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Theory of radiation reaction and atom self-energies: all-order perturbation theory of the generalized non-relativistic Lamb shift

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Abstract. We describe a natural all-order decorrelation procedure for the interaction of a single two-level atom with all modes of the radiation field which replaces the semi-classical boson approximation for the atom by an exact fermion treatment. In consequence the vacuum Lamb shift appears as twice the Bethe shift for each level separately instead of the limiting neo-classical shift obtained in the Bose theory.

Stimulated emission and absorption modify the Einstein A coefficient and the vacuum shift is extended to include a field dependent shift. Mass renormalization terms apparently particular to the two-level atom, one field dependent the other not, also arise; but the kinetic mass renormalization which appears in the boson theory is identically eliminated. The all-order decorrelated perturbation theory yields an equation of motion for the single-atom dipole moment which includes those reported from operator radiation reaction theory recently; but it also generalizes these by including the effects of stimulated processes.

The method is extended to a many-atom case in which it becomes necessary to modify the procedure slightly. The theory gives exponential decay of the dipole density waves travelling through an attenuator and the decay constant is modified by stimulated terms proportional to the field intensity. There is corresponding exponential growth in the amplifier.

1. Introduction

The quantum electrodynamics of spontaneous emission is well understood in both non-relativistic and relativistic formulations of perturbation theory (cf, eg, Power 1964, Kroll 1965 as well as Low 1952 for the relativistic problem). Further, Weisskopf and Wigner (1930) long since gave us a dynamical theory of spontaneous emission using Dirac's method of 'variation of constants' for the Schrödinger wavefunction. Nevertheless it is natural to wish to provide a dynamical theory of spontaneous emission which exhibits the radiation damping mechanism as a radiation reaction of the type first considered (in a c number theory) by Lorentz (1909)‡. Moreover in modern quantum optics it has become desirable to be able to treat the intense field optics of a many-atom system systematically without *ad hoc* inclusion of damping and radiative level shifting processes which may in any case apply only to single atoms coupled to weak or vanishing fields.

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‡ See especially the 1952 edition of this book (New York: Dover) §§ 27, 28, 37 and 38, and note 18.

In this series of papers we therefore develop a theory of *operator* reaction fields which is applicable to systems of one or more atoms each with two or more energy levels: the theory covers the problems of spontaneous emission, stimulated emission and absorption, and radiative level shifts due both to the vacuum (the Lamb shift) and to imposed fields. It is interesting to note that the recent optical resolution of hyperfine structure in sodium (Hänsch *et al* 1971) and similar work (eg Schallow 1973) makes a one-atom theory of radiative level shifts with this degree of generality very desirable at this time. The N atom theory also includes the theory of super-radiance, due in the first instance to Dicke (1954) in a natural way as a radiation reaction field theory.

Recently Jaynes and co-workers (Jaynes and Cummings 1963, Crisp and Jaynes 1969, Stroud and Jaynes 1970, Jaynes 1973) have studied a 'neo-classical' theory of spontaneous emission and level shifts which is essentially non-linear and agrees with Bethe's perturbation theory of the Lamb shift only to order of magnitude and then only in the long-time limit. A number of workers (for example Bullough *et al* 1972, Bullough 1973, Ackerhalt *et al* 1973) have already reported, however, that the neo-classical theory is equivalent to a non-linear operator reaction field theory in which operator products are systematically decorrelated. They also show in more or less degree that if the non-linear operator theory is not decorrelated the results do agree with Bethe's for the shifts† and Weisskopf's and Wigner's for the dynamical evolution of the radiation rate. Operator reaction field theory as such, however, is still only briefly reported and it is the aim of this series of papers to present a comprehensive theory of this type in a completeness greater than was possible in earlier reports.

The theory is both approximate and to an extent internally inconsistent (Bullough 1973, Bullough *et al* 1973). The inconsistencies arise only if the number of field modes is unbounded but reaction field theory is rather sensitive to exposing these. One approximation is to make the usual rejection of certain terms as 'mass renormalization' terms. These are actually identical in form with those arising at order e^2 in perturbation theory and show that although the theory is dynamical (that is valid for all time) it is still an order e^2 theory. This is a consequence of a second approximation apparently required to simplify the effect of the reaction field: perhaps the most challenging problem remaining in reaction field theory is to find an exact solution of even the simplest problem of a single atom coupled to the vacuum field.

These facts mean that a check on the dynamical theory is needed and one has already been briefly reported (Bullough and Caudrey 1971). Since the report is brief and has apparently been misunderstood (compare Ackerhalt *et al* 1973 and our comments in Bullough *et al* 1973) we shall preface this series of papers on reaction field theory with a paper which gives complete account of this somewhat different approach to the problem of a coupled matter field system. It is an all-order perturbation theory which yields as its main result the equations of motion (4.12) for the dipole moment of a single two-level atom valid precisely to order e^2. These equations contain field-dependent effects and have all the generality previously described. We regain directly comparable results specifically by operator reaction field methods in later papers; and there we are also able to draw correspondence with the technique of master equations developed especially by Agarwal (1970, 1971a, 1971b, 1973a, 1973b). This correspondence is one of complete equivalence and serves as a further check on both the reaction field and perturbation theories.

In this paper we consider the problem of a collection of two-level atoms in an electromagnetic field. This field is divided into two parts. The first of these is quantized and is

† For this see also Agarwal (1973a).

specified as an initial condition on the density matrix at $t = -\infty$ by an initial Foch state vector with non-vanishing occupation numbers in one or more field modes. The second part is a 'probe' field which is assumed to be classical and of low intensity. The mode of calculation is to find a linear response relation for the atomic system in the quantized field induced by the semi-classical field. Later in this series we show how the totally quantized reaction field theory reproduces both the non-linear features due to the quantized field in the present calculation as well as the features due to the 'external' semi-classical probe.

The § 2 which follows describes the system of fields and atoms in detail as well as some of the work on linear response theory which has already been done on it. In § 3 we describe a new decorrelation procedure for one atom in which the field is decorrelated and not the atomic system as in earlier work. The § 4 gives an example of how the method works for a specific distribution of occupation numbers for the quantized field and shows that the field not only produces stimulated emission but also modifies the Lamb shift. In this section we derive the main result (4.12) of the paper.

In § 5 the method of all-order perturbation theory is generalized to a many-atom system. It becomes necessary to decorrelate the atomic system as well as the field in this case and the outcome is the same as if the one-atom case could simply be used to provide a formula for the atomic polarizability in an otherwise totally classical theory. Finally § 6 is a discussion of the results. It also assesses the advantages and disadvantages of the particular form of all-order perturbation theory from which these results have been obtained.

2. Description of system and earlier work

Our system consists of N atoms situated at the points $\boldsymbol{x}_i$ ($i = 1, 2, \ldots, N$) in an electromagnetic field. We define a dipole density operator

$$\boldsymbol{p}(\boldsymbol{x}, t) = e \sum_i \delta(\boldsymbol{x} - \boldsymbol{x}_i) \boldsymbol{r}_i(t) \tag{2.1}$$

where $e\boldsymbol{r}_i(t)$ is the dipole operator for the ith atom. All operators are conveniently taken in the interaction representation. In the dipole approximation we can take the interaction as the interaction density

$$H_{\text{int}}(\boldsymbol{x}, t) = -\boldsymbol{p}(\boldsymbol{x}, t) \cdot (\boldsymbol{e}(\boldsymbol{x}, t) + \boldsymbol{E}_{\text{ext}}(\boldsymbol{x}, t)) \tag{2.2}$$

where $\boldsymbol{e}(\boldsymbol{x}, t)$ is a field operator and $\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}, t)$ is the classical externally applied field.

The total hamiltonian is

$$H = \sum_{\boldsymbol{k}, \lambda} \hbar ck (a^\dagger_{\boldsymbol{k}, \lambda} a_{\boldsymbol{k}, \lambda} + \tfrac{1}{2}) + H_{\text{matter}} + \sum_{\boldsymbol{x}} H_{\text{int}}(\boldsymbol{x}, t). \tag{2.3}$$

The summation over $\boldsymbol{x}$ on $H_{\text{int}}(\boldsymbol{x}, t)$ is to be interpreted as an integration. The modes of the field are labelled by wavevector $\boldsymbol{k}$ and polarization index λ ($\lambda = 1$ or 2). The first term in the hamiltonian (2.3) is therefore the usual free-field hamiltonian. Since $\boldsymbol{E}$ is a classical field the hamiltonian associated with this is immaterial to the problem. The hamiltonian H_{matter} is the hamiltonian of the free matter. For the moment it is sufficient to know that H_{matter} has eigenstates which are product states of the eigenstates $|s_i\rangle$ of the hamiltonians for each one of the free atoms i.

The field operator $\boldsymbol{e}(\boldsymbol{x}, t)$ is a total field operator which at $\boldsymbol{x}_i$ implicitly includes the fields from all other atoms $j \neq i$. It is not necessarily simply the transverse part of the field. Power and Zienau (1959) show that in the dipole approximation, with $\boldsymbol{E}_{\text{ext}} \equiv \boldsymbol{0}$, $\boldsymbol{e}$ can be the transverse part of the field providing certain contact terms are included in the hamiltonian. We look carefully at these contact terms later in this series but ignore them here.

From the hamiltonian (2.3) it is possible to derive the classical integral equation

$$\boldsymbol{P}(\boldsymbol{x}, \omega) = \sum_i \delta(\boldsymbol{x}-\boldsymbol{x}_i)\boldsymbol{\alpha}_i(\omega) \cdot \left(\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}, \omega) + \int \mathbf{F}(\boldsymbol{x}, \boldsymbol{x}'; \omega) \cdot \boldsymbol{P}(\boldsymbol{x}', \omega)\, \mathrm{d}\boldsymbol{x}' \right). \tag{2.4}$$

The argument has been sketched (Bullough *et al* 1968, Obada and Bullough 1969) but has not yet been published at length. However it is sufficient for our purpose here to note the following: $\boldsymbol{P}(\boldsymbol{x}, \omega)$ is an expectation value which can now be interpreted as the classical dipole density; it has been Fourier transformed on the time t so that it is now a function of frequency ω. The tensor $\boldsymbol{\alpha}_i(\omega)$ is the Kramers–Heisenberg polarizability tensor for the ith atom:

$$\boldsymbol{\alpha}_i(\omega) = \frac{2e^2}{\hbar} \sum_{s_i \neq 0_i} \frac{\omega_{s_i} \langle 0_i|\boldsymbol{r}_i(0)|s_i\rangle \langle s_i|\boldsymbol{r}_i(0)|0_i\rangle}{\omega_{s_i}^2 - (\omega + \mathrm{i}\delta)^2} \tag{2.6}$$

in which the frequencies $\omega_{s_i} \equiv \hbar^{-1}(E_{s_i} - E_{0_i})$ and E_{s_i} and E_{0_i} are the excited and ground state energies of the free ith atom; δ is a positive infinitesimal.

The tensor $\mathbf{F}(\boldsymbol{x}, \boldsymbol{x}'; \omega)$ is the classical propagator for dipole fields:

$$\mathbf{F}(\boldsymbol{x}, \boldsymbol{x}'; \omega) \equiv (\nabla\nabla + k_0^2 \mathbf{U}) \exp(\mathrm{i}k_0|\boldsymbol{x}-\boldsymbol{x}'|)|\boldsymbol{x}-\boldsymbol{x}'|^{-1} \tag{2.7}$$

in which $k_0 \equiv \omega c^{-1}$ and $\mathbf{U}$ is the unit tensor. The result (2.4) is an approximate result in which an all-order perturbation theory is systematically decorrelated at each order. The propagator (2.7) is an exact consequence of this decorrelation procedure.

The procedure is to expand the density matrix as a series of nested commutators. The expanded density matrix is used to calculate the expectation value $\boldsymbol{P}(\boldsymbol{x}, t)$ of the dipole density operator $\boldsymbol{p}(\boldsymbol{x}, t)$. Because of the parity of the dipole operator the series is a series in e^2 although H_{int} is linear in e. The decorrelation replaces a term like

$$[[\boldsymbol{r}_i(t), \boldsymbol{r}_i(t') \cdot \boldsymbol{e}(\boldsymbol{x}_i, t')], \boldsymbol{r}_j(t'') \cdot \boldsymbol{e}(\boldsymbol{x}_j, t'')] \tag{2.8a}$$

by

$$\langle 0_i|[\boldsymbol{r}_i(t), \boldsymbol{r}_i(t')]|0_i\rangle \cdot [\boldsymbol{e}(\boldsymbol{x}_i, t'), \boldsymbol{e}(\boldsymbol{x}_j, t'')] \cdot \boldsymbol{r}_j(t'') \tag{2.8b}$$

a pattern which can be continued throughout the commutator nest. The state $|0_i\rangle$ is the ground state of atom i: in the interaction representation $[\boldsymbol{r}_i(t), \boldsymbol{r}_j(t')] = 0$ for $i \neq j$. It will be noted that since $\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}, t)$ commutes with all operators it will survive from the interaction (2.2) only in the last term of the commutator nest. The result is therefore linear in $\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}, t)$ but this is precisely the result we need for a linear response theory.

The propagator $\mathbf{F}$ emerges from (2.8*b*) because of the result of Jordan and Pauli (1928) that the unequal space–time commutator of two free-field operators is a c number. The theory sketched here is a causal theory and the Fourier transform of the causal part of this commutator is precisely $\mathbf{F}(\boldsymbol{x}, \boldsymbol{x}'; \omega)$:

$$\int_{-\infty}^{\infty} \frac{\mathrm{i}}{\hbar} [\boldsymbol{e}(\boldsymbol{x}, t), \boldsymbol{e}(\boldsymbol{x}', t')] \theta(t-t')\, \mathrm{e}^{\mathrm{i}\omega(t-t')}\, \mathrm{d}t' = \mathbf{F}(\boldsymbol{x}, \boldsymbol{x}'; \omega). \tag{2.9}$$

In this $\theta(t)$ is the step function. Note that the field operator $\boldsymbol{e}(\boldsymbol{x}, t)$ in (2.2) becomes a free-field operator in the interaction representation: it is the $\theta(t-t')$ which plays a vital role in picking up longitudinal contributions to the field (a point we must discuss in detail elsewhere). To ensure convergence at the lower limit $t' = -\infty$ we interpret ω as $\omega+\mathrm{i}\delta$ in (2.9).

The Fourier transform of the causal part of the decorrelated single-atom dipole–dipole commutator is the Kramers–Heisenberg polarizability for that atom:

$$\int_{-\infty}^{\infty} \frac{\mathrm{i}}{\hbar}\langle 0_i|[\boldsymbol{er}_i(t), \boldsymbol{er}_i(t')]|0_i\rangle\theta(t-t')\,\mathrm{e}^{\mathrm{i}\omega(t-t')}\,\mathrm{d}t' = \boldsymbol{\alpha}_i(\omega). \tag{2.10}$$

We shall suppose the states so chosen that $\boldsymbol{r}_{i0_s} \equiv \langle 0_i|\boldsymbol{r}_i|s_i\rangle$ is the same as $\boldsymbol{r}_{is0}$. Comparison of (2.10) with (2.9) suggests that the decorrelation procedure adopted is equivalent to assuming that the dipole operators $\boldsymbol{r}_i(t)$ are Bose-type operators. The Bose approximation is thought to be good for few photons amongst many atoms few of which are in an excited state (compare, eg, Hopfield 1958).

We see this approximation is a Bose approximation very precisely by restricting the discussion to a single spinless two-level atom with ground state $|0\rangle$ and excited state $|s\rangle$ chosen so that the matrix elements of the dipole operator are given by

$$\boldsymbol{er}_{0s} = \boldsymbol{er}_{s0} = ex_{0s}\hat{\boldsymbol{u}} \tag{2.11a}$$

where $\hat{\boldsymbol{u}}$ is a fixed unit vector. Then at time $t = 0$ we can put

$$\boldsymbol{er} = ex_{0s}\hat{\boldsymbol{u}}\sigma_x = ex_{0s}\hat{\boldsymbol{u}}(\sigma_+ + \sigma_-) \tag{2.11b}$$

where

$$\sigma_\pm = \tfrac{1}{2}(\sigma_x \pm \mathrm{i}\sigma_y) \tag{2.11c}$$

and σ_x, σ_y (and σ_z) are the Pauli spin matrices. The atomic hamiltonian H_{matter} is now given by

$$H_{\text{matter}} \equiv \tfrac{1}{2}\hbar\omega_s\sigma_z \equiv H_0. \tag{2.12}$$

In the interaction representation at time t we find

$$\sigma_x(t) = \exp(\mathrm{i}\hbar^{-1}H_0t)\sigma_x\exp(-\mathrm{i}\hbar^{-1}H_{0t}) = \exp(\mathrm{i}\omega_st)\sigma_+ + \exp(-\mathrm{i}\omega_st)\sigma_-, \tag{2.13}$$

and the commutator becomes

$$[\boldsymbol{er}(t), \boldsymbol{er}(t')] = -e^2x_{0s}^2\hat{\boldsymbol{u}}\hat{\boldsymbol{u}}2\mathrm{i}\sin\omega_s(t-t')[\sigma_-, \sigma_+]. \tag{2.14}$$

Thus the decorrelation procedure used by Bullough *et al* amounts to assuming a boson commutation relation for the operators $\sigma_\pm$,

$$[\sigma_-, \sigma_+] = 1. \tag{2.15}$$

In fact, of course, they obey fermion commutation relations†

$$\begin{aligned}[\sigma_-, \sigma_+] &= -\sigma_z \\ [\sigma_-, \sigma_+]_+ &= 1.\end{aligned} \tag{2.16}$$

† A single two-level atom evolves in a Hilbert space spanned by the states $|s\rangle$ and $|0\rangle$. Any linear operator on this space has a 2×2 matrix representation. A complete basis set of operators can be chosen to satisfy an SU_2 Lie algebra. Hence (2.15).

The classical integral equation (2.4) with the Kramers–Heisenberg polarizability now given by

$$\boldsymbol{\alpha}(\omega) = \frac{2e^2\omega_s x_{0s}^2 \hat{\boldsymbol{u}}\hat{\boldsymbol{u}}}{\hbar[\omega_s^2 - (\omega + \mathrm{i}\delta)^2]} \tag{2.17}$$

follows from (2.15) and not (2.16). In future we call this approximate theory the pseudo-boson theory.

For a single particle at $\boldsymbol{x}_i$ (2.4) in the pseudo-boson theory reduces to

$$\boldsymbol{P}_i(\omega)\delta(\boldsymbol{x}-\boldsymbol{x}_i) = \alpha(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}} \cdot \delta(\boldsymbol{x}-\boldsymbol{x}_i)(\boldsymbol{E}_{\mathrm{ext}}(\boldsymbol{x}, \omega) + \mathbf{J}_0(\omega) \cdot \boldsymbol{P}_i(\omega)) \tag{2.18}$$

where we have put

$$\boldsymbol{P}(\boldsymbol{x}, \omega) = \boldsymbol{P}_i(\omega)\delta(\boldsymbol{x}-\boldsymbol{x}_i)$$

$$\boldsymbol{\alpha}(\omega) = \alpha(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}}$$

and

$$\mathbf{J}_0(\omega) \equiv \int \mathbf{F}(\boldsymbol{x}, \boldsymbol{x}'; \omega)\delta(\boldsymbol{x}-\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}' = J_0(\omega)\,\mathbf{U}.$$

Thus

$$\boldsymbol{P}_i(\omega) = \gamma(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}} \cdot \boldsymbol{E}_{\mathrm{ext}}(\boldsymbol{x}_i, \omega) \tag{2.19}$$

where

$$\gamma(\omega) = \frac{\alpha(\omega)}{1 - \alpha(\omega)J_0(\omega)}. \tag{2.20}$$

This solution is purely formal, however, as $J_0(\omega)$ is divergent

$$\begin{aligned}\mathbf{J}_0(\omega) &= \int \mathbf{F}(\boldsymbol{x}, \boldsymbol{x}'; \omega)\delta(\boldsymbol{x}-\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}' \\ &= \int (\nabla\nabla + k_0^2\,\mathbf{U})\exp(\mathrm{i}k_0|\boldsymbol{x}-\boldsymbol{x}'|)|\boldsymbol{x}-\boldsymbol{x}'|^{-1} \\ &\quad \times \frac{1}{(2\pi)^3}\int \exp(-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}'))\,\mathrm{d}\boldsymbol{k}\,\mathrm{d}\boldsymbol{x}' \\ &= \left(-\frac{2}{3\pi}\int_0^\infty k^2\,\mathrm{d}k + \frac{4}{3\pi}k_0^2\int_0^\infty \mathrm{d}k + \tfrac{2}{3}\mathrm{i}k_0^3\right)\mathbf{U}. \end{aligned} \tag{2.21}$$

We shall use the symbol

$$K_0 \equiv \frac{2c}{\pi\omega_s}\int_0^\infty \mathrm{d}k$$

in the later papers although we may restrict the upper limit to $k_{\max} = c^{-1}\omega_{\max} < \infty$. The cubic divergence in (2.21) is connected with the contact terms omitted from the hamiltonian (2.3) and we shall not analyse this term here: with this term ignored

$$J_0(\omega) = \tfrac{2}{3}(k_s k_0^2 K_0 + \mathrm{i}k_0^3) \tag{2.22}$$

and

$$\gamma(\omega) = \frac{2e^2\hbar^{-1}x_{0s}^2\omega_s}{\omega_s^2-\omega^2-\frac{4}{3}e^2x_{0s}^2\hbar^{-1}(k_sk_0^2K_0+ik_0^3)} \tag{2.23a}$$

$$\simeq \frac{e^2\hbar^{-1}x_{0s}^2}{\omega_s-\omega-\frac{2}{3}e^2x_{0s}^2\hbar^{-1}(k_s^3K_0+ik_s^3)} \tag{2.23b}$$

near resonance. The width of this resonance is

$$\Gamma_0 = \frac{4}{3}\frac{e^2x_{0s}^2\omega_s^3}{\hbar c^3} \tag{2.24}$$

which is both the Einstein A coefficient and the Weisskopf and Wigner (1930) spontaneous emission width. There is no stimulated emission in this theory. The Lamb shift in Bethe's form is also excluded and must be identified instead with the apparent shift of ω_s

$$-\tfrac{2}{3}e^2x_{0s}^2\hbar^{-1}k_s^3K_0. \tag{2.25}$$

This is the long-time limit of the dynamical shift obtained by Stroud and Jaynes (1970).

The divergence of K_0 is caused by the dipole approximation. If we use a modified version of the dipole approximation given by the substitution

$$e\boldsymbol{r}_i(t)\delta(\boldsymbol{x}-\boldsymbol{x}_i) \rightarrow \frac{\mathrm{e}}{(2\pi)^3}\int \exp -\mathrm{i}\boldsymbol{k}.(\boldsymbol{x}-\boldsymbol{x}_i)(\boldsymbol{r}_i(t)\exp \mathrm{i}\boldsymbol{k}.\boldsymbol{r}_i(t))\,\mathrm{d}\boldsymbol{k} \tag{2.26}$$

(this has the effect of moving the site of the dipole from that of the centre of the atom to that of the electron in the atom which is responsible for the dipole) then the theory coincides with the long-time limit of the neo-classical Lamb shift theory of Crisp and Jaynes (1969).

It is helpful to interpret the linear response relation (2.19)

$$\boldsymbol{P}_i(\omega) = \gamma(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}}.\boldsymbol{E}_{\mathrm{ext}}(\boldsymbol{x}_i,\omega)$$

with $\gamma(\omega)$ given by (2.23a) in the time domain. For simplicity we suppose $\boldsymbol{E}_{\mathrm{ext}}(\boldsymbol{x}_i,\omega)$ is parallel to $\hat{\boldsymbol{u}}$. Then

$$[\omega_s^2-\omega^2-\tfrac{4}{3}e^2x_{0s}^2\omega_s\hbar^{-1}(k_sk_0^2K_0+ik_0^3)]P(\omega) = 2e^2\hbar^{-1}x_{0s}^2\omega_sE_{\mathrm{ext}}(\boldsymbol{x}_i,\omega) \tag{2.27}$$

and by Fourier inversion on ω and writing $E(t)$ for $E_{\mathrm{ext}}(\boldsymbol{x}_i,t)$ we get

$$\ddot{P}(t)+\omega_s^2P(t)-\Gamma_0\omega_s^{-2}(\dddot{P}(t)-K_0\omega_s\ddot{P}(t)) = 2e^2\hbar^{-1}x_{0s}^2\omega_sE(t). \tag{2.28}$$

This form emphasizes the connection of the pseudo-boson theory with Jaynes' work. We shall see later in this series that (2.28) is equivalent to assuming the Bose commutation relations (2.15) for the atom and using an operator reaction field

$$\frac{2}{3}\frac{\hat{\boldsymbol{u}}}{c^3}\dddot{p}(t)-\frac{2}{3}\frac{K_0}{c^3}\omega_s\hat{\boldsymbol{u}}\ddot{p}(t). \tag{2.29}$$

This form of field really follows directly from the form of (2.21).

3. A different decorrelation procedure

The lack of stimulated emission in the pseudo-boson theory is due to the decorrelation approximation used. This ensures that the field operators appear only in the form of c

number commutators which do not depend on the field states. In order to overcome this difficulty we shall change the decorrelation procedure so as to retain the fermion character of the commutation relations for the matter operators, (2.13). Unfortunately the calculation becomes intractable with no decorrelation so we decorrelate the *field* operators by replacing the *anti*-commutator of two such operators by its expectation value:

$$[\boldsymbol{e}(\boldsymbol{x}, t), \boldsymbol{e}(\boldsymbol{x}', t')]_+ \rightarrow \langle \mathrm{ph}|\,[\boldsymbol{e}(\boldsymbol{x}, t), \boldsymbol{e}(\boldsymbol{x}', t')]_+|\mathrm{ph}\rangle \tag{3.1a}$$

in which $|\mathrm{ph}\rangle$ is the initial state of the field (at $t = -\infty$). More precisely we replace

$$[\boldsymbol{e}(\boldsymbol{x}, t)+\boldsymbol{E}_{\mathrm{ext}}(\boldsymbol{x}, t), \boldsymbol{e}(\boldsymbol{x}', t')+\boldsymbol{E}_{\mathrm{ext}}(\boldsymbol{x}', t')]_+ \tag{3.1b}$$

at each stage where it may be identified, by the right-hand side of (3.1*a*): once we agree to replace products of two fields by their expectation value this amounts to retaining only the linear terms in $\boldsymbol{E}(\boldsymbol{x}, t)$ which is all we need for any linear response theory. We shall see that the anti-commutator (3.1*b*) comes up in a natural way in the theory once we use the fermion commutation relations (2.13) for the atom.

We use the same perturbation expansion as before, namely

$$\begin{aligned}\langle \boldsymbol{p}(\boldsymbol{x}, t)\rangle = {} & \mathrm{Tr}\{\rho \boldsymbol{p}(\boldsymbol{x}, t)\}+\frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t} \mathrm{d}t_1 \int \mathrm{d}\boldsymbol{x}_1\, \mathrm{Tr}\{\rho[\boldsymbol{p}(\boldsymbol{x}, t), H_{\mathrm{int}}(\boldsymbol{x}_1, t_1)]\} \\ & +\left(\frac{1}{\mathrm{i}\hbar}\right)^2 \int_{-\infty}^{t} \mathrm{d}t_1 \int \mathrm{d}\boldsymbol{x}_1 \int_{-\infty}^{t} \mathrm{d}t_2 \int \mathrm{d}\boldsymbol{x}_2\, \mathrm{Tr}\{\rho[[\boldsymbol{p}(\boldsymbol{x}, t), H_{\mathrm{int}}(\boldsymbol{x}_1, t_1)], H_{\mathrm{int}}(\boldsymbol{x}_2, t_2)]\} \\ & + \ldots \end{aligned} \tag{3.2}$$

where ρ is the density operator of the system in the infinite past before the interaction is adiabatically 'switched on'. This initial density operator is a product of the initial density operator ρ_0 for the matter and the field density operator $|\mathrm{ph}\rangle\langle \mathrm{ph}|$.

We put $e(t) \equiv \hat{\boldsymbol{u}} \cdot (\boldsymbol{e}(\boldsymbol{x}_i, t)+\boldsymbol{E}_{\mathrm{ext}}(\boldsymbol{x}_i, t))$. The skeletons of the first few commutator nests in (3.2) are then

$$[\sigma_x(t), \sigma_x(t_1)e(t_1)] = 2\mathrm{i} \sin \omega_s(t-t_1)\sigma_z e(t_1) \tag{3.3}$$

$$\begin{aligned}&[[\sigma_x(t), \sigma_x(t_1)e(t_1)], \sigma_x(t_2)e(t_2)] \\ &\quad = 2\mathrm{i} \sin \omega_s(t-t_1)[\sigma_z e(t_1), \sigma_x(t_2)e(t_2)] \\ &\quad = 2\mathrm{i} \sin \omega_s(t-t_1)\{\sigma_z\sigma_x(t_2)[e(t_1), e(t_2)]_+ - [\sigma_z, \sigma_x(t_2)]_+ e(t_2)e(t_1)\} \\ &\quad \rightarrow 2\mathrm{i} \sin \omega_s(t-t_1)\langle \mathrm{ph}|\,[e(t_1), e(t_2)]_+|\mathrm{ph}\rangle \sigma_z\sigma_x(t_2)\end{aligned} \tag{3.4}$$

$$\begin{aligned}&[[[\sigma_x(t), \sigma_x(t_1)e(t_1)], \sigma_x(t_2)e(t_2)], \sigma_x(t_3)e(t_3)] \\ &\quad \rightarrow 2\mathrm{i} \sin \omega_s(t-t_1)\langle \mathrm{ph}|\,[e(t_1), e(t_2)]_+|\mathrm{ph}\rangle\,[\sigma_z\sigma_x(t_2), \sigma_x(t_3)]e(t_3) \\ &\quad = 2\mathrm{i} \sin \omega_s(t-t_1)\langle \mathrm{ph}|\,[e(t_1), e(t_2)]_+|\mathrm{ph}\rangle 2 \cos \omega_s(t_2-t_3) \times \sigma_z e(t_3).\end{aligned} \tag{3.5}$$

Before the step to (3.4) we use the fact that $\sigma_z(0) = \sigma_z(t_2)$ in interaction representation and that $[\sigma_z, \sigma_x]_+ = 0$. Before the final step to (3.5) we use

$$[\sigma_z\sigma_x(t_2), \sigma_x(t_3)] \equiv \sigma_z\sigma_x(t_2)\sigma_x(t_3)-\sigma_x(t_3)\sigma_z\sigma_x(t_2) = \sigma_z[\sigma_x(t_2), \sigma_x(t_3)]_+ .$$

From (3.3) and (3.5) we now see that the pattern is established. By substituting these results in the perturbation expansion, retaining only linear terms in $\boldsymbol{E}_{\mathrm{ext}}$ and Fourier

transforming with respect to time to eliminate the convolution integrals we reach the result

$$\boldsymbol{P}_i(\omega) = -(\rho_{ss}-\rho_{00})\alpha(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}}\cdot(\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}_i,\omega)+J_0^+(\omega)\alpha^+(\omega)\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}_i,\omega) + J_0^+(\omega)\alpha^+(\omega)J_0^+(\omega)\alpha^+(\omega)\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}_i,\omega)+\ldots). \tag{3.6}$$

This is equivalent to

$$\boldsymbol{P}_i(\omega) = \gamma^+(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}}\cdot\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}_i,\omega) \tag{3.7}$$

where

$$\gamma^+(\omega) = \frac{-(\rho_{ss}-\rho_{00})\alpha(\omega)}{1-J_0^+(\omega)\alpha^+(\omega)}. \tag{3.8}$$

We have taken the atomic density matrix ρ_0 to be diagonal

$$\rho_0 = \begin{pmatrix}\rho_{ss} & 0\\ 0 & \rho_{00}\end{pmatrix}; \tag{3.9}$$

$\alpha^+(\omega)$ corresponds to $\alpha(\omega)$ with the expectation value of the commutator now replaced by the anti-commutator which is already a c number:

$$\alpha^+(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}} = \int_{-\infty}^{\infty}\frac{\mathrm{i}}{\hbar}[e\boldsymbol{r}_i(t), e\boldsymbol{r}_i(t')]_+\theta(t-t')\,\mathrm{e}^{\mathrm{i}\omega(t-t')}\,\mathrm{d}t' = \frac{1}{\hbar}e^2x_{0s}^2\frac{2\omega}{\omega_s^2-(\omega+\mathrm{i}\delta)^2}\hat{\boldsymbol{u}}\hat{\boldsymbol{u}}. \tag{3.10}$$

This c number appears at the final step to (3.5) as noted. Notice the ω in the numerator instead of the ω_s in the expectation value of the commutator (2.17).

Similarly $J_0^+(\omega)$ corresponds to $J_0(\omega)$ but is now an expectation value:

$$\mathbf{J}_0^+(\omega) = \int \mathbf{F}^+(\boldsymbol{x},\boldsymbol{x}';\omega)\delta(\boldsymbol{x}-\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}' \tag{3.11}$$

$$\mathbf{F}^+(\boldsymbol{x},\boldsymbol{x}';\omega) = \int_{-\infty}^{\infty}\frac{\mathrm{i}}{\hbar}\langle\mathrm{ph}|[\boldsymbol{e}(\boldsymbol{x},t),\boldsymbol{e}(\boldsymbol{x}',t')]_+|\mathrm{ph}\rangle\theta(t-t')\,\mathrm{e}^{\mathrm{i}\omega(t-t')}\,\mathrm{d}t' = \int\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3}\sum_\lambda\hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda}\hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda}(2n_{\boldsymbol{k}}^{(\lambda)}+1)\left(\frac{k}{k-k_0}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')}-\frac{k}{k+k_0}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')}\right) \tag{3.12}$$

where $n_{\boldsymbol{k}}^{(\lambda)}$ is the occupation number for photons of wavevector $\boldsymbol{k}$ and polarization $\hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda}$ ($\lambda = 1$ or 2).

In general unlike $\mathbf{J}_0(\omega)$, $\mathbf{J}_0^+(\omega)$ is not isotropic, ie $\mathbf{J}_0^+(\omega)\neq J_0^+(\omega)\mathbf{U}$. We have, however, defined the scalar

$$J_0^+(\omega) = \hat{\boldsymbol{u}}\cdot\mathbf{J}_0^+(\omega)\cdot\hat{\boldsymbol{u}}. \tag{3.13}$$

We cannot easily express (3.7) with $\gamma^+(\omega)$ given by (3.8) and $J_0^+(\omega)$ given by (3.13) with (3.11) and (3.12) as an equation of motion because $J_0^+(\omega)$ depends on ω in a slightly complicated way. It simplifies considerably in typical cases and it is particularly simple in the case of an isotropic unpolarized field.

4. Equations of motion in an isotropic unpolarized field

If the field is unpolarized $n_{\boldsymbol{k}}^{(1)} = n_{\boldsymbol{k}}^{(2)}$. In our brief report (Bullough and Caudrey 1971) we chose $n_{\boldsymbol{k}}^{(1)} = n_{\boldsymbol{k}}^{(2)} = \frac{1}{2}n_{\boldsymbol{k}}$ and for the isotropic field then chose $n_{\boldsymbol{k}} = n_k$ for all $\boldsymbol{k}$. The factor of one half does not follow conventional usage and we shall not make this choice here. We choose instead $n_{\boldsymbol{k}}^{(1)} = n_{\boldsymbol{k}}^{(2)} = n_k$ for all $\boldsymbol{k}$. Then

$$\mathbf{F}^{+}(\boldsymbol{x}, \boldsymbol{x}'; \omega) = \frac{1}{\pi}\int_0^\infty \frac{2k_0}{k^2 - k_0^2}\,\mathrm{d}k\,(\nabla\nabla + k^2\,\mathbf{U})(2n_k + 1)\left(\frac{\sin k|\boldsymbol{x}-\boldsymbol{x}'|}{|\boldsymbol{x}-\boldsymbol{x}'|}\right). \tag{4.1}$$

In this isotropic field case $\mathbf{J}_0^{+}(\omega)$ is also isotropic and

$$J_0^{+}(\omega) = \frac{4}{3\pi}k_0\int_0^\infty (2n_k + 1)\frac{k^3\,\mathrm{d}k}{k^2 - k_0^2}. \tag{4.2}$$

The imaginary part depends on $n_{|k_0|}$:

$$\operatorname{Im} J_0^{+}(\omega) = \tfrac{2}{3}k_0^3(2n_{|k_0|} + 1)\operatorname{sgn} k_0 \tag{4.3}$$

in which $\operatorname{sgn} k_0$ is the sign of $k_0 \equiv \omega c^{-1}$. The real part, however, depends on all the field modes. If we choose the admittedly rather artificial distribution

$$\begin{aligned} n_k = n &= \text{constant} && \text{for } a < k < b\ (a < |k_0| < b) \\ &= 0 && \text{otherwise} \end{aligned}$$

then we get

$$\operatorname{Re} J_0^{+}(\omega) = \frac{4}{3\pi}k_0^3\ln\left(\frac{m_e c}{\hbar|k_0|}\right) + \frac{4}{3\pi}k_0\int_0^{kc} k\,\mathrm{d}k + \frac{4}{3\pi}k_0 n\left[k_0^2\ln\left(\frac{b^2 - k_0^2}{k_0^2 - a^2}\right) + b^2 - a^2\right] \tag{4.4}$$

in which the first logarithmic term has been cut off at the reciprocal Compton wavelength $k_C = m_e c\hbar^{-1}$. The second term which would otherwise be quadratically divergent is also cut off there. It has to be interpreted as a mass renormalization in two-level atom theory.

We now have

$$\gamma^{+}(\omega) = \frac{-(\rho_{ss} - \rho_{00})2\hbar^{-1}e^2x_{0s}^2\omega_s}{\omega_s^2 - \omega^2 - 2\hbar^{-1}e^2x_{0s}^2\omega J_0^{+}(\omega)} \simeq \frac{-(\rho_{ss} - \rho_{00})\hbar^{-1}e^2x_{0s}^2}{\omega_s - \omega - \hbar^{-1}e^2x_{0s}^2 J_0^{+}(\omega_s)} \tag{4.5}$$

near the physical resonance supposed close to $\omega = +\omega_s$. There is a resonance width which appears to be

$$\Gamma = 2\hbar^{-1}e^2x_{0s}^2\operatorname{Im} J_0^{+}(\omega_s) = (2n_{k_s} + 1)\Gamma_0. \tag{4.6}$$

This is not just the usual width Γ_0 corrected for stimulated *emission* and we were mistaken in saying this in our brief report (see Bullough and Caudrey 1971 below equation (13) noting that with the convention of $\frac{1}{2}n$ instead of n (4.6) is just $(n_{k_s} + 1)\Gamma_0$). The width (4.6) includes the effect of stimulated absorption as well as emission. This must be so since $\gamma^{+}(\omega)$ is a dynamical result which leads to an equation of motion as did $\gamma(\omega)$ in § 2.

The shift in resonance frequency is given by

$$\Delta\omega_s = -\hbar^{-1}e^2x_{0s}^2 \operatorname{Re} J_0^+(\omega_s)$$
$$= -\frac{4}{3\pi}\hbar^{-1}e^2x_{0s}^2k_s^3 \ln\left(\frac{m_ec}{\hbar k_s}\right) - \frac{4}{3\pi}\hbar^{-1}e^2x_{0s}^2k_s\int_0^{k_C} k\,\mathrm{d}k$$
$$-\frac{4}{3\pi}\hbar^{-1}e^2x_{0s}^2\left[k_s^3n\ln\left(\frac{b^2-k_s^2}{k_s^2-a^2}\right)+k_sn(b^2-a^2)\right]. \tag{4.7}$$

The first logarithmic term is precisely twice the non-relativistic Bethe (1947) formula for the Lamb shift. This is to be expected since both energy levels move towards one another by the amount given by the Bethe single-level shift. We use the symbol Δ for this first term.

The second term would diverge quadratically without cut-off: it can be identified as precisely twice the static electromagnetic mass renormalization term which appears in second-order perturbation theory for the level shifts (Feynman and Hibbs 1965, Bullough 1969). It is worth noting that in level-shift perturbation theory for the many-level atom we obtain for each level

$$\frac{1}{3\pi\hbar^2}\frac{e^2}{c}\sum_{s\neq t}2(E_s-E_t)x_{ts}^2\int_0^{k_C}k\,dk = \frac{e^2}{3\pi\hbar m_ec}\int_0^{k_C}k\,\mathrm{d}k \tag{4.8}$$

after using the Thomas–Reiche–Kuhn sum rule for oscillator strengths. Each level is therefore shifted by the same amount and the spacing between any two levels is unaffected. On the other hand in the two-level atom the ground state contributes a single term proportional to $2\hbar^{-1}(E_s-E_0)x_{0s}^2 = 2\omega_sx_{0s}^2$ and the excited state contributes one proportional to $2\hbar^{-1}(E_0-E_s)x_{0s}^2$ so that the two terms simply add.

It might appear from this that to the approximation which is (4.7) certainly an e^2 approximation the renormalization problem is solved. Unfortunately whilst the second term in (4.7) is a particular and apparently spurious feature of the two-level atom model so is the elimination of the linearly divergent term which appeared previously in (2.24). Although this term is the source of the Stroud and Jaynes (1970) shift it appears in Bethe's (1947) theory as the kinetic mass renormalization term (Feynman and Hibbs 1965). In the many-level atom the analogue of (4.8) is the level dependent result

$$\frac{e^2}{3\pi\hbar^3c^2}\left(\sum_{s\neq t}2(E_s-E_t)^2x_{ts}^2\right)\int_0^{k_C}\mathrm{d}k = \frac{4}{3\pi}\frac{e^2}{\hbar c^2}\frac{\langle t|p^2|t\rangle}{2m_e^2}\int_0^{k_C}\mathrm{d}k \tag{4.9}$$

in which p is the momentum operator. In general the spacing between two levels depends on the two levels. However, in two-level atom theory two terms $2\hbar^{-2}(E_s-E_t)^2x_{0s}^2$ will cancel. This is one explanation why no term in $K_0 = (2\pi)^{-1}k_s\int_0^{k_C}\mathrm{d}k$ appears in (4.7) and it reinforces the view that (4.7) is an e^2 result equivalent to second-order perturbation theory.

The other logarithmic term is a generalization of the Lamb shift to include the effect of occupied field modes: it has been called the 'lamp' shift! It obviously vanishes for a symmetric distribution of field modes so that

$$b^2-k_s^2 = k_s^2-a^2.$$

We use the symbol Δ_1 for this term.

The remaining term proportional to $n(b^2-a^2)$ does not vanish even in this particular case. It obviously generalizes the term in $\int_0^{k_C} k\,\mathrm{d}k$ for the vacuum. It will vanish for the many-level atom in second-order perturbation theory as pointed out by Knight (1972) again because of the result (4.8). The situation surrounding any field-dependent kinetic mass renormalization term proportional to (4.9) is different: in perturbation theory *two* stimulated terms mutually cancel as Knight (1972) and Saunders and Bullough (1973) show†.

In our brief report (Bullough and Caudrey 1971) of this all-order perturbation theory for the two-level atom we suggested that the term in (4.7) proportional to $n(b^2-a^2)$ should be observable in sufficiently intense isotropic fields: but the argument from (4.5) to (4.7) shows that despite the all-order calculation the result (4.7) is actually an e^2 result. To this order our suggestion is therefore mistaken for the reason pointed out by Knight. We were concerned at that time to report consequences of the two-level atom theory. However we now know that identical results for the two-level atom can be obtained by reaction field theory and that an extension to the many-level atom can be made which reproduces all the results of second-order perturbation theory. The problem of extending the theory beyond order e^2 has not been solved.

A conceptual difficulty remains even at order e^2: if the term in $\int_0^{k_C} k\,\mathrm{d}k$ in (4.7) is interpreted as a mass renormalization level by level then this becomes field dependent as $\int_0^{k_C}(2n_k+1)k\,\mathrm{d}k$ in an isotropic field. The situation is different in relativistic theory where quadratically divergent terms cancel. We have not explored the present problem in this context.

We now return to (3.7) and calculate the main result of this paper. This result is the equation of motion analogous to (2.27) but now based on $\gamma^+(\omega)$ instead of $\gamma(\omega)$.

We observe that because of the sgn k_0 in (4.3) we have as in (4.5)

$$\gamma^+(\omega) \simeq \frac{-(\rho_{ss}-\rho_{00})\hbar^{-1}e^2x_{0s}^2}{\omega_s-\omega-\hbar^{-1}e^2x_{0s}^2J_0^+(\omega_s)} \tag{4.10a}$$

for $\omega > 0$. But for $\omega < 0$

$$\gamma^+(\omega) \simeq \frac{-(\rho_{ss}-\rho_{00})\hbar^{-1}e^2x_{0s}^2}{\omega_s+\omega-\hbar^{-1}e^2x_{0s}^2\{J_0^+(\omega_s)\}^*}. \tag{4.10b}$$

We can now see the essential mathematical role played by the factor ω rather than ω_s in the numerator of (3.10): it preserves the sign of the energy shift as well as the causal property—both poles are in the lower half plane.

To the same approximation as (4.10) we have for all ω that

$$\gamma^+(\omega) = -\frac{(\rho_{ss}-\rho_{00})\hbar^{-1}e^2x_{0s}^2}{\omega_s^2-\omega^2-2\omega_s\hbar^{-1}e^2x_{0s}^2\,\mathrm{Re}(J_0^+(\omega_s))-2i\omega\hbar^{-1}e^2x_{0s}^2\,\mathrm{Im}(J_0^+(\omega_s))} \tag{4.11}$$

† Stenholm (1972, pp 1–122, § 2.2) reviews the 'light shifts' obtained in e^2 order perturbation theory first discussed by Barrat and Cohen-Tannoudji (1961, see also Series 1970). These shifts appear to us incorrect in at least two points: first, the calculation omits all negative-frequency contributions which means that the magnitude of the shifts can only be one half of our shifts based on (4.4); second there is no distinction between the physical and non-physical parts of the shifts so that, and because of the omission of the negative frequency contributions, there is a field dependent kinetic mass apparently contributing to the shift. Further, the calculation does not make clear that the width takes the form (4.6) since for the *single* level considered it approximates to $(n_{k_s}+1)\Gamma_0$. We shall show in a later paper that it is the width (4.6) which appears in the spectrum although we find in this case that n_{k_s} must be evaluated at the vacuum shifted wavenumber $k_s' \equiv k_s - c^{-1}\Delta$.

so that

$$\ddot{P}(t)+\omega_s^2 P(t)+(2n+1)\Gamma_0\dot{P}(t)-2\omega_s\left(\Delta+\Delta_1+\Delta_2+\frac{4}{3\pi}\hbar^{-1}e^2x_{0s}^2k_s\int_0^{k_C}k\,\mathrm{d}k\right)P(t)$$
$$=-2\omega_s(\rho_{ss}-\rho_{00})\hbar^{-1}e^2x_{0s}^2E(t). \tag{4.12a}$$

It can be seen also that because (4.3) has the factor k_0^3 rather than k_s^3 we could replace the damping term by $-(2n+1)\Gamma_0\omega_s^{-2}\ddot{P}(t)$. This is equivalent to arguing from (4.12*a*) that $\ddot{P}(t)\simeq-\omega_s^2P(t)$ which will be true to $O(\Gamma_0\omega_s^{-1})$ if the field occupation number n is small enough since $E(t)$ is vanishingly weak. In fact because $n_{|k_0|}$ appears in (4.3) and the ω in the numerator of (3.10) introduces a factor ω^4 into the damping term the time Fourier transform of this term is still more complicated.

The same sort of thing is true of the shift, for in (4.12*a*) the terms Δ, Δ_1, and Δ_2 are respectively the first, third and fourth terms in (4.7). The forms of $J^+(\omega)$ and $\alpha^+(\omega)$ show that the form of (4.13*a*) based on the precise result (3.8) for $\gamma^+(\omega)$ is considerably more complicated. In a recent report (Bullough *et al* 1973) we quoted the results as

$$\ddot{P}(t)+\omega_s^2P(t)-(2n+1)\omega_s^{-2}\Gamma_0\ddot{\dot{P}}(t)-2\omega_s\left(\Delta+\Delta_1+\Delta_2+\frac{\Gamma_0}{2\pi}\omega_s^{-2}\omega_c^2\right)P(t)$$
$$=-2\omega_s(\rho_{ss}-\rho_{00})\hbar^{-1}e^2x_{0s}^2E(t) \tag{4.12b}$$

although a different notation was used there: we chose this form as typifying the situation although the fundamental status of the $\ddot{P}(t)$ rather than the $\dot{P}(t)$ raises an interesting question not yet solved. In (2.28) in contrast $\ddot{\dot{P}}(t)$ appears directly.

In weak enough fields described by small enough n and vanishing $E(t)$ the solution of (4.12*b*) which has a vanishing derivative as $t=0$ is approximately

$$P(t)=P(0)\exp[-\tfrac{1}{2}(2n+1)\Gamma_0t]\cos\Omega t \tag{4.13a}$$

in which

$$\Omega=\omega_s-\left(\Delta+\Delta_1+\Delta_2+\frac{1}{2\pi}\Gamma_0\omega_s^{-2}\omega_C^2\right) \tag{4.13b}$$

($\omega_C\equiv ck_C\equiv m_ec^2\hbar^{-1}$). This solution is a slowly-varying amplitude and phase solution of the type we make much use of later: it is applicable to order $\Gamma_0\omega_s^{-1}$ and hence to order e^2 if but only if n is small enough. Note again that although the isotropic field with the single parameter n is very artificial it is clear how to perform the more intricate but conceptually no different calculations for physically more realistic fields.

The reaction field analogous to (2.29) must now break into two parts for positive and negative frequencies ω respectively. We interpret the ω in the numerator of (3.10) to act as though it has the magnitude $\omega_s\,(>0)$ but preserves the sign of ω. In this case we see by inspection of (4.3) and (4.6) that one guess at the reaction fields to replace (2.29) is the positive and negative frequency part fields

$$e^{(\pm)}(t)=\frac{1}{3c^3}\left(\pm\frac{1}{\pi}\mathrm{i}\omega_C^2\dot{p}(t)\mp\mathrm{i}K_1\ddot{p}(t)\right)+\frac{2}{3c^3}\ddot{p}^{(\pm)}(t) \tag{4.14a}$$

where

$$K_1\equiv\frac{2}{\pi}\ln\left(\frac{\omega_C}{\omega_s}\right). \tag{4.14b}$$

We show in a later paper to what extent this guess is confirmed by reaction field theory itself. The guess is imperfect because the total reaction field $e(t) \equiv e^{(+)}(t)+e^{(-)}(t)$ and proves still to be given by (2.29); but the significant parts of the fields are correctly described by (4.14).

The general result of § 3 raises a number of other questions. One is the relation of results like (4.12) for incoherent Fock state fields to the rather different results which have been obtained (eg by Lamb 1965) for single atoms coupled to strongly *classical* fields. This question is best answered by the reaction field theory and will be treated in a paper (Hassan and Bullough 1974) where the effect of the free field in reaction field theory is analysed in depth.

5. Many atoms

Now let us return to our system of N atoms situated at the points $\boldsymbol{x}_i$ $(i = 1, 2, \ldots, N)$. It becomes necessary to follow a hybrid decorrelation procedure in this case. This is because while we use the fermion commutation relations for two matter operators acting on the same atom, two matter operators acting on different atoms commute with one another as boson operators:

$$[er_i(t), er_j(t')] = 0, \qquad i \neq j. \tag{5.1}$$

We still decorrelate the field operators as before by replacing an anti-commutator by its expectation value. However, it also becomes necessary to decorrelate the matter operators. One way of doing this is as follows. As the commutator nests are being built up, at some stages there will appear terms containing the operator $\sigma_z^{(i)}$. (The operators $\sigma_x^{(i)}$, $\sigma_y^{(i)}$, and $\sigma_z^{(i)}$ are the Pauli spin matrices as before but they act on the state vectors of the ith atom only.) If this term contains no other matter operators acting on the ith atom and no field operators referring to the site $\boldsymbol{x}_i$ then $\sigma_z^{(i)}$ is replaced by its expectation value $(\rho_{ss}-\rho_{00})$ (assumed to be the same for all atoms).

Using the notation $e_i(t) = \hat{\boldsymbol{u}} \cdot \boldsymbol{e}(\boldsymbol{x}_i, t)$ for the field operators, (3.3)–(3.5) are replaced by

$$\sum_j [\sigma_x^{(i)}(t), \sigma_x^{(j)}(t_1)e_j(t_1)] = 2\mathrm{i} \sin \omega_s(t-t_1)\sigma_z^{(i)}e_i(t_1) \tag{5.2}$$

$$\begin{aligned}\sum_{j,k} [[\sigma_x^{(i)}(t), \sigma_x^{(j)}(t_1)e_j(t_1)], \sigma_x^{(k)}(t_2)e_k(t_2)] \\ \rightarrow 2\mathrm{i} \sin \omega_s(t-t_1)\{\langle \mathrm{ph}|[e_i(t_1), e_i(t_2)]_+|\mathrm{ph}\rangle \sigma_z^{(i)}\sigma_x^{(i)}(t_2) \\ + \sum_{k\neq i} [e_i(t_1), e_k(t_2)]\sigma_z^{(i)}\sigma_x^{(k)}(t_2)\} \\ \rightarrow 2\mathrm{i} \sin \omega_s(t-t_1)\{\langle \mathrm{ph}|[e_i(t_1), e_i(t_2)]_+|\mathrm{ph}\rangle \sigma_z^{(i)}\sigma_x^{(i)}(t_2) \\ + \sum_{k\neq i} [e_i(t_1), e_k(t_2)](\rho_{ss}-\rho_{00})\sigma_x^{(k)}(t_2)\}\end{aligned} \tag{5.3}$$

$$\begin{aligned}\sum_{j,k,l} [[[\sigma_x^{(i)}(t), \sigma_x^{(j)}(t_1)e_j(t_1)], \sigma_x^{(k)}(t_2)e_k(t_2)], \sigma_x^{(l)}(t_3)e_l(t_3)] \\ \rightarrow 2\mathrm{i} \sin \omega_s(t-t_1)\{\langle \mathrm{ph}|[e_i(t_1), e_i(t_2)]_+|\mathrm{ph}\rangle 2 \cos \omega_s(t_2-t_3)\sigma_z^{(i)}e_i(t_3) \\ + \sum_{k\neq i} [e_i(t_1), e_k(t_2)](\rho_{ss}-\rho_{00})2\mathrm{i} \sin \omega_s(t_2-t_3)\sigma_z^{(k)}e_k(t_3).\end{aligned} \tag{5.4}$$

Again the pattern is established.

Equation (3.6) becomes

$$\boldsymbol{P}_i(\omega) = -(\rho_{ss}-\rho_{00})\alpha(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}} \cdot \Big[\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}_i,\omega)+\Big(J_0^+(\omega)\alpha^+(\omega)\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}_i,\omega) - \sum_{k\neq i}\mathsf{F}(\boldsymbol{x}_i,\boldsymbol{x}_k;\omega)\cdot\hat{\boldsymbol{u}}(\rho_{ss}-\rho_{00})\alpha(\omega)\hat{\boldsymbol{u}}\cdot\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}_k,\omega)\Big)+\ldots\Big]. \tag{5.5}$$

After some manipulation this can be reduced to

$$\boldsymbol{P}_i(\omega) = \hat{\boldsymbol{u}}\gamma^+(\omega)\Big(\hat{\boldsymbol{u}}\cdot\boldsymbol{E}_{\text{ext}}(\boldsymbol{x}_i,\omega)+\sum_{k\neq i}\hat{\boldsymbol{u}}\cdot\mathsf{F}(\boldsymbol{x}_i,\boldsymbol{x}_k;\omega)\cdot\hat{\boldsymbol{u}}\hat{\boldsymbol{u}}\cdot\boldsymbol{P}_k(\omega)\Big), \tag{5.6}$$

which is equivalent to

$$\boldsymbol{P}(\boldsymbol{x},\omega) = \gamma^+(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}}\cdot\sum_i\delta(\boldsymbol{x}-\boldsymbol{x}_i)\Big(\boldsymbol{E}_{\text{ext}}(\boldsymbol{x},\omega)+\int_{V-v}\mathsf{F}(\boldsymbol{x},\boldsymbol{x}';\omega)\boldsymbol{P}(\boldsymbol{x}',\omega)\,\mathrm{d}\boldsymbol{x}'\Big) \tag{5.7}$$

where $V-v$ is all space except for a sphere of vanishingly small radius centred on $\boldsymbol{x}' = \boldsymbol{x}$. This excludes self-terms which of course are already contained in $\gamma^+(\omega)$.

The main point of this result is that it shows within the decorrelation process that the intra-molecular photon propagator (carrying the reaction field) is $\mathsf{F}^+(\boldsymbol{x},\boldsymbol{x}';\omega)$ defined by (3.1*a*). In contrast the intermolecular field is carried by $\mathsf{F}(\boldsymbol{x},\boldsymbol{x}';\omega)$ defined in (2.7). This result is supported by the equation of motion methods since $\mathsf{F}(\boldsymbol{x},\boldsymbol{x}';\omega)$ is the Green function of Maxwell's equations (viewed as operator equations or not). However, equation (5.7) is actually linearized and compared directly with (2.4): the only change is the replacement of $\gamma(\omega)$ by $\gamma^+(\omega)$ so its solution is immediate.

We follow the procedure of Bullough *et al* (1968) and Bullough (1968). We ensemble average over atomic sites $\boldsymbol{x}_i$. With

$$n_0 \equiv \Big\langle\sum_{i=1}^{N}\delta(\boldsymbol{x}-\boldsymbol{x}_i)\Big\rangle_{\text{av}}$$

we find the approximate integral equation for $\boldsymbol{P}(\boldsymbol{x},\omega)$ (now ensemble averaged)

$$\boldsymbol{P}(\boldsymbol{x},\omega) = \gamma^+(\omega)\hat{\boldsymbol{u}}\hat{\boldsymbol{u}}\cdot\Big(\boldsymbol{E}_{\text{ext}}(\boldsymbol{x},\omega)+n_0\int_{V-v}\mathsf{F}(\boldsymbol{x},\boldsymbol{x}';\omega)\cdot\boldsymbol{P}(\boldsymbol{x}',\omega)\,\mathrm{d}\boldsymbol{x}'\Big). \tag{5.8}$$

We have again extracted a small sphere of volume v about the point $\boldsymbol{x}$ to ensure convergence of the integral. V is now the region occupied by atoms. The solution is

$$\boldsymbol{P}(\boldsymbol{x},\omega) = \hat{\boldsymbol{u}}P(\omega)\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}$$

if, but only if, $k = m\omega c^{-1}$ where $m(\omega)$ satisfies the dispersion relation

$$m^2(\omega)-1 = 4\pi n_0\gamma^+(\omega)(1-\tfrac{4}{3}\pi n_0\gamma^+(\omega))^{-1}. \tag{5.9}$$

Since $\gamma^+(\omega)$ is given by (3.8) we find

$$m^2(\omega)-1 = \frac{-8\pi n_0(\rho_{ss}-\rho_{00})e^2x_{0s}^2\omega_s\hbar^{-1}}{\omega_s^2-\omega^2+\frac{8}{3}\pi(\rho_{ss}-\rho_{00})n_0e^2x_{0s}^2\hbar^{-1}\omega_s-2\omega e^2x_{0s}^2\hbar^{-1}J_0^+(\omega)}. \tag{5.10}$$

The level shift is now corrected by the Lorentz field terms which however depend on the

initial state occupation $\rho_{ss}-\rho_{00}$ in agreement with results obtained by Saunders and Bullough (1973) by second-order perturbation theory.

The Lamb shift and its generalizations do not depend on the state occupation but the damping does. The refractive index m is complex and the sign of $\mathrm{Im}(m)$ is determined by that of the product $-(\rho_{ss}-\rho_{00})\,\mathrm{Im}\,J^{+}(\omega)$. In the attenuator $\rho_{ss}=0$ and $\rho_{00}=1$ so the wave $e^{ik.x}$ damps exponentially. In the amplifier $\rho_{ss}=1$ and $\rho_{00}=0$ and the wave *grows* exponentially: the damping constant (positive or negative) depends on the field described by the parameter n through $J^{+}(\omega)$. It is difficult to determine at this stage what real features of the amplifier are contained in this theory: it is a fermion theory in the self-interactions but is a pseudo-boson theory otherwise. Saunders and Bullough (1973) note what appear to be inadequacies in a pseudo-boson theory of the amplifier in taking account of all the damping processes. Significant non-linear features are certainly missed in reaching the linear integral equation (5.8). A pseudo-boson theory of the amplifier without the $\gamma^{+}(\omega)$ was sketched by Doniach (1963).

6. Discussion

The fermion decorrelation procedure we have described is a natural procedure alternative to the decorrelated all-order perturbation theory used for a pseudo-boson theory. It appears to be the correct procedure for a quantal theory of self-interactions since it agrees with the results of second-order perturbation theory. It is therefore an order e^2 theory but is strong enough to yield the main result which is the equations of motion (4.12). These equations contrast sharply with the comparable equation (2.28) in the pseudo-boson theory, and this contrast already indicates the very different content of the neo-classical theory due to Jaynes and others and the second quantized theory. The reaction field theory to be developed in the papers to follow only emphasizes this point.

It is perhaps worth pointing out that when first reported in 1971 the calculation was the first to obtain the total vacuum shift of the energy spacing in a natural way as Δ rather than $\frac{1}{2}\Delta$. Weisskopf–Wigner theory, for example, produces $\frac{1}{2}\Delta$ as does the resolvant method described by Kroll (1965), for example. This is the shift of the upper state only, is due to making a rotating-wave approximation too early in the calculation (compare Bullough 1973, Ackerhalt *et al* 1973, Agarwal 1973a) and then can be corrected for the Lamb shift of the ground state by rather arbitrary methods like that of Kroll (1965) who formally introduces the exact ground state energy. Ackerhalt *et al* (1973) also quote this particular result but their argument is unsound.

The theory is also good enough to obtain the field-dependent shifts Δ_1 and Δ_2 in agreement with perturbation theory. These terms simply do not appear in the pseudo-boson theory. For this reason they appear as a consequence only of the self-interactions in the many atom theory of § 5. The interatomic interactions are there carried by the propagator $\mathbf{F}$ and emerge from the Bose commutation relations which apply to interatomic processes.

However, we have found difficulty in extending this particular method to systems of atoms with more than two levels. It seems very probable that the propagator $\mathbf{F}^{+}$ is the correct propagator for the calculation of self-interaction at order e^2; but we have so far made most progress on the problem of the many-level atom by applying operator reaction field theory to it. We have also found it easier, for example, to calculate the emitted spectrum corresponding to the result (4.12) by reaction field methods.

We therefore develop the theory of this field in a following paper.

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