will depend on Z^4, interestingly enough, and, because of $\beta^2 = (\frac{v}{c})^2$, will be of the same order of magnitude as the velocity dependent energies previously suggested as responsible for the Lamb shift. The evaluation of the integral, however, presents some difficulties because of the β^2 factor. The velocity which one wants is a supposed velocity of the $\vec{E}_-$ field everywhere in space. There is little justification for the supposition that this velocity would be independent of spatial coordinates and could be factored out of the integral, perhaps as $\langle \beta \rangle_{n\ell m}$ or $\langle \beta^2 \rangle_{n\ell m}$. Even then, the expectation values would yield an averaged velocity over the wave function region which might be inappropriate for the electric field region. On the other hand, a coordinate dependent definition of $\vec{v}$ such as $\vec{v}_{n\ell m} \equiv \frac{\vec{j}_{n\ell m}}{\rho_{n\ell m}}$ is equally troublesome. There is, however, another way of arriving at the effect of β^2 in the integral based on the previous magnetic field calculation. This field, after all, apparently includes a proper account of $\vec{v}$ ($\vec{B} = \frac{\gamma}{c} \left(\frac{k_m}{k_e}\right)^{1/2} |\vec{v}||\vec{E}|$). One can thus find the effect of β^2 on an integral such as that above from the following comparison:

$$U_{E_{211}} = \frac{1}{8\pi k_e} \int \vec{E}_{211} \cdot \vec{E}_{211} d^3r = U_{E_r} + U_{E_\theta}$$

$$= \frac{A_0^2}{k_e a_o} (51 + .83) = 2.45 \text{ eV} ,$$

according to previous calculations, but

$$\Delta U_{E_{211}} = \frac{1}{8\pi k_e} \int \beta^2 \vec{E}_{211} \cdot E_{211} d^3r$$

$$= \frac{1}{8\pi k_m} \int \vec{B}_{211} \cdot \vec{B}_{211} d^3r = 3.3 \times 10^{-6} \text{ eV} .$$

Since $\vec{E}_{211}$ does not differ much from $\vec{E}_+$ (in form) throughout most of space, one can conclude that

$$\Delta U_{E_+E_-} = \frac{1}{8\pi k_e} \int \beta^2 \vec{E}_+ \cdot \vec{E}_- d^3r \cong \frac{(3.3 \times 10^{-6})}{(2.45)} \cdot \frac{Z^2}{8\pi k_e} \int \vec{E}_+ \cdot \vec{E}_- d^3r$$

$$= (1.347 \times 10^{-6}) Z^2 U_{E_+E_-}$$

$$= (1.347 \times 10^{-6}) \frac{k_e e^2 Z^4}{8a_o} .$$

For hydrogen, this gives

$$\Delta U_{E_+E_-} = 4.59 \times 10^{-6} \text{ eV} ,$$

which corresponds to a frequency, which is now hypothesized to be the $2^2P_{1/2} \rightarrow 2^2S_{1/2}$ Lamb shift, of

$$\nu = 1110 \text{ MHz}.$$

It is not necessary to include the factor $\frac{2}{3}$ in this analysis since $\vec{B}(r,\Theta)$ is the <u>total</u> magnetic field of the $^2P_{1/2}$ $(m_j = \pm\frac{1}{2})$ state $|\frac{1}{2}, \pm\frac{1}{2}\rangle = R(r)(\frac{1}{3})^{1/2}\ [\pm\sqrt{2}\ Y_{1,\pm1}(\mp) \mp Y_{1,0}(\pm)]$, implying a velocity $\vec{v}$ in the ϕ direction (since $\vec{B}(r,\Theta) \propto \vec{v} \times \vec{E}(r,\Theta)$) and a corresponding $\Delta\vec{E}$ change in the electric field of the whole state $|\frac{1}{2}, \pm\frac{1}{2}\rangle$. The level shift also is in the right direction. $\Delta U_{E_+E_-}$ will be negative since $\vec{E}_+$ and $\vec{E}_-$ are in opposite directions. In keeping with the correspondence between field energies and mechanical energies, this implies a lowering of the $^2P_{1/2}$ state. This is in agreement with experiment, which confirms that the S state is higher in energy than the P state. The quantum electrodynamic explanation of the Lamb shift predicts that the S state will be raised, in contrast to the present theory; however, the relative shifts are exactly the same and the two theories are therefore experimentally indistinguishable (ns → np).

In order to provide some idea of the magnitudes of the $^2P_{1/2} \leftrightarrow {}^2S_{1/2}$ Lamb shifts for various cases and the corresponding predictions of the present Z^4 relationship, the results are listed and compared in Table 1. The numbers given for the present theory show simply the Z^4 variation and are unadjusted for nuclear size effects, for example, which, just as in the quantum electrodynamic calculations, would make important corrections. The importance of the good general agreement to the overall subject of a classical theory of radiative transitions lies in the direct way in which one can apparently carry the principles of classical electrodynamics to the quantum mechanical realm.

TABLE 1

LAMB SHIFT FREQUENCIES FOR THE $2^2P_{1/2} \leftrightarrow 2^2S_{1/2}$ TRANSITION IN HYDROGENIC ATOMS AND IONS

Ion	Experiment	This Theory*
Hydrogen (H)	1057.8 MHz	1,110 MHz
Deuterium (D)	1,059 MHz	1,110 MHz
Helium ($^4_2He^+$)	14,040 MHz	17,760 MHz
Lithium ($^6_3Li^{+2}$)	62,800 MHz	89,910 MHz
Carbon ($^{12}_6C^{+5}$)	780,000 MHz	1,438,560 MHz
Oxygen ($^{16}_8O^{+6}$)	2,210,000 MHz	4,546,560 MHz

*Nuclear size effect and other effects will make important corrections to these values.

V. OTHER APPLICATIONS OF CLASSICAL IDEAS

Spontaneous emission has played an important part in the long controversy over the relative merits of quantum electrodynamics and semiclassical theories. Until recently it was considered to be a phenomenon which presented great problems for the latter, since in the usual perturbation theory calculation there would be no interaction Hamiltonian whose matrix elements could be said to "cause" the spontaneous transition, there being no radiation incident as in the case of stimulated emission or absorption. The usual quantum theoretical explanation invokes the fluctuations of the vacuum radiation field as the perturbation which triggers the release of the stored energy of an atom, in the form of a photon. By 1927 Dirac had already derived the correct Einstein A coefficient for the probability of the resulting transition.[4] Jaynes has recently introduced a new semiclassical theory, however, which also predicts the A coefficient and, in addition, attributes the cause of the spontaneous transition to the classically familiar effect of radiation reaction, the response of the atom to the electromagnetic wave which it is itself emitting.[22] This idea is wholly compatible with the completely classical viewpoint of the present study since it provides an electromagnetic field to which the "transition state" formalism of Section II can be applied, and which is also of precisely the right frequency to be in "resonance" with the transition, with resultant large effects, as for the photoeffect discussion in Section II. The prediction of the correct A coefficient, however, is

not quite sufficient to allow a complete derivation of the blackbody spectrum. The semiclassical theory of spontaneous emission is therefore reexamined in the following discussion in a slightly different way. The A coefficient is obtained generally in the manner of Jayne's theory, but it is proved that there exists a spontaneous transition mechanism only from a state of higher energy to one of lower energy. This is enough to allow a rigorous derivation of the Planck formula. The discussion of solutions of the $\dot{c}_i$ equations for spontaneous emission also provides an opportunity for a demonstration of the origin of the Lamb shift according to Jayne's theory and leads to an analysis of the time development of a Compton transition, under the somewhat unrealistic conditions hypothesized in Section III. Since all of these subjects depend in various ways on the $\dot{c}_i$ equations and since most recent work in the field of semiclassical radiation theory is concerned with the solution of these equations for particular conditions, a brief summary of the usual treatment of them is given first and a new method of solution in introduced which enables one to avoid one of the main (although incorrect) approximations invariably used, the "rotating wave approximation."

A. THE USUAL SEMICLASSICAL THEORY OF THE $\dot{c}_i$ EQUATIONS

It is desired to calculate the change with time of the transition state wave function given by Eq. (1) of Section II under the influence of an electromagnetic field. The restriction to a two level transition is again made in the interest of simplicity. The analysis is still

realistic for the usual case of some type of resonant interaction between the field and a many level atom, which can effectively pick out the two appropriate states. If the field is represented by the vector potential $\vec{A}$, the progress of the transition from ψ_1 to ψ_2 is given by Eqs. (6), the "$\dot{c}_i$ equations,"

$$i\hbar\dot{c}_1 = c_1\langle u_1|\hat{H}' + \hat{H}''|u_1\rangle + c_2\langle u_1|\hat{H}' + \hat{H}''|u_2\rangle e^{-i\omega_{21}t}$$

$$i\hbar\dot{c}_2 = c_1\langle u_2|\hat{H}' + \hat{H}''|u_1\rangle e^{i\omega_{21}t} + c_2\langle u_2|\hat{H}' + \hat{H}''|u_2\rangle ,$$

where

$$\hat{H}' = \frac{ie\hbar}{mc}\left(\frac{k_e}{k_m}\right)^{1/2}\vec{A}\cdot\nabla ,$$

$$\hat{H}'' = \frac{k_e e^2}{2k_m mc^2}\vec{A}^2 , \text{ and}$$

$$\omega_{21} \equiv \omega_2 - \omega_1 \equiv \frac{1}{\hbar}(E_2 - E_1) .$$

If one assumes that the field is a monochromatic wave of frequency $\omega \cong \omega_{21}$,

$$\vec{A} = A\vec{\varepsilon}_1 \cos(\vec{k}\cdot\vec{r} - \omega t) ,$$

whose amplitude is small compared to that of the atomic fields, then one can neglect $\hat{H}''$ compared to $\hat{H}'$ and use the fact that $\hat{H}'$ gives zero matrix elements if the two states are the same to obtain

$$i\hbar\dot{c}_1 = c_2 H'_{12} e^{-i\omega_{21}t} \quad , \quad i\hbar\dot{c}_2 = c_1 H'_{21} e^{i\omega_{21}t} \tag{6'}$$

where $H'_{ij} \equiv \langle u_i | \hat{H}' | u_j \rangle$. One can now transform H'_{12} and H'_{21} by the use of $\nabla = -\frac{m}{\hbar^2}(\hat{H}_0\vec{r} - \vec{r}\hat{H}_0)$ to

$$H'_{ij} = \frac{ie\hbar}{mc}\left(\frac{k_e}{k_m}\right)^{1/2} A \frac{m}{\hbar}\omega_{ji}\,\vec{\varepsilon}_1 \cdot \langle u_i | \vec{r} | u_j \rangle \cos\omega t \ .$$

But from $\vec{E} = -\nabla V - \frac{1}{c}\left(\frac{k_e}{k_m}\right)^{1/2}\dot{\vec{A}}$

$$\vec{E} = \frac{1}{c}\left(\frac{k_e}{k_m}\right)^{1/2} A\,\vec{\varepsilon}_1\,\omega \sin\omega t \ ,$$

and, except for a phase difference,

$$H'_{12} \langle = \rangle \vec{E} \cdot \langle u_1 | e\vec{r} | u_2 \rangle = \langle u_1 | \vec{d} \cdot \vec{E} | u_2 \rangle \ ,$$

where $\vec{d}$ is the dipole moment operator. Thus the Hamiltonian for this two level system can also be written in another familiar form which shows the classical interaction energy of a dipole moment in an electric field:

$$\hat{H} = \hat{H}_0 + \hat{H}' = \hat{H}_0 - \vec{d} \cdot \vec{E} \ .$$

$\hat{H}_0$ is the atomic Hamiltonian among whose energy eigenfunctions are ψ_1 and ψ_2.

The usual procedure[29] for using this $\vec{d} \cdot \vec{E}$ form of $\hat{H}$ to analyze the two level transition begins by limiting consideration to the

two-dimensional Hilbert space spanned by ψ_1 and ψ_2. The matrix elements of the operators in the Hamiltonian are

$$\langle 1|\hat{H}_0|1\rangle = E_1 , \quad \langle 2|\hat{H}_0|2\rangle = E_2 , \quad \langle 1|\hat{H}_0|2\rangle = \langle 2|\hat{H}_0|1\rangle = 0$$

and

$$\langle 1|\hat{\vec{d}}|2\rangle = \vec{d}_{12} , \quad \langle 2|\hat{\vec{d}}|1\rangle = \vec{d}_{12}^{\,*} , \quad \langle 1|\hat{\vec{d}}|1\rangle = \langle 2|\hat{\vec{d}}|2\rangle = 0 .$$

In this two-dimensional space the complete Hamiltonian can therefore be written

$$\hat{H} = \frac{1}{2}(E_2 + E_1)\hat{I} + \frac{1}{2}(E_2 - E_1)\hat{\sigma}_3 - \begin{pmatrix} \vec{d}_r^{\,0} - i\vec{d}_i & \vec{d}_r + i\vec{d}_i \\ 0 & \end{pmatrix} \cdot \vec{E}$$

where $\hat{I}$ is the two-dimensional unit matrix and $\hat{\sigma}_1$, $\hat{\sigma}_2$ and $\hat{\sigma}_3$ are the Pauli matrices. The dipole moment operator $\hat{\vec{d}}$ can be written $\hat{\vec{d}} = \vec{d}_r\hat{\sigma}_1 - \vec{d}_i\hat{\sigma}_2$ in H and the Heisenberg equation of motion for an operator $\hat{O}$,

$$-\frac{\hbar}{i}\dot{\hat{O}} = [\hat{O},\hat{H}] ,$$

can be used to determine the time rates of change of $\hat{\sigma}_1$, $\hat{\sigma}_2$, and $\hat{\sigma}_3$:

$$\dot{\hat{\sigma}}_1 = -\omega_{21}\hat{\sigma}_2 + \frac{2}{\hbar}(\vec{d}_i\cdot\vec{E})\hat{\sigma}_3$$

$$\dot{\hat{\sigma}}_2 = \omega_{21}\hat{\sigma}_2 + \frac{2}{\hbar}(\vec{d}_r\cdot\vec{E})\hat{\sigma}_3$$

$$\dot{\hat{\sigma}}_3 = -\frac{2}{\hbar}(\vec{d}_r\cdot E)\hat{\sigma}_2 - \frac{2}{\hbar}(\vec{d}_i\cdot\vec{E})\hat{\sigma}_1$$

Expectation values of these equations, assuming that operator products can be factored as $\langle \hat{\vec{E}}\hat{\sigma}_3 \rangle = \langle \hat{\vec{E}} \rangle \langle \hat{\sigma}_3 \rangle$, for example, are

$$\dot{s}_1 = -\omega_{21} s_2 + \frac{2}{\hbar} \vec{d}_i \cdot \vec{E}\, s_3$$

$$\dot{s}_2 = \omega_{21} s_1 + \frac{2}{\hbar} \vec{d}_r \cdot \vec{E}\, s_3$$

$$\dot{s}_3 = -\frac{2}{\hbar} \vec{d}_i \vec{E}\, s_1 - \frac{2}{\hbar} \vec{d}_r \cdot \vec{E}\, s_2 ,$$

where $s_i = \langle \hat{\sigma}_i \rangle$. One can prove that these equations imply that $s_1^2 + s_2^2 + s_3^2 = 1$. Several simplifying assumptions are made in most instances. It is usually adequate to assume that the transition has $\Delta m = 0$ and to adjust the phases of the states so that $\vec{d}_i$ is zero. If E_d is the component of $\vec{E}$ along $\vec{d}$ and $\kappa \equiv \frac{2}{\hbar} |\vec{d}|$, the semiclassical atomic equations take the form

$$\dot{s}_1 = -\omega_{21} s_2$$

$$\dot{s}_2 = \omega_{21} s_1 + \kappa E_d s_3$$

$$\dot{s}_3 = -\kappa E_d s_2 .$$

Referring to the form of the Hamiltonian $\hat{H}$, one can see the physical significance of s_1, s_2, and s_3. $\frac{1}{2} \hbar \omega_{21} s_3$ represents the internal energy of the atom relative to the average energy $\frac{1}{2}(E_1 + E_2)$, which can be redefined as the zero of energy, and s_1 and s_2 are components of the dipole moment of the atom. $\vec{s}$ is a unit vector known as the "pseudospin"

vector and the semiclassical equations above, which describe the path of $\vec{s}$ over a unit sphere during a transition, are known as the "optical Bloch" equations since they are analogous to the equations treated by Bloch for spin precession in magnetic resonance.

The "pseudospin" equations are generally solved by transforming everything into a rotating coordinate system in which important and unimportant terms can be easily discerned. This is called the "rotating wave approximation" and was first used in the magnetic resonance problems. The three equations above can be written in terms of an angular velocity vector $\vec{\Omega}$ (sometimes called a "torque"!?):

$$\dot{\vec{s}} = \vec{\Omega} \times \vec{s}$$

where

$$\vec{\Omega} = (-\kappa E_d,\ 0,\ \omega_{21}) \ .$$

The situation can be roughly represented by the diagram in Figure 6. Since $\kappa E_d << \omega_{21}$, $\vec{\Omega}$ points almost in the 3 direction. An idea of the magnitudes of the two nonzero components of $\vec{\Omega}$ in a practical case may be obtained by calculating the field strength required for them to be equal. Therefore if $\hbar\kappa E \cong \hbar\omega_{21} \sim 1$ eV and $\hbar\kappa \sim ea_o$ for a typical dipole moment, then $E \cong 1V/a_0 \sim 10^8$ V/cm. Such an electric field would be many orders of magnitude larger than that of any reasonable resonance experiment. Also $E \cong \frac{k_e e}{a_o^2}$, the atomic field.

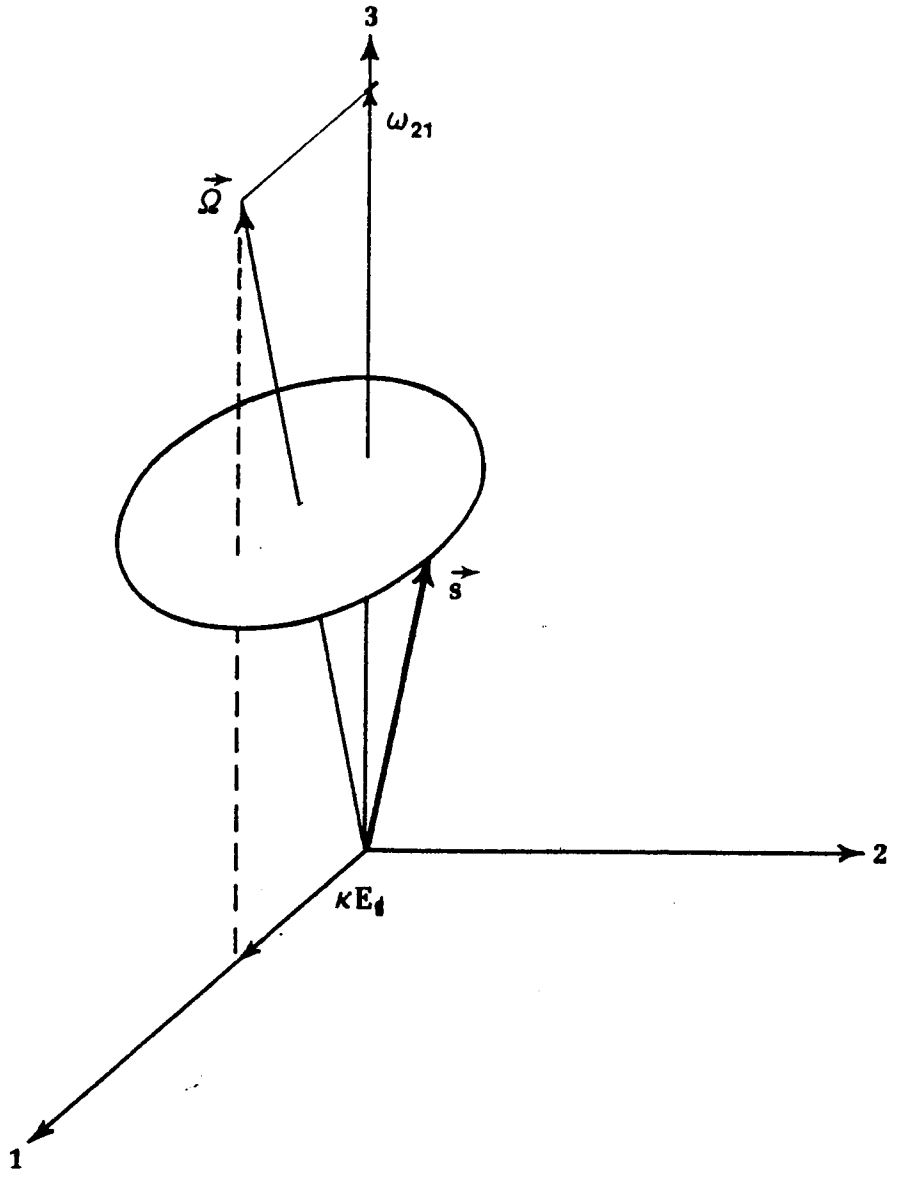

Figure 6. The precession of the unit pseudospin vector $\vec{s}$ about the "angular velocity" vector $\vec{\Omega}$.

Since E_d will change rapidly with time at a frequency $\omega \sim \omega_{21}$, $\vec{\Omega}$ will move rapidly about the approximate direction 3, and can be written as the sum of one large constant vector and two small time dependent ones ($E = \frac{1}{2} E_d$):

$$\vec{\Omega} = \vec{\Omega}^{+} + \vec{\Omega}^{-} + \vec{\Omega}^{o} = (-\kappa E \cos \omega t, -\kappa E \sin \omega t, 0)$$
$$+ (-\kappa E \cos \omega t, +\kappa E \sin \omega t, 0)$$
$$+ (0, 0, \omega_{21}) .$$

If one then transforms to a coordinate system rotating about 3 with angular velocity ω, then $\vec{\Omega}^{+}$ becomes a constant while $\vec{\Omega}^{-}$ rotates with angular velocity 2ω and is said to have little long term effect. Therefore the "rotating wave approximation" consists of ignoring $\vec{\Omega}^{-}$ and writing the "pseudospin" equations in terms of $\vec{\Omega}^{o}$ and $\vec{\Omega}^{+}$ as

$$\dot{s}_1 = -\omega_{21} s_2 - \kappa E \, s_3 \sin \omega t$$

$$\dot{s}_2 = \omega_{21} s_1 + \kappa E \, s_3 \cos \omega t$$

$$\dot{s}_3 = -\kappa E (s_2 \cos \omega t - s_1 \sin \omega t) .$$

In the rotating coordinate frame the "pseudospin" $\vec{\rho} = (u,v,w)$ satisfies

$$\dot{\vec{\rho}} = \vec{\Omega}' \times \vec{\rho} .$$

where

$$\vec{\Omega}' \equiv (-\kappa E, 0, \omega_{21} - \omega) ,$$

or:

$$\dot{u} = -(\omega_{21}-\omega)v$$

$$\dot{v} = +(\omega_{21}-\omega)u + \kappa E w$$

$$\dot{w} = - Ev \ ,$$

and (near resonance) all optical frequencies have disappeared. Again $\frac{1}{2}\hbar\omega_{21}w$ represents the energy of the atom and u and -v are the components of the dipole moment in phase and 90° out of phase with the field E.

The same equations can be obtained in a simpler way[22] directly from the $\dot{c}_i$ equations, Eqs. (6'). The substitution

$$c_1 = c_1' e^{i\omega_1 t} \ , \quad c_2 = c_2' e^{i\omega_2 t}$$

transforms these into (dropping primes)

$$i\hbar\dot{c}_1 = E_1 c_1 - \vec{d}\cdot\vec{E}\, c_2$$

$$i\hbar\dot{c}_2 = E_2 c_2 - \vec{d}\cdot\vec{E}\, c_1 \ ,$$

where H_{12}' has been written as $-\vec{d}\cdot\vec{E}$. If one again assumes $\vec{E}$ and $\vec{d}$ to be in the same direction and introduces $\langle d\rangle = d(c_1 c_2^* + c_1^* c_2)$ and $\langle H_0\rangle = \frac{1}{2}\hbar\omega_{21}(c_1 c_1^* - c_2 c_2^*)$, these equations then show that the new variables satisfy

$$\frac{d^2}{dt^2}\langle d\rangle + \omega_{21}^2 \langle d\rangle = -\kappa\langle H_0\rangle E$$

$$\frac{d}{dt}\langle H_0\rangle = E\,\frac{d}{dt}\langle d\rangle \ ,$$

where $\kappa \equiv \frac{2}{\hbar} d$. The second derivative can be eliminated by multiplying the first of these equations by $\langle \dot{d} \rangle$ and integrating:

$$(\langle \dot{d} \rangle)^2 + \omega_{21}^2 \langle d \rangle^2 + \kappa \langle H_0 \rangle^2 = \text{constant} .$$

The constant is evaluated by using the normalization $c_1^2 + c_2^2 = 1$ in this equation and is found to be equal to $d^2\omega_{21}^2$. Since this equation resembles the equation of a sphere, it can be put explicitly in the form $s_1^2 + s_2^2 + s_3^2 = 1$ by the substitution

$$\langle \dot{d} \rangle + i\omega_{21} \langle d \rangle = id\omega_{21} e^{i\omega t}(s_1 + is_2) , \quad \langle H_0 \rangle = \frac{1}{2} h\omega_{21} s_3 .$$

The physical meaning of s_1, s_2, and s_3 can be demonstrated by taking the imaginary part of the first by these equations,

$$\langle d \rangle = d(s_1 \cos \omega t - s_2 \sin \omega t) ,$$

which shows that s_1 is the component of the dipole moment in phase with the electric field and s_2 the component 90° out of phase with it (assuming $E(t) = E \cos \omega t$). The same substitution in the dynamical equations for $\langle d \rangle$, $\langle \dot{d} \rangle$, and $\langle H_0 \rangle$ yields

$$\dot{s}_1 = (\omega - \omega_{21}) s_2 + \kappa s_3 E \sin \omega t$$

$$\dot{s}_2 = -(\omega - \omega_{21}) s_1 + \kappa s_3 E \cos \omega t$$

$$\dot{s}_3 = -\kappa E(s_1 \sin \omega t + s_2 \cos \omega t) ,$$

if the 2ω frequency terms are neglected. These equations are equivalent to the "optical Bloch equations" obtained in the previous ($\vec{\Omega}$) derivation for the time dependence of the "pseudospin" $\vec{s}$.

The problem, of course, with these methods of solution of the $\dot{c}_i$ equations is that the "counter rotating" 2ω terms cannot really be dropped. Although one can argue that the long term path of $\vec{s}$ on the unit sphere does not depend on them, it is apparent that they will appear in c_1 and c_2 and also, therefore, in the oscillating transition charge and current densities ($c_1 c_2^* \rho_{12*}$ and $c_1 c_2^* \vec{j}_{12*}$). It thus appears incorrect in any semiclassical derivation which discusses and uses ρ or $\vec{j}$, for one simply to drop them, as was done in the previous discussion of the photoelectric effect, and as is done more elegantly in the rotating wave approximation. Before one can attempt to apply the $\dot{c}_i$ equations to more difficult problems then, one must determine how they must be solved in the present simple case of a two level transition at resonance ($\omega \sim \omega_{21}$), where it cannot be considered acceptable to omit any terms for whatever reason.

B. A NEW EXACT SOLUTION OF THE $\dot{c}_i$ EQUATIONS

Abandoning the foregoing standard semiclassical and neoclassical methods, one can perhaps find some clues for a correct solution in the original simple expressions describing the time development of the transition wave function, Eqs. (6'):

$$i\hbar\dot{c}_1 = c_2 H_{12} e^{-i\omega_{21}t}, \quad i\hbar\dot{c}_2 = -c_1 H_{12} e^{i\omega_{21}t}.$$

As in the preceding discussion, only two active levels, $\psi_1 = u_1 e^{-i\omega_1 t}$ and $\psi_2 = u_2 e^{-i\omega_2 t}$ are considered, H_{12} is given by

$$H_{12} = \langle u_1 | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}\cdot\nabla | u_2 \rangle ,$$

and incident monochromatic light is assumed:

$$\vec{A} = A \vec{\varepsilon}_1 \cos (\vec{k} \cdot \vec{r} - \omega t) .$$

Since the wave functions are confined to a volume with dimensions on the order of a_0 and radiation of optical frequencies will have a wavelength many times larger than this,

$$\frac{2\pi}{k} = \lambda >> a_0 ,$$

the usual (dipole) approximation can be made:

$$\vec{A} \cong A \vec{\varepsilon}_1 \cos \omega t = \frac{1}{2} A \vec{\varepsilon}_1 (e^{i\omega t} + e^{-i\omega t}) .$$

With A written in this way one can see that the main problem one is faced with in Eqs. (6') is the combination of a real oscillatory radiation term with a complex term from the wave functions, and that the rotating wave approximation amounts simply to the elimination of terms of the form

$$e^{\pm i(\omega_{21}+\omega)t} \simeq e^{\pm 2i\omega t} .$$

This would then leave the following very simple equations for radiation exactly at resonance ($\omega_{21} - \omega = 0$):

$$i\hbar\dot{c}_1 = c_2 H_{12} \quad , \quad i\hbar\dot{c}_2 = -c_1 H_{12} \ .$$

With $H_{12} = \langle u_1 | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \frac{1}{2} A \vec{\varepsilon}_1 \cdot \nabla | u_2 \rangle$, these equations can be solved almost trivially, yielding correct time dependences and correct transition "speeds" for two level cases. However, although everyone recognizes that the "counterrotating" terms are the only impediment to this procedure and that they must somehow not really belong in the equations, they cannot legitimately just be erased because they are "nonresonant." But at any rate, it appears that one is in some manner close to the right method since the above equations conserve matter ($c_1(t)^2 + c_2(t)^2 = 1$) and provide the usual matrix elements (H_{12}) for a transition.

There are several things that one might try in order to eliminate the 2ω terms from Eqs. (6'). One could ask whether the transition wave function $c_1\psi_1 + c_2\psi_2$ satisfies the Schrödinger equation with only the $\vec{A}_c = A \vec{\varepsilon}_1 e^{i\omega t}$ part of the vector potential. In quantum electrodynamics, after all, the two complex parts of the vector potential are completely separated, one going with a creation operator and the other with an annihilation operator. If radiation of two or more frequencies, only one of which is the resonant frequency, is incident on the two level system, the system might be expected to respond only to the resonant part of the field, at least as far as the interlevel transition under consideration is concerned. The hypothesis might therefore be made that

the Schrödinger equation can essentially "pick out" the frequency which will cause the transition. Then the fact that Eqs. (6') describe the physical situation accurately and can make $c_1\psi_1 + c_2\psi_2$ exactly the correct wave function for the problem might justify the use of $\vec{A}_c$. This line of reasoning, however, would introduce a problem in another area. The derivation of the continuity equation and the expression for the current density in Eq. (7) require that A be real. Here $\vec{A}_c = \vec{A}_r + i\vec{A}_i$ and the continuity equation would become

$$\partial_t(e\psi\psi^*) = -\nabla \cdot [\vec{j}_\psi - \frac{e^2}{mc}\left(\frac{k_e}{k_m}\right)^{1/2} \psi\psi^* \vec{A}_r] - \frac{2e}{\hbar c}\left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}_i \cdot \vec{j}_\psi ,$$

where $\vec{j}_\psi = \frac{e\hbar}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*)$. There would be introduced therefore an unusual extra term depending on $\vec{A}_i = A_i\vec{\epsilon}_1 \sin(\vec{k}\cdot\vec{r} - \omega t)$ which might describe a rapid creation and annihilation of charge density during the transition, although there would be no net change in total charge. The divergence term would be the same as before, with $\vec{A}_r = A_r\vec{\epsilon}_1 \cos(\vec{k}\cdot\vec{r} - \omega t)$, and apparently could still contain the expression for the total current density. However, in addition to this troublesome extra term in the continuity equation, there are other considerations which argue against the above hypothesis. One cannot provide any good reason why all components of the vector potential in which the two level atom is immersed should not enter the momentum term $\left(\frac{h}{i}\nabla - \frac{e}{c}\left(\frac{k_e}{k_m}\right)^{1/2}\vec{A}\right)$ in the same way. Arguing by analogy with classical mechanics, one would expect that the total $\vec{A}$ should affect the relative momentum term <u>and</u> the center of mass momentum term, both according to the foregoing relation. It is much

more reasonable to assume that $\vec{A}$ <u>total</u> goes into the Schrödinger equation, and thereby into the $\dot{c}_i$ equations, but that their solution is only influenced greatly by the resonant frequency. This argument also implies that one could not assume that part of a field affects the relative coordinates and another part the center of mass coordinates. All of the field must affect all of the coordinates. One remaining possibility for eliminating the 2ω frequency terms in Eqs. (6') is suggested by the fact that there is only a simple phase change between the wave functions which satisfy the Schrödinger equation with $\vec{A} = A\,\vec{\epsilon}_1 \cos \omega t$ and $\vec{A} = A\,\vec{\epsilon}_1 \sin \omega t$. One could accomplish the same thing in Eqs. (6') with the substitution $t \to T - \frac{\pi}{2\omega}$. Then

$$i\hbar\partial_t c_1(T - \tfrac{\pi}{2\omega}) = c_2(T - \tfrac{\pi}{2\omega})H_{12} \sin \omega t\, e^{-i\omega_{21}(T - \frac{\pi}{2\omega})}$$

$$= ic_2(T - \tfrac{\pi}{2\omega})H_{12} \sin \omega T\, e^{-i\omega_{21}T} ,$$

and similarly for the $\dot{c}_2$ equation. Then if one could assume $c_{1,2}(t \pm \frac{\pi}{2\omega}) \cong c_{1,2}(t)$, this equation could be added to its original form, with the result

$$2i\hbar\dot{c}_1 = c_2 H_{12}(\cos \omega t + i \sin \omega t)e^{-i\omega_{21}t}$$

$$= c_2 H_{12} .$$

A similar result would apply to $\dot{c}_2$, and one would apparently have obtained the same simple equations as if the 2ω terms had been dropped. The flaw in this treatment is that, although the approximation

$c_1(t \pm \frac{\pi}{2\omega}) = c_1(t)$ seems valid since $\frac{1}{2\pi\omega}$, the period of the wave, is very short compared to the transition time, the reasoning is circular. The approximation of a slow change of c_1 and c_2 is effectively the same as saying that there can be no 2ω frequencies in the equations which describe $\dot{c}_1$ and $\dot{c}_2$, Eqs. (6').

Based on the clues revealed in the foregoing discussion, however, one can show that there exists a simple and exact method of handling Eqs. (6'), by taking a slightly different approach to the problem. Since the trouble comes partly from the complex nature of wave functions, one can examine the possibilities of some generalization or combination of them which will allow a coupling with a real field. In addition, in a dipole transition there will be an angular momentum change in ψ, which should somehow be related to the electromagnetic angular momentum of the radiation. An exact solution to the $\dot{c}_i$ equations then follows and correct account is taken of the transfer of angular momentum between system and radiation if one begins with circularly polarized incident light rather than linearly polarized and adopts a particular orientation of the atomic coordinate system. The incident $\vec{A}$ is therefore assumed to be

$$\vec{A} = A(\vec{\varepsilon}_1 \cos(\vec{k}\cdot\vec{r} - \omega t) - \vec{\varepsilon}_2 \sin(\vec{k}\cdot\vec{r} - \omega t)\ ,$$

as shown in Figure 7, the minus sign $(-\vec{\varepsilon}_2)$ implying right circularly polarized (RCP) radiation. The atom is oriented as shown, with the wave functions ψ_1 and ψ_2 assumed to be those of an electron in a central potential V(r).

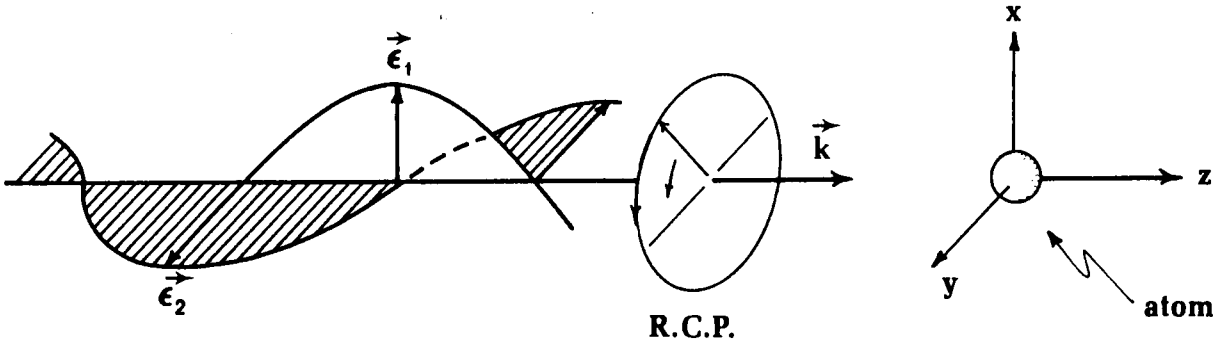

Figure 7. Right circularly polarized radiation incident on an atom. The atomic coordinate system is oriented as shown. The angular momentum flux density in the field is given by

$$\Phi_L = \vec{n}_k \cdot \overleftrightarrow{M} ,$$

where $\vec{n}_k = \frac{\vec{k}}{|\vec{k}|}$, $\overleftrightarrow{M} = \overleftrightarrow{T} \times \vec{r}$, and $\overleftrightarrow{T}$ is the Maxwell stress tensor,

$$\overleftrightarrow{T} = \frac{1}{4\pi} \left[\frac{\vec{E}\vec{E}}{k_e} + \frac{\vec{B}\vec{B}}{k_m} - \frac{1}{2} \overleftrightarrow{I} \left(\frac{E^2}{k_e} + \frac{B^2}{k_m} \right) \right] .$$

Therefore $\Phi_L = 0$ unless there is some absorption by the atom. There is then an xy plane variation of the fields and $\langle \Phi_L \rangle_{\text{time}} \neq 0$.

The matrix element $H_{12}(t)$ is now given by

$$H_{12}(t) = \langle u_1 | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A} \cdot \nabla | u_2 \rangle$$

$$= \langle u_1 | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} A \vec{\varepsilon}_1 \cdot \nabla | u_2 \rangle \cos \omega t$$

$$+ \langle u_1 | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} A \vec{\varepsilon}_2 \cdot \nabla | u_2 \rangle \sin \omega t \ .$$

Transforming these into dipole matrix elements by use of $\nabla = -\frac{m}{\hbar^2} (\hat{H}_0 \vec{r} - \vec{r} \hat{H}_0)$, one obtains

$$H_{12}(t) = \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} A \frac{m}{\hbar} \omega_{21} [\vec{\varepsilon}_1 \cdot \langle u_1 | \vec{r} | u_2 \rangle \cos \omega t$$

$$+ \vec{\varepsilon}_2 \cdot \langle u_1 | \vec{r} | u_2 \rangle \sin \omega t]$$

$$= \frac{ie}{c} \left(\frac{k_e}{k_m}\right)^{1/2} A \omega_{21} [X \cos \omega t + Y \sin \omega t] \ ,$$

where $X = \langle u_1 | x | u_2 \rangle$ and $Y = \langle u_1 | y | u_2 \rangle$. Now

$$X = A_{n\ell m} A_{n'\ell'm'} \int_0^\infty R_{n'\ell'} \, r \, R_{n\ell} r^2 dr \int_0^\pi P_{\ell'}^{m'} \sin\theta \, P_\ell^m \sin\theta \, d\theta$$

$$\times \int_0^{2\pi} e^{-im'\phi} \cos\phi \, e^{im\phi} \, d\phi \equiv K \int_0^{2\pi} \cos\phi \, e^{i(m-m')\phi} \, d\phi \ ,$$

and

$$Y = K \int_0^{2\pi} e^{-im'\phi} \sin\phi \, e^{im\phi} \, d\phi \ .$$

So $X = K\pi$ iff $m' = m \pm 1$ while

$$Y = K \times \int_0^{2\pi} \frac{1}{2i} \left(e^{i(m-m'+1)} - e^{-i(m-m'-1)}\right) d\phi$$

$$= K \times \begin{cases} \frac{\pi}{i} \ , & m' = m + 1 \\ -\frac{\pi}{i} \ , & m' = m - 1 \end{cases} .$$

Therefore if $m' = m - 1$ for example, $X = K\pi$, $Y = K\pi i$, and

$$H_{12}(t) = \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} A\omega_{21} K\pi(\cos \omega t + i \sin \omega t) \ .$$

This $H_{12}(t)$ then has just the right factor to cancel $e^{-i\omega_{21}t}$ at resonance and the $\dot{c}_i$ equations are again in the simple form

$$\dot{c}_1 = c_2 H'_{12} \ , \quad \dot{c}_2 = -c_1 H'_{12} \ ,$$

where here

$$H'_{12} = \langle u_1 | \frac{e}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} A\vec{\varepsilon}_1 \cdot \nabla | u_2 \rangle \ .$$

The "decoupled" equations, of course, are of the form $\ddot{c}_1 + c_1 H'^2_{12} = 0$, with obvious solutions. The same procedure can be extended to more general polarizations by reorienting the atomic coordinates. As long as

the situation is adjusted so that angular momentum transferral is correct, Eqs. (6') describing the dynamics of the transition will assume a simple, easily soluble form. Apparently, a certain amount of elliptical polarization is necessary for an electric dipole transition, since $\Delta\ell = \pm 1$ for the system. For strictly linear polarized radiation there is no way to apply the present argument and, indeed, there seem to be no nonsingular physical solutions to Eqs (6') at all. This fact may have recently received some experimental confirmation in certain results which have been interpreted as photon "antibunching".[25] In these experiments, a linearly polarized laser beam is used to drive a resonant two level transition in single atoms of an atomic beam. Evidence of a transition is obtained by the radiation emitted by the atom in a direction perpendicular to both the incident light beam and the atomic beam. The delay or absence of transitions which is found has been interpreted as due to "antibunching" of the incident laser photons. The discussion above indicates, however, that it is possible that the result is caused by the initial linear polarization of the light.

C. SPONTANEOUS EMISSION AND THE BLACKBODY SPECTRUM

One can now finally proceed to solve Eqs. (6) for spontaneous emission with no rotating wave type approximations, without ignoring any terms because of the frequencies they contain. In this case it is desired to use the $\vec{A}$ field produced by various parts of the radiating charge density itself as the field which causes the transition through Eqs. (6). It is assumed that the two states involved are connected

through a dipole transition and thus the $\dot{c}$ equations [Eqs. (6')] are again

$$i\hbar\dot{c}_1 = c_2 H_{12} e^{-i\omega_{21}t} \quad , \quad i\hbar\dot{c}_2 = -c_1 H_{12}^* e^{i\omega_{21}t} \quad ,$$

where

$$H_{12} = \langle u_1 | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A} \cdot \nabla | u_2 \rangle \quad .$$

There is no external $\vec{A}$ incident, the vector potential in H_{12} arising in this case from the transition current density $\vec{j}_\psi$ itself by means of Eq. (9). The time dependent parts of $\vec{j}_\psi$ are

$$\vec{j}_\psi(t) = c_1 c_2^* \frac{e\hbar}{2im} (u_2^* \nabla u_1 - u_1 \nabla u_2^*) e^{i\omega_{21}t} + c_1^* c_2 \frac{e\hbar}{2im} (u_1^* \nabla u_2 - u_2 \nabla u_1^*) e^{-i\omega_{21}t} .$$

In accord with the above discussion of conservation of angular momentum, one should check the state of polarization of $\vec{j}_\psi$. This current density can be written as

$$\vec{j}_\psi = \frac{e\hbar}{2im} (\vec{j}_r + i\vec{j}_i) e^{i\omega_{21}t} + \frac{e\hbar}{2im} (\vec{j}_r - i\vec{j}_i) e^{-i\omega_{21}t}$$

$$= \frac{e\hbar}{m} (\vec{j}_i \cos \omega_{21}t + \vec{j}_r \sin \omega_{21}t) \quad ,$$

and it can be seen that $\vec{j}_\psi$ will produce elliptically polarized radiation in general since $\vec{j}_r$ and $\vec{j}_i$ will be in different directions. Following the argument of Jaynes, one can assume that the electron will experience only the effects of the transverse part of this current density, and

that, since the retardation is small over the wave function region, the following expansion for $\vec{A}$ is allowable:

$$\vec{A} = \frac{(k_e k_m)^{1/2}}{c} \iiint \vec{j}_t \frac{(\vec{r}', t-R/c)}{R} d^3r'$$

$$\cong \frac{(k_e k_m)^{1/2}}{c} \left(\iiint \frac{\vec{j}_t(\vec{r}', t)}{R} d^3r' - \frac{1}{c} \frac{d}{dt} \iiint \vec{j}_t(\vec{r}', t) d^3r' \right), \qquad (17)$$

where $\vec{j}_t$ indicates the transverse component of the current density $\vec{j}_\psi(t)$ above.[22] If the first term of this expression for $\vec{A}$, the "unretarded" term, is substituted in H_{12}, this part of the matrix element becomes

$$H'_{12} = \frac{k_e i e^2 \hbar^2}{2 i m^2 c^2} (c_1 c_2^*) e^{i\omega_{21} t} \langle u_1 | \iiint (u_2'^* \nabla' u_1' - u_1' \nabla' u_2'^*)_t \frac{1}{|\vec{r} - \vec{r}'|} d^3r' \cdot \nabla | u_2 \rangle$$

$$+ \frac{k_e i e^2 \hbar^2}{2 i m^2 c^2} (c_1^* c_2) e^{-i\omega_{21} t} \langle u_1 | \iiint (u_1'^* \nabla u_2' - u_2' \nabla u_1'^*)_t \frac{1}{|\vec{r} - \vec{r}'|} d^3r' \cdot \nabla | u_2 \rangle,$$

and according to Jaynes this part of H_{12} accounts for the Lamb shift.[50] In Jaynes' formulation, the second term of this expression is ignored because it contributes an $e^{-2i\omega t}$ term to the equations. The remaining H'_{12} term, $H'_{12} = c_1 c_2^* M e^{i\omega_{21} t}$, will then contribute an imaginary term to the $\dot{c}_i$ Eqs. (6') which will appear as a frequency shift (time dependent because $|c_1|$ and $|c_2|$ are factors). In the present derivation, considerations similar to those used in the incident wave circular polarization case lead to the conclusion that the second term of H'_{12} will be identically

zero for those wave functions appropriate for a spontaneous transition. This can be shown in the same manner as is done below for the other H_{12} term, that involving the second term of the self $\vec{A}$ in Eq. (17). Thus H'_{12} still has the form

$$H'_{12} = c_1 c_2^* M e^{i\omega_{21}t} ,$$

where M is real. As will be shown, the effect of H'_{12} is then again to introduce phase changes in the solutions c_1 and c_2. For the present discussion of spontaneous emission, the details of its evaluation are unimportant, as long as it is known that it is of the above form and has no influence on the time variation of the amplitudes $|c_1|$ and $|c_2|$. The second term of Eq. (17), the "slightly retarded" part of $\vec{A}$, gives

$$H''_{12} = \frac{k_e i e^2 \hbar^2}{2m^2 c^3} (c_1 c_2^*)\omega_{21} e^{i\omega_{21}t} \langle u_1 | \iiint (u_2'^* \nabla' u_1' - u_1' \nabla' u_2'^*)_t d^3r' \cdot \nabla | u_2 \rangle$$

$$+ \frac{k_e i e^2 \hbar^2}{2m^2 c^3} (c_1^* c_2)\omega_{21} e^{-i\omega_{21}t} \langle u_1 | \iiint (u_1'^* \nabla u_2' - u_2' \nabla u_1'^*)_t d^3r' \cdot \nabla | u_2 \rangle .$$

This part of H_{12} correctly accounts for spontaneous emission, yielding the proper Einstein A coefficient and appropriate $c_i(t)$ solutions through Eqs. (6').

The way in which the previous new exact method of solving the $\dot{c}_i$ equations applies in the present case can be outlined for the same wave functions ($\Delta m_\ell = \pm 1$) as were used in that discussion, since the various integrals have already been evaluated. With slight modification the

same argument can be applied to a $\Delta m_\ell = 0$ transition. Thus, using integration by parts and employing $\frac{\hbar}{i}\nabla = \frac{im}{\hbar}(\hat{H}_0\vec{r} - \vec{r}\hat{H}_0)$, one can first transform the inner (prime) integrals in the H''_{12} expression:

$$\int(u_2'^*\nabla u_1' - u_1'\nabla u_2'^*)d^3r' = 2\int u_2'^*\nabla u_1 d^3r'$$

$$= \frac{-2m}{\hbar^2}(E_2 - E_1)\langle u_2|\vec{r}|u_1\rangle \ ,$$

$$\int(u_1'^*\nabla u_2' - u_2'\nabla u_1'^*)d^3r' = -2\int u_2'\nabla u_1^* d^3r'$$

$$= \frac{2m}{\hbar^2}(E_2 - E_1)\langle u_1|\vec{r}|u_2\rangle \ .$$

The same $|u_1\rangle$ and $|u_2\rangle$ as were used in the circular polarization case above then yield

$$\langle u_2|\vec{r}|u_1\rangle = \langle u_2|x\vec{i} + y\vec{j} + z\vec{k}|u_1\rangle$$

$$= K\pi(\vec{i} + i\vec{j})$$

and

$$\langle u_1|\vec{r}|u_2\rangle = K\pi(\vec{i} - i\vec{j}) \ ,$$

with the former definition of K. The inner prime integrals in H''_{12} can be factored out and the two terms of H''_{12} will then involve the following factors, respectively:

$$\langle u_2|\vec{r}|u_1\rangle \cdot \langle u_1|\vec{r}|u_2\rangle = (K\pi)^2(\vec{i} + i\vec{j})\cdot(\vec{i} - i\vec{j})$$

$$= (K\pi)^2(1 + 1) ,$$

$$\langle u_1|\vec{r}|u_2\rangle \cdot \langle u_1|\vec{r}|u_2\rangle = (K\pi)^2(\vec{i} - i\vec{j})\cdot(\vec{i} - i\vec{j})$$

$$= (K\pi)^2(1 - 1)$$

$$= 0 .$$

The second term of H''_{12} will therefore be zero. Using $\int \vec{j}'_t \, d^3r' = \frac{2}{3} \int \vec{j}' \, d^3r'$, one finally obtains

$$H''_{12} = \frac{2}{3} \frac{k_e e^2}{\hbar c^3} \omega_{21}^3 \, |\langle u_1|\vec{r}|u_2\rangle|^2 \, c_1 c_2^* \, e^{i\omega_{21}t} ,$$

$$= \frac{1}{2} A_{12} \, c_1 c_2^* \, e^{i\omega_{21}t} , \qquad (18)$$

where A_{12} is the usual Einstein A coefficient and H''_{12} has the correct factor to cancel $e^{-i\omega_{21}t}$ in Eqs. (6').

The contributions to the transverse self field matrix element $H_{12} = H'_{12} + H''_{12}$ can now be collected and substituted into Eqs. (6'), yielding

$$\dot{c}_1 = c_2(\tfrac{1}{2} A_{12} + iM)c_1 c_2^* \quad , \quad \dot{c}_2 = -c_1(\tfrac{1}{2} A_{12} + iM)c_1^* c_2 ,$$

or, since $c_1 c_1^* + c_2 c_2^* = 1$,

$$\dot{c}_1 = c_1(\tfrac{1}{2} A_{12} + iM)(1 - |c_1|^2) \quad , \quad \dot{c}_2 = -c_2(\tfrac{1}{2} A_{12} + iM)(1 - |c_2|^2) .$$

If one tries a solution of the form

$$c_1 = |c_1| e^{iK_1(t)} ,$$

in the $\dot{c}_1$ equation and equates real and imaginary parts, then

$$|\dot{c}_1| = |c_1|(1 - |c_1|^2)\tfrac{1}{2}A_{12} \quad , \quad \dot{K}_1(t)|c_1| = |c_1|(1 - |c_1|^2)M .$$

$K_1(t)$ then obeys $\dot{K}_1(t) = (1 - |c_1|^2)M = |c_2|^2 M$ and will have a slow time variation. Similarly the $\dot{c}_2$ equation and the substitution

$$c_2 = |c_2| e^{iK_2(t)}$$

yields

$$|\dot{c}_2| = -|c_2|(1 - |c_2|^2)\tfrac{1}{2}A_{12} \quad , \quad \dot{K}_2(t) = (1 - |c_2|^2)M = |c_1|^2 M .$$

One can now see how the imaginary parts of a matrix element (M in this case) could alter the frequency of the radiation being emitted. $\vec{j}$ contains a factor $c_1 c_2^*$ which can be written ($\sigma_{ij} \equiv c_i c_j^*$)

$$\sigma_{12} = c_1 c_2^* = |c_1||c_2| e^{iM\int(\sigma_{22}-\sigma_{11})dt} .$$

Since $\sigma_{22}(= c_2 c_2^* = |c_2|^2)$ and σ_{11} will have a slow time variation, the frequency shift in σ_{12} will have a small time dependence. Jaynes has shown that several of the frequency shifts from this sort of effect seem to agree with the corresponding Lamb shifts. According to the present

solution for σ_{12}, however, whenever $|c_1|$ and $|c_2|$ are significantly different from zero and there is a large radiation current density ($|\sigma_{12}| >> 0$), the frequency shift will be small. It will in fact be zero at the point of maximum emission ($|c_1| = |c_2|$). For a complete transition, also, the time averaged shift in frequency will be zero. Thus a detectable shift by this means will result only when all atoms involved are excited inefficiently and remain near a particular state ($|c_1| \cong 0$, $|c_2| \cong 1$). But this is precisely the condition of all of the experimental measurements of 1S → 2P, 2S transitions, which have involved samples of hydrogen or deuterium gas containing tremendous numbers of atoms.[47,48] Irradiation of these samples by 1216 Å or 2430 Å (in the two photon case) ultraviolet light can be considered to produce excitations of particular atoms only slightly above the ground state ($1S_{1/2}$). There is then a substantial frequency shift ($\sigma_{11} \equiv c_1 c_1^* \cong 0$, $\sigma_{22} \cong 1$) equivalent to .278 cm^{-1} (including a vacuum polarization contribution). If an experiment could be arranged to "see" an entire 1S - 2S, P transition there should be no Lamb shift of the line. Now although this has not been accomplished for such n = 1 to n = 2 cases, it has been the principal method for determining the $2S_{1/2} - 2P_{1/2}$ transition frequency.[39] A beam of hydrogen atoms traverses a region of microwave radiation of the appropriate frequency in these methods, allowing very efficient excitation of the transition. Moreover, only complete transitions are observed since the atoms emerging in a particular state constitute the signal. Therefore Jaynes' sort of shift would average to zero and only other possible contributions to a level shift,

such as the "static" effects of Section IV, would be observable. Thus the existence of two distinct causes for Lamb shift frequencies corresponds exactly to two very different ways of measuring them.

The equations for the amplitudes of c_1 and c_2, which are of more concern for the present purposes, are solved in the following manner.[51] With the notation $\frac{1}{2} A_{12} \equiv A$, the substitution $|c_1| = ue^{At}$ in the $|\dot{c}_1|$ equation gives

$$\dot{u} = -A\, u^3\, e^{2\,At} .$$

Then

$$\int_{u_0}^{u} u^{-3} du = -A \int_{t_0}^{t} e^{2\,At}\, dt$$

can easily be solved to obtain

$$u = (e^{2\,At} - e^{2At_0} + \frac{1}{u_0^2})^{-1/2} .$$

Therefore

$$|c_1| = e^{At}\, (e^{2\,At} + C)^{-1/2}$$

and

$$\sigma_{11} = \frac{1}{Ce^{-A_{12}t} + 1} . \tag{19}$$

Similarly

$$\sigma_{22} = \frac{e^{-A_{12}t}}{Ce^{-A_{12}t} + 1} ,$$

and with the choice C = 1 for the constant of integration, these solutions will be as shown in Figure 8. The important facts to note in the context of spontaneous emission are that Eqs. (19) provide a consistent, matter conserving ($\sigma_{11} + \sigma_{22} = 1$) description of the phenomenon which predicts the correct Einstein A coefficient for the transition probability, through Eq. (18). There is one other important characteristic of a spontaneous transition revealed in Eq. (18), which is not obvious, and at first glance might appear of little consequence. This characteristic can be seen if it is noted that the symbol ω_{21} is defined by

$$\omega_{21} \equiv \omega_2 - \omega_1 \equiv \frac{1}{\hbar} (E_2 - E_1) ,$$

and that careful account has been taken of the sign of this energy difference in Eq. (18). One can therefore state that if $E_2 > E_1$, $A_{12} > 0$ and σ_{11} must begin at zero and go to one. Thus the transition must go from $|2\rangle$ to $|1\rangle$. There can be no spontaneous transition from state $|1\rangle$ to $|2\rangle$ if $E_2 > E_1$. In Figure 8, the time development of the higher energy state is always given by the dotted curve σ_{22}, and so inherent in Eq. (18) is proof that there cannot be a spontaneous transition from lower to higher energy. This fact, in turn, is a necessary condition for obtaining the correct form of the blackbody spectrum.

Based on the preceding facts then, the blackbody frequency distribution can be obtained rigorously by means of Einstein's simple procedure. If one considers a two level transition $|1\rangle \leftrightarrow |2\rangle$ at a certain frequency in the walls of a blackbody cavity, one must assume

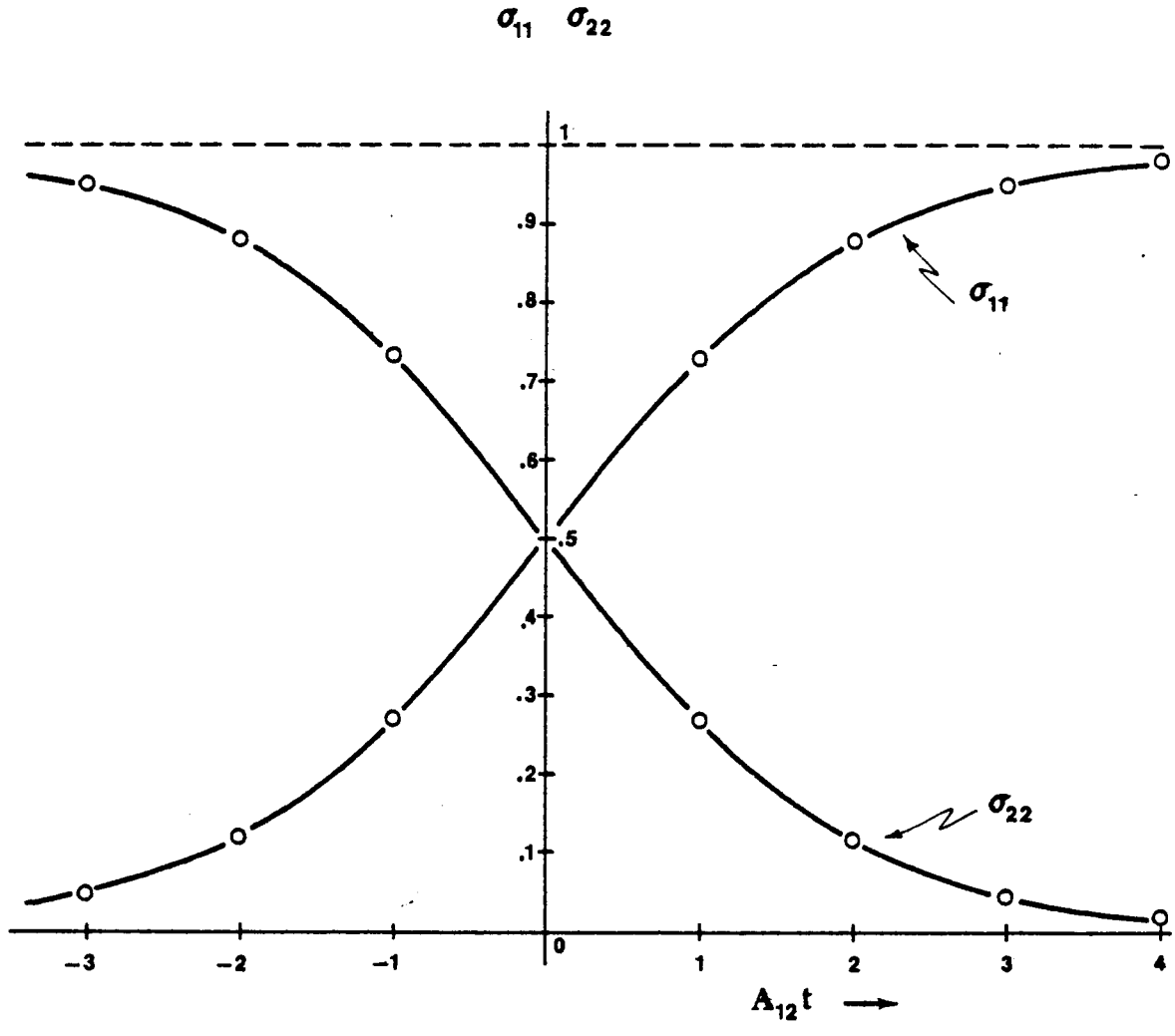

Figure 8. Time development of a spontaneous transition.

the ratio of number of atoms in the upper state N_2 to number in the lower N_1 to be

$$\frac{N_2}{N_1} = e^{-(E_2-E_1)/kT} .$$

Equal numbers n go up or down since equilibrium exists; therefore the ratio of transition probabilities is

$$\frac{P_1}{P_2} = \frac{n/N_1}{n/N_2} = e^{-(E_2-E_1)/kT} .$$

But one can now state that

$$P_1 = \frac{4\pi^2 e^2 k_e}{3\hbar^2} |\langle 1|\vec{r}|2\rangle|^2 \frac{I(\omega)}{c} = B_{12} \frac{I(\omega)}{c}$$

for stimulated upward transitions and

$$P_2 = B_{12} \frac{I(\omega)}{c} + A_{12}$$

for stimulated and spontaneous downward transitions. Therefore

$$e^{-\frac{\hbar\omega}{kT}} = \left(\frac{4\pi^2 e^2 k_e}{3\hbar^2} |\langle 1|\vec{r}|2\rangle|^2 \frac{I(\omega)}{c}\right) \div \left(\left(\frac{4\pi^2 e^2 k_e}{3\hbar^2} \frac{I(\omega)}{c} + \frac{4e^2 k_e \omega^3}{3\hbar c^3}\right) |\langle 1|\vec{r}|2\rangle|^2\right)$$

or, for the energy density in $\Delta\omega$,

$$\frac{I(\omega)}{c} \Delta\omega = \frac{\hbar\omega^3 \Delta\omega}{\pi^2 c^3 (e^{\hbar\omega/kT} - 1)} .$$

D. THE $\dot{c}_i$ EQUATIONS FOR THE COMPTON EFFECT

It is of interest now to turn to a final application of the preceding semiclassical methods and to attempt to apply the above analysis of the spontaneous transition "self field" $\dot{c}_i$ equations to a problem which was left unsolved in Section III. There it was stated that a realistic account of the time development of a single Compton transition, as expressed in the $B_1(t)$ and $B_2(t)$ coefficients, would require the inclusion of the secondary radiation emitted by the changing wave functions. One now has the necessary tools to do this. It is important to note first, however, that the conditions assumed in Section III are unrealistic, at least at the incident radiation wavelengths where there is any detectable difference between the Thompson and Klein-Nishina predictions for the scattering. The initial use of x-rays in Compton scattering work has been almost universally abandoned in favor of shorter wavelength and more easily obtainable γ-rays from radioactive materials.[52] Radiation at these wavelengths almost certainly exhibits some "photon-like" properties, as has been shown to some extent in Section III. Specifically such radiation will consist of short pulses in time, in addition to any spatial aspects of discreteness, and therefore cannot really be treated as a monochromatic plane wave of infinite length as has been done in the present work. Realistically, one would have to take into account the pulse envelope time dependence, and then the probability of a certain event could come out to be a function of the scattering angle. In the present case, however, one can only assume that a linear, infinite plane wave must be interpreted for modern

experiments as a beam of "photon" pulses superimposed. Then since the intensity ratios account for the angular dependence of the scattering, one should expect that the time development of a Compton transition in the present treatment should not necessarily depend on angle. This is what is found in the following analysis. The discussion is probably more valuable in indicating how one might account microscopically for absorption of radiation and certain other phenomena than in describing accurately an individual Compton event.

One can begin with a straightforward evaluation of the Lorentz gauge vector and scalar potentials produced by the charge and current densities in the Compton effect.[53] These are, in the notation of Section III:

$$
\begin{aligned}
\vec{j} &= \frac{e\hbar}{2im}\,(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{e^2}{mc}\left(\frac{k_e}{k_m}\right)^{1/2}\vec{A}\psi\psi^* \\
&= \frac{e\hbar}{2im}\left(\left(c_1^*Q_1^* + c_2^*Q_2^*\, e^{-i(\vec{q}\cdot\vec{r}-\omega_q t)}\right)\left(c_2Q_2 i\vec{q}\, e^{i(\vec{q}\cdot\vec{r}-\omega_q t)}\right)\right. \\
&\quad \left. - \left(c_1Q_1 + c_2Q_2\, e^{i(\vec{q}\cdot\vec{r}-\omega_q t)}\right)\left(c_2^*Q_2^*\,(-i\vec{q})e^{-i(\vec{q}\cdot\vec{r}-\omega_q t)}\right)\right) \\
&\quad - \frac{e^2}{mc}\left(\frac{k_e}{k_m}\right)^{1/2}\vec{\varepsilon}_1\,\frac{A_{inc.}}{2}\left(\left(c_1^2Q_1^2 + c_2^2Q_2^2\right)2\cos\,(\vec{k}_1\cdot\vec{r}-\omega_1 t)\right. \\
&\quad + c_1^*Q_1^*c_2Q_2\, e^{i(\vec{k}_2\cdot\vec{r}-\omega_2' t)} + c_1Q_1c_2^*Q_2^*\, e^{-i(\vec{k}_2'\cdot\vec{r}-\omega_2' t)} \\
&\quad \left. + c_1^*Q_1^*c_2Q_2\, e^{-i(\vec{k}_2\cdot\vec{r}-\omega_2 t)} + c_1Q_1c_2^*Q_2^*\, e^{i(\vec{k}_2\cdot\vec{r}-\omega_2 t)}\right) \\
&= \vec{j}_\psi + j_{\vec{A}} + ① + ② + ③ + ④\,, \qquad (19)
\end{aligned}
$$

where $\vec{k}_2' = \vec{k}_1 + \vec{q}$, $\vec{k}_2 = \vec{k}_1 - \vec{q}$, and

$$\rho = e\psi\psi^* = e\left(c_1^2Q_1^2 + c_2^2Q_2^2 + c_1c_2^*Q_1Q_2^* \, e^{-i(\vec{q}\cdot\vec{r}-\omega_q t)} + c_1^*c_2Q_1^*Q_2 \, e^{i(\vec{q}\cdot\vec{r}-\omega_q t)}\right) .$$

The vector potential produced by $\vec{j}$ is again given by

$$\vec{A}_{self} = \frac{1}{c}(k_e k_m)^{1/2} \iiint \frac{\vec{j}(\vec{r}', t-R/c)}{R} d^3r'$$

$$\simeq \frac{1}{c}(k_e k_m)^{1/2} \iiint \frac{\vec{j}(\vec{r}', t)}{R} d^3r' - \frac{1}{c^2}(k_e k_m)^{1/2} \frac{d}{dt} \iiint \vec{j}(\vec{r}', t) d^3r',$$

giving a "near zone" $\vec{A}_s$ and a "slightly retarded" $\vec{A}_s'$. The method of evaluation of the "near zone" $\vec{A}_s$ can be illustrated by use of ③ and ④ (the Compton radiation terms). The $R^{-1} \equiv |\vec{r} - \vec{r}'|^{-1}$ factor can be expressed as

$$\frac{1}{R} = \frac{1}{|\vec{r} - \vec{r}'|} = \frac{(4\pi)}{(2\pi)^3} \int \frac{1}{k^2} e^{i\vec{k}\cdot\vec{R}} d^3k .$$

Substitution of ③ and ④ in the "unretarded" part of the $\vec{A}_{self}$ expression, with the notation $\sigma_{ij} = c_i c_j^* Q_i Q_j^*$, yields

$$\vec{A}_s = \left(-\frac{e^2}{mc}\left(\frac{k_e}{k_m}\right)^{1/2} \frac{1}{2} A_1 \vec{\varepsilon}_1\right) \frac{(k_e k_m)^{1/2}}{c} \frac{4\pi}{(2\pi)^3} \int_k \iiint_{\vec{r}'} \left(\sigma_{12} \, e^{i(\vec{k}_2\cdot\vec{r}-\omega_2 t)} + \sigma_{21} \, e^{-i(\vec{k}_2\cdot\vec{r}-\omega_2 t)}\right) e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \, d^3r' \, \frac{1}{k^2} d^3k$$

$$= C \int \frac{1}{k^2} e^{i(\vec{k}\cdot\vec{r})} \left(\iiint_{\vec{r}'} e^{i(\vec{k}_2 - \vec{k})\cdot\vec{r}'} \, d^3r' \right) d^3k\sigma_{12} \, e^{-i\omega_2 t}$$

$$+ C \int \frac{1}{k^2} e^{i(\vec{k}\cdot\vec{r})} \left(\iiint_{\vec{r}'} e^{-i(\vec{k}_2 + \vec{k})\cdot\vec{r}'} \, d^3r' \right) d^3k\sigma_{21} \, e^{i\omega_2 t}$$

where $C = -r_0 \frac{1}{2} A_1 \vec{\varepsilon}_1 \frac{4\pi}{(2\pi)^3}$. The $\vec{r}'$ integration gives $(2\pi)^3\delta^3(\vec{k}_2 - \vec{k}) \cong V \delta^3_{\vec{k}_2\vec{k}}$ and therefore

$$\vec{A}_s(\vec{r},t) = \frac{1}{k_2^2} (2\pi)^3 C \sigma_{12} e^{i(\vec{k}_2\cdot\vec{r} - \omega_2 t)} + \frac{1}{k_2^2} (2\pi)^3 C \sigma_{21} e^{-i(\vec{k}_2\cdot\vec{r} - \omega_2 t)} .$$

Thus the unretarded vector potential from ③ and ④ depends on $\vec{r}$ and t in exactly the same way as do ③ and ④ themselves. In a similar way, every other term of $\vec{j}$ gives an unretarded $\vec{A}_s$ of the same form as itself. The term of $\vec{j}$ in Eq. (19) which is independent of time,

$$\vec{j}_{const.} = \frac{e\hbar}{m} \sigma_{22} \vec{q} ,$$

is assumed to make no contribution to $\vec{A}_s$. For the second term in the expansion of $\vec{A}_{self}$, $\vec{A}_s'$, only the terms of $\vec{j}$ which are independent of $\vec{r}$ will give a nonzero integration. If $\vec{j}_{const.}$ is again ignored, this means that

$$\vec{A}_s' = 0 .$$

The total vector potential in the interaction volume V, including the incident field $\vec{A}_{inc.}$ and the above self field contributions, is then given by the following expression:

$$\vec{A}_T = \vec{A}'_s + \vec{A}_s + \vec{A}_{inc.}$$

$$= \frac{(k_e k_m)^{1/2}}{c} 4\pi \left\{ \frac{e\hbar}{2im} \left(\sigma_{21}\, i\vec{q}\, e^{i(\vec{q}\cdot\vec{r}-\omega_q t)} + \sigma_{12}\, i\vec{q}\, e^{-i(\vec{q}\cdot\vec{r}-\omega_q t)} \right) \frac{1}{q^2} - \frac{1}{2} \frac{e^2}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} A_{inc.} \vec{\varepsilon}_1 \right.$$

$$\times \left(\frac{1}{k_1^2} (\sigma_{11} + \sigma_{22})\, 2\cos(\vec{k}'_1\cdot\vec{r} - \omega_1 t) + \frac{1}{k_2'^2} \sigma_{21}\, e^{i(\vec{k}_2\cdot\vec{r}-\omega'_2 t)} \right.$$

$$+ \frac{1}{k_2'^2} \sigma_{12}\, e^{-i(\vec{k}'_2\cdot\vec{r}'-\omega_2 t)} + \frac{1}{k_2^2} \sigma_{21}\, e^{-i(\vec{k}_2\cdot\vec{r}-\omega_2 t)}$$

$$\left. \left. + \frac{1}{k_2^2} \sigma_{12}\, e^{i(\vec{k}_2\cdot\vec{r}-\omega_2 t)} \right) \right\} + \frac{1}{2} A_{inc.} \vec{\varepsilon}_1 \left(e^{i(\vec{k}_1\cdot\vec{r}-\omega_1 t)} + e^{-i(\vec{k}_1\cdot\vec{r}-\omega_1 t)} \right).$$

It is necessary now to determine which terms of $\vec{A}_T$ contribute to $H'_{ij} = \langle u_i | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}_T \cdot \nabla | u_j \rangle$ or $H''_{ij} = \langle u_i | \frac{e^2}{m^2c^2} \left(\frac{k_e}{k_m}\right) \vec{A}_T \cdot \vec{A}_T | u_j \rangle$. By substitution of the above expression for $\vec{A}_T$ in H''_{ij}, it is found that many terms of $\vec{A}_T^2$ contribute to H''_{ij} but that they always give a real H''_{ij} which, divided by ih, turn out to give only phase shifts to c_1 and c_2, in every case. For example H''_{12} will have a nonzero term from

$$\left(\frac{1}{2} A\vec{\varepsilon}_1\, e^{-i(k_1\cdot\vec{r}-\omega_1 t)} \right) \cdot \left(\frac{-1}{2k_2^2} A\varepsilon_1 \frac{e^2}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \sigma_{12}\, e^{i(\vec{k}_2\cdot\vec{r}-\omega_2 t)} \right)$$

$$= K''_{12}\sigma_{12}\, e^{-i(\vec{q}\cdot\vec{r}-\omega_q t)},$$

where K''_{12} is a constant. The contribution to H''_{12} from this term will be ($\sigma'_{ij} \equiv c_i c_j^*$)

$$\frac{-k_e e^3}{k_2^2 m^2 c^4} \pi A^2 \sigma'_{12} = C''_{12} \sigma'_{12} \ .$$

When this is substituted in the $\dot{c}_i$ equations, the c_1 equation, for example, will be in the form

$$\dot{c}_1 = (\text{other terms})\ c_1 + (\text{other terms} + \frac{C''_{12}}{i\hbar}\ \sigma'_{12}) c_2 \ ,$$

and this σ'_{12} term can be rewritten as

$$\dot{c}_1 = \ldots + iM\ c_1 c_2^* c_2 = \ldots + iM\ c_1 (1 - c_1^2) \ .$$

c_1 can be factored out, leaving an imaginary slowly varying part $iM|c_2|^2$, which depends only on the absolute value of c_2. As shown previously, this then affects only the phase of c_1. One can show that <u>every</u> contribution to H''_{11}, H''_{12}, H''_{21}, and H''_{22} from $\vec{A}_T^2$ follows this same pattern. There are no terms which determine the variation of $|c_1|$ or $|c_2|$.

The same conclusions result from consideration of the $H'_{ij} = \langle u_i | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}_T \cdot \nabla | u_j \rangle$ term in the $\dot{c}_i$ equations, where again $\vec{A}_T$ $(= \vec{A}_s + \vec{A}'_s + \vec{A}_{inc.})$ is given by the expression on the previous page. $\vec{A}_T$ is explicitly real, including any arbitrary choices for Q's in $\sigma_{ij} = c_i c_j^* Q_i Q_j^*$, and so the ∇ operating on $|u_j\rangle$ introduces $i\vec{q}$ (if $\neq 0$), the i then cancelling the i in the constant coefficient of the matrix element. Therefore H'_{ij} is real (or 0) and the $i\hbar$ from the left sides of the $\dot{c}_i$ equations makes $\frac{H'_{ij}}{i\hbar}$ imaginary. As shown above, σ_{ij} enters in such a way that c_1 or c_2 can be factored out, leaving terms which will affect only the <u>phase</u> of c_1 and c_2. For example,

$$H'_{12} = \langle Q_1^* | (K'_{12})(i\hbar)\, \sigma_{12}(\vec{q}) e^{-i(\vec{q}\cdot\vec{r}-\omega_q t)} \cdot \nabla | Q_2\, e^{i\vec{q}\cdot\vec{r}} \rangle$$

$$= \langle Q_1^* | (K'_{12})(i\hbar)\sigma_{12}(\vec{q}) \cdot (i\vec{q}) e^0 | Q_2 \rangle$$

$$= \langle Q_1^* | (K'_{12})(-\hbar)\vec{q}^2 \sigma_{12} | Q_2 \rangle = C'_{12}\sigma'_{12}$$

where K'_{12} and C'_{12} are real constants. The $\dot{c}_1$ equation is:

$$i\hbar\, \dot{c}_1 = (H'_{11} + H''_{11})c_1 + (H'_{12} + H''_{12})c_2$$

$$= (H'_{11} + H''_{11})c_1 + (C'_{12}\sigma'_{12} + H''_{12})c_2 \,.$$

Therefore,

$$\dot{c}_1 = (\ \ldots\ )c_1 + \frac{C'_{12}}{i\hbar}\, c_1 c_2^* c_2$$

$$= (\ \ldots\ )c_1 + \frac{C'_{12}}{i\hbar}\, |c_2|^2 c_1$$

This term therefore affects only the phase of c_1. The same argument applies to every term of H'_{11}, H'_{12}, H'_{21}, H'_{22}. There are again no terms which control the $|c_1|$ and $|c_2|$ time dependence.

Still working under the assumption that the potentials are expressed in the Lorentz gauge, one must also examine the effects of the scalar potential Φ, which obeys the inhomogeneous wave equation

$$\nabla^2\Phi - \frac{1}{c^2}\,\partial_t^2\Phi = -4\pi k_e \rho \,.$$

Therefore

$$\Phi = \iiint \frac{-4\pi k_e \rho(t-R/c)}{-4\pi R} d^3r'$$

$$= k_e \iiint \frac{\rho(t - R/c)}{|\vec{r} - \vec{r}'|} d^3r'$$

$$= k_e \iiint \frac{\rho(\vec{r}', \vec{t})}{R} - \frac{k_e}{c} \frac{d}{dt} \iiint \rho(\vec{r}', t) d^3r' + \ldots .$$

If the expression for the transition charge density $\rho = e\psi\psi^*$ given previously is substituted in the above formula the scalar potential becomes

$$\Phi = 4\pi k_e e \left(\sigma_{12} e^{-i(\vec{q}\cdot\vec{r}-\omega_q t)} + \sigma_{21} e^{i(\vec{q}\cdot\vec{r}-\omega_q t)} \right) ,$$

where constant terms are again omitted. The same arguments apply as previously since Φ is real and $\frac{\Phi}{i\hbar}$ is imaginary, and σ_{ii} enters just as in the H'_{ij} $(\vec{A} \cdot \nabla)$ case. Therefore Φ also only produces a c_1 or c_2 phase change.

It is perhaps necessary to be more precise about the physical reality of the situation. As in Section III, one is not concerned simply with plane wave functions. The case can be compared with that of the separation of the hydrogen atom problem into center of mass coordinates and relative coordinates. The Schrödinger equation for the center of mass coordinates is a free particle equation with a plane wave solution

$$\psi_{CM} = e^{i(\vec{q}\cdot\vec{R}_{CM}-\omega_{CM}t)} .$$

But this does not affect the usual relative coordinate solution, which

effectively limits the H atom to a volume with a radius of only a few Bohr radii. That is, $\psi(\vec{r},t) = \psi_{CM}(\vec{r},t)\psi_{n\ell m}(\vec{r},t)$. One must then think of ψ_{CM} as superimposed over, and limited by the extent of, the relative coordinate solution. As discussed in Section III, it is possible to assume that the same sort of thing occurs in the case of a single electron, except that the equation obeyed by the relative coordinates is not known. One can hypothesize some "structure" function which is unknown but slowly varying with respect to the superimposed free particle solution, as shown in Figure 2, p. 26.

The physical "transition" wave function can then be assumed to be

$$\psi = c_1 f_1(\vec{r})\psi_1 + c_2 f_2(\vec{r})\psi_2 ,$$

which satisfies

$$\left(- \frac{\hbar^2}{2m} \nabla^2 + \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A} \cdot \nabla + \frac{k_e e^2}{2k_m mc^2} \vec{A}^2 \right) \psi = - \frac{\hbar}{i} \partial_t \psi .$$

This insures that

$$\vec{j} = \frac{e\hbar}{2m} (\psi^* \nabla\psi - \psi \nabla\psi^*) - \frac{e^2}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}\psi\psi^*$$

no matter what the form of ψ. The assumption that $f_1(r)$ and $f_2(r)$ are slowly varying implies that

$$\nabla(f_1(\vec{r})\psi_1(\vec{r},t)) = f_1(\vec{r})\nabla\psi_1 + \psi_1 \nabla f(\vec{r})$$

$$\tilde{=} f_1(\vec{r})\nabla\psi_1 ,$$

and therefore that free particle ψ_1 and ψ_2 are appropriate and furthermore, that the current densities produced by f_1 and f_2 are negligible.

One may now consider the effect of these "structure" functions on the matrix elements in the $\dot{c}_i$ equations. Again the constant terms of $\vec{A}_T$ have been dropped and only the physical, time varying parts retained. Then writing out the matrix element components which depend on $f_1(\vec{r})$ and $f_2(\vec{r})$, one obtains:

$$H'_{11\ im} = \langle Q_1^* f_1(\vec{r}) | \frac{ie\hbar}{me} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}_T \cdot \nabla f_1(\vec{r}) | Q_1 \rangle$$

$$H'_{22\ im} = \langle Q_2^* f_2(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}_T \cdot \nabla f_2(\vec{r}) | Q_2 e^{i\vec{q}\cdot\vec{r}} \rangle$$

$$H'_{12\ im} = \langle Q_1^* f_1(\vec{r}) | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}_T \cdot \nabla f_2(\vec{r}) | Q_2 e^{i\vec{q}\cdot\vec{r}} \rangle$$

$$H'_{21\ im} = \langle Q_2^* f_2(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} | \frac{ie\hbar}{mc} \left(\frac{k_e}{k_m}\right)^{1/2} \vec{A}_T \cdot \nabla f_1(\vec{r}) | Q_1 \rangle$$

Now only the constant terms of $\vec{A}_T$, which have been assumed to have no real existence, would contribute to $H'_{11\ im}$ and $H'_{22\ im}$. Therefore $H'_{11\ im} = H'_{22\ im} = 0$. For $H'_{12\ im}$, only

$$\vec{A}_{-\vec{q}} = 4\pi \frac{1}{q^2} \frac{(k_e k_m)^{1/2}}{c} \frac{e\hbar}{2m} \sigma_{12}\, \vec{q}\, e^{-i(\vec{q}\cdot\vec{r}-\omega_q t)}$$

contributes. $H'_{12\ im}$ becomes

$$H'_{12\ im} = \frac{k_e e^2 i\hbar^2}{2m^2c^2} 4\pi \frac{1}{q^2} \sigma_{12}\, G\, e^{i\omega_q t} \equiv i\hbar\, M\, \sigma'_{12}\, e^{i\omega_q t}$$

where $G = \langle Q_1^* f_1(\vec{r}) | \vec{q} \cdot \nabla | Q_2 f_2(\vec{r}) \rangle$. Similarly $H'_{21\ im}$ is

$$H'_{21\ im} = \frac{k_e e^2 i\hbar^2}{2m^2c^2} 4\pi \frac{1}{q^2} \sigma_{21}\, (-G) e^{-i\omega_q t} \equiv -i\hbar\, M\, \sigma'_{21}\, e^{-i\omega_q t} ,$$

when use is made of $\vec{A}_{\vec{q}}$ and partial integration.

Finally, then one can include all of the contributions to the matrix elements discussed above in the $\dot{c}_i$ equations:

$$i\hbar\dot{c}_1 = [H''_{11} + H'_{11}]c_1 + [H''_{12} + H'_{12} + H'_{12\ im}]c_2$$

$$i\hbar\dot{c}_2 = [H''_{21} + H'_{21} - H'_{12\ im}] + [H''_{22} + H'_{22}]c_2 .$$

Now since $H'_{ij} + H''_{ij}$ involve only the amplitudes of c_1 and c_2, a factor $e^{iK_{1,2}(t)}$ in $c_{1,2}$ accounts for all imaginary parts and one is left with the following equations which describe the time variation of $|c_1|$ and $|c_2|$:

$$|\dot{c}_1| = M|c_2 c_2^*|c_1 = M(1 - |c_1|^2)|c_1|$$

$$|\dot{c}_2| = -Mc_1 c_1^*|c_2 = -M(1 - |c_2|^2)|c_2| .$$

These equations have the same form as those solved previously for spontaneous emission and they therefore provide a consistent mechanism for a Compton event. That is, in the notation of Section III,

$$|c_1| \equiv B_1 \text{ and } |c_2| \equiv B_2 ,$$

they imply

$$(B_1(t))^2 + (B_2(t))^2 = 1$$

and a time dependence as shown in Figure 7, p. 78. Again it must be remembered, however, that they could only apply exactly to a Compton transition involving monochromatic plane wave radiation of infinite duration.

This last application of semiclassical ideas has thus brought the overall discussion back to its first major example, the Compton effect. But at the same time, this return to a previously treated semiclassical problem with new semiclassical methods epitomizes the philosophy which may serve to unify the apparently unrelated subject matter of Sections III, IV, and V. This underlying principle in essence is that it is of paramount importance that classical concepts of space and time not be abandoned in the search for explanations of physical phenomena. Quantum electrodynamics has of course been one of the foremost theories which has at least in part forsaken such classical restraints. Various of its adherents, at one time or another, have cited most of the phenomena discussed in the present work the Lamb shift, spontaneous emission, blackbody radiation, the photoelectric effect, the discrete nature of Compton scattering, as evidence against semiclassical theories. This fact is partly responsible for the choice of subjects here. Another is simply that the present explanations of these subjects seem to be

excellent examples of the value of retaining a foundation of classical ideas of time, space, and fields in a physical realm which can never be experienced directly.

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28. This would depend on the time dependence of the coefficients. In general these changes are slow compared to the wave function frequencies.

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33. All equations such as (5) which contain electromagnetic quantities are written with the constants k_e and k_m so that they be expressed in any system of units according to the following:

Units	k_e	k_m
MKS	$\frac{1}{4\pi\varepsilon_o}$	$\frac{\mu_o}{4\pi}$
Gaussian	1	1
Heavyside-Lorentz	$\frac{1}{4\pi}$	$\frac{1}{4\pi}$
esu	1	$\frac{1}{c^2}$
emu	c^2	1

34. This is actually incorrect but is equivalent to the usual semiclassical procedure. The correct method of handling $(\omega+\omega_{21})$ is treated in Section VB.

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43. The rest mass energy of a particle or the static self energy in its electric field do not enter into consideration. Note the cancellation of the rest mass terms in the Dirac equation and the contributions to the energy in the nonrelativistic Schrödinger equation.

44. The P level is lowered here in contrast to other derivations (Bethe, Welton) where the S level is raised (due to the r=0 behavior of the s wave function). There is no experimental difference.

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50. A question arises concerning the consistency of the assertion that the transverse self vector potential produces observable effects while in Section IV the energies due to the self fields are taken to be unobservable. An identification of all the terms involved can be made by writing the entire potential energy operator for a particle in an electromagnetic field:

$$\hat{u}|\psi\rangle = \left(q\Phi + \frac{i\hbar q}{mc}\left(\frac{k_e}{k_m}\right)^{1/2} \vec{A} \cdot \nabla\right)|\psi\rangle .$$

If the scalar and vector potentials produced by the particle wave function itself are included and the self vector potential further broken into transverse and longitudinal parts, the complete potentials in $\hat{u}$ are

$$\Phi = \Phi_{ext} + \Phi_{self} , \quad \vec{A} = \vec{A}_{ext} + \vec{A}_{self,t} + \vec{A}_{self,\ell} .$$

With regard to the self terms in particular, it can be shown that for any one stationary state ψ the Φ_{self} term gives a self potential energy due to the location of ρ_ψ in Φ_{self} which is equal to

$$\frac{1}{8\pi k_e} \int \vec{E}^2 d^3r .$$

Similarly the A_{self} term, which for a stationary ψ is wholly longitudinal, gives a self potential energy equal to

$$\frac{1}{2c}\left(\frac{k_e}{k_m}\right)^{1/2} \int \vec{j} \cdot \vec{A}_{self,\ell} d^3r = \frac{1}{8\pi k_m} \int \vec{B}^2 d^3r .$$

These are the field energies which are calculated in Section IV and assumed to be unobservable, as they are also in QED (Harris, Heitler) and in classical electrodynamics (Heitler, Jackson).

In particular for the classical Abraham-Lorentz evaluation of the self force on an electron, $\vec{A}_{self}$ is expanded just as Jaynes does. The "unretarded" term giving rise to

$$\frac{4}{3} \dot{\vec{v}} \frac{U_{self}}{c^2} ,$$

the second ("retarded") term to $-\frac{2}{3}\frac{k_e e^2}{c^3} \ddot{\vec{v}}$. These are respectively the electromagnetic mass times acceleration force and radiation reaction force. The question in these terms is whether or not any part of the unretarded $\vec{A}$ term of Jaynes can be observable since U_{self} has already been declared unobservable. Let it suffice to say that the Abraham-Lorentz derivation has also a separate electrostatic force term which is actually the force corresponding to the U_{self} energy. It is really this term which must be assumed unobservable.

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53. The complete expressions for these charge and current densities are retained in this discussion in contrast to that of Section VC in which it is assumed that only the transverse part of the self vector potential was felt by the electron. This entire analysis is meant only to be illustrative of some approaches which might be useful for a complete description of a Compton transition.

VITA

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