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Theory of radiation reaction and atom self-energies: an operator reaction field

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Abstract. We derive an operator field which includes the radiation reaction and self-fields for a single two-level atom in operator form. The field generalizes in a natural way the *c*-number theory of radiation reaction and frequency shifts due to Lorentz. By a trivial extension the operator field can be applied to the more complicated cases of a single multi-level atom and the super-radiant problem of N atoms on the same site where these are coupled either to the vacuum or the vacuum and additional imposed quantized fields. By further extension it also applies to the case of N atoms on different sites.

Explicit expressions for positive and negative frequency parts of the total operator field are given in terms of arbitrary dipole operator sources and are apparently valid for times $t \gg \omega_{max}^{-1} \gg \omega_{max}^{-1}$ where ω_{x} is the atomic resonance and ω_{max} a cut-off used systematically throughout the theory. The theory is internally consistent for $\omega_{max} < \infty$ but must then be approximated in order to be applicable. In this case, or if the approximation is 'improved' by $\omega_{max} \to \infty$ the fields either cease to be Heisenberg operators or break the equal-time matter-field commutation relations. These inconsistencies reflect those implicit in the mass renormalization problem.

The discussion is specialized to the spontaneous emission of a single two-level atom. The motion is described by three coupled nonlinear operator equations. Within a slowly varying amplitude approximation (sva) the dipole operator satisfies a damped oscillator equation with damping constant the Einstein A coefficient and with the natural frequency shifted from the atomic resonance by Δ just twice Bethe's expression for the Lamb shift of single levels. The spectrum of spontaneous emission is calculated: it is Lorentzian but peaked about the resonance shifted by Δ .

The svA is shown to be valid to first order in e^2 . The results therefore agree identically with those of second-order perturbation theory in the short-time limit but remain valid to the same order e^2 for all later times.

1. Introduction

In a previous paper (Bullough *et al* 1974, to be referred to as I) we used linear response theory in the form of an all-order perturbation theory to derive the spontaneous and stimulated emission rates, the Lamb shift, and the field-dependent generalized Lamb shift ('lamp' shift) for a single two-level atom in an ambient radiation field. The main point of these papers, however, is to set up a radiation reaction field theory of these phenomena. Reaction field theory has played a fundamental role in radiation theory since it was first introduced by Lorentz (1909)[†]. The importance of a reaction field

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

theory for a single atom at the present time lies in the natural way in which it fits into the theory of many-atom systems interacting with fields of arbitrary intensity.

In this paper we derive an operator field which contains an operator reaction field within it and generalize in a natural way the *c*-number theory of radiation reaction and frequency shifts due to Lorentz. Unfortunately when one attempts to consider the limit as the number of electromagnetic field modes tends to infinity the self- and reaction-field theory (sFT) is internally inconsistent. This shows itself as in I in the usual non-relativistic divergences and in addition and in consequence in the breakdown of the equal-time matter-field commutation relations. We shall therefore be concerned to show that the sFT is consistent with all known results in non-relativistic perturbation theory, with the results of I and with those obtained, for example, by the master equation methods exploited particularly by Agarwal (1970, 1971a, b, 1973a, b).

The work of checking the sFT is, however, largely deferred to a later paper. In this paper we can merely develop the theory of the operator fields themselves and consider the particular problem of a single two-level atom coupled to the vacuum.

The plan of the paper is as follows: In § 2 we derive the total field operator as a linear combination of matter and free field operators; the total field operator is derived in a form not restricted to the case of a single two-level atom. In § 3 we derive appropriate forms of the negative and positive frequency parts of the total field operator and show in the case of a single two-level atom how these simplify providing the imposed fields are weak. In § 4 we derive and investigate the operator equations of motion for a single two-level atom initially in the vacuum state. We find the Lamb shift is the doubled Bethe shift Δ obtained in I: the equation of motion for the expectation value of the dipole operator agrees with that derived in I for this case. In § 5 we calculate the auto-correlation function for a single initially inverted atom in the vacuum field. The emission spectrum is Lorentzian and resonant about the atomic frequency with Lamb shift Δ .

2. The total field operator

In this section the problem of a single two-level atom in its radiation reaction field is considered. The results obtained are however of greater generality; they apply, for example, to the single multi-level atom and to the problem first considered by Dicke (1954) of N super-radiant atoms on the same site and can be extended to N atoms on different sites.

We work in dipole approximation and second quantization. We take as the Hamiltonian

$$H = \frac{1}{2}\hbar\omega_{s}\sigma_{z} + \sum_{\boldsymbol{k},\lambda} \hbar\omega_{\boldsymbol{k}}(a^{\dagger}_{\boldsymbol{k},\lambda}a_{\boldsymbol{k},\lambda} + \frac{1}{2}) - \boldsymbol{p} \cdot \boldsymbol{e}.$$
(2.1)

In this (\mathbf{k}, λ) labels a mode of the free field with wavevector \mathbf{k} and polarization index λ ($\lambda = 1 \text{ or } 2$); $\omega_k = ck$. The field \mathbf{e} can be written as

$$\boldsymbol{e} = \mathrm{i} \sum_{\boldsymbol{k},\lambda} \left(\frac{2\pi\hbar\omega_{\boldsymbol{k}}}{V} \right)^{1/2} \hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda} (a_{\boldsymbol{k},\lambda} - a_{\boldsymbol{k},\lambda}^{\dagger})$$
(2.2)

where $\hat{\mathbf{e}}_{\mathbf{k},\lambda}$ is the unit vector defining the polarization direction of the mode (\mathbf{k},λ) and $a_{\mathbf{k},\lambda}$ and $a_{\mathbf{k},\lambda}^{\dagger}$ are the photon creation and annihilation operators which obey the commutation relations

$$[a_{\mathbf{k},\lambda}, a_{\mathbf{k}',\lambda'}^{\dagger}] = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\lambda\lambda'}.$$
(2.3)

The two-level atom has eigenstates $|s\rangle$ and $|0\rangle$ with energies E_s and E_0 respectively; $E_s - E_0 = \hbar\omega_s$. The operator σ_z is a Pauli spin operator such that the eigenvalues of $\frac{1}{2}\hbar\omega_s\sigma_z$ are $\pm\frac{1}{2}\hbar\omega_s$.

The matrix element of the x component of the atomic dipole operator ex is

$$e\langle 0|x|s\rangle \equiv ex_{0s} = ex_{s0}$$

as in I: we shall now use p for this. In second-quantized notation the total dipole operator p is $\hat{u}p\sigma_x$ in which \hat{u} is a unit vector in the x direction and σ_x is a second Pauli spin operator. We introduce the third Pauli spin operator σ_y to complete, with the addition of the unit operator, an SU₂ Lie algebra. The spin operators $\boldsymbol{\sigma} = (\sigma_x \sigma_y \sigma_z)$ thus satisfy the usual commutation relations

$$\boldsymbol{\sigma} \times \boldsymbol{\sigma} = 2\mathbf{i}\boldsymbol{\sigma}.\tag{2.4}$$

The spin operators σ commute with the photon operators $a_{\mathbf{k},\lambda}$, $a_{\mathbf{k},\lambda}^{\dagger}$. Hence we have the commutation relation

$$[\boldsymbol{e}(t), \boldsymbol{\sigma}(t)] = \boldsymbol{0}. \tag{2.5}$$

We now construct the total field operator e(t) of equation (2.2). Heisenberg's equations of motion together with the commutation relation (2.3) yield

$$\dot{a}_{\boldsymbol{k},\lambda} = -\mathrm{i}\omega_{\boldsymbol{k}}a_{\boldsymbol{k},\lambda} + \hbar^{-1}\boldsymbol{p}\cdot\hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda} \left(\frac{2\pi\hbar\omega_{\boldsymbol{k}}}{V}\right)^{1/2}$$
(2.6*a*)

$$\dot{a}_{\boldsymbol{k},\lambda}^{\dagger} = +\mathrm{i}\omega_{k}a_{\boldsymbol{k},\lambda}^{\dagger} + \hbar^{-1}\boldsymbol{p}\cdot\hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda}\left(\frac{2\pi\hbar\omega_{k}}{V}\right)^{1/2}.$$
(2.6b)

Hence

$$a_{\boldsymbol{k},\lambda}(t) = a_{\boldsymbol{k},\lambda}(0) \,\mathrm{e}^{-\imath\omega_{\boldsymbol{k}}t} + \hbar^{-1} \,\mathrm{e}^{-\imath\omega_{\boldsymbol{k}}t} \,\int_{0}^{t} \boldsymbol{p}(t') \cdot \hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda} \left(\frac{2\pi\hbar\omega_{\boldsymbol{k}}}{V}\right)^{1/2} \,\mathrm{e}^{\imath\omega_{\boldsymbol{k}}t'} \,\mathrm{d}t' \qquad (2.7a)$$

$$a_{\boldsymbol{k},\lambda}^{\dagger}(t) = a_{\boldsymbol{k},\lambda}^{\dagger}(0) \, \mathrm{e}^{\mathrm{i}\omega_{\boldsymbol{k}}t} + \hbar^{-1} \, \mathrm{e}^{\mathrm{i}\omega_{\boldsymbol{k}}t} \, \int_{0}^{t} \boldsymbol{p}(t') \, \boldsymbol{\cdot} \, \boldsymbol{\hat{\epsilon}}_{\boldsymbol{k},\lambda} \, \left(\frac{2\pi\hbar\omega_{\boldsymbol{k}}}{V}\right)^{1/2} \mathrm{e}^{-\mathrm{i}\omega_{\boldsymbol{k}}t'} \, \mathrm{d}t'. \tag{2.7b}$$

Thus the total field operator of equation (2.2) is

$$\boldsymbol{e}(t) = \boldsymbol{e}_{0}(t) + \left(\frac{\mathrm{i}2\pi}{V}\right) \sum_{\boldsymbol{k},\lambda} \omega_{\boldsymbol{k}} \left(\mathrm{e}^{-\mathrm{i}\omega_{\boldsymbol{k}}t} \int_{0}^{t} \boldsymbol{\epsilon}_{\boldsymbol{k},\lambda} \boldsymbol{\epsilon}_{\boldsymbol{k},\lambda} \cdot \boldsymbol{p}(t') \, \mathrm{e}^{\mathrm{i}\omega_{\boldsymbol{k}}t'} \, \mathrm{d}t' - \mathrm{CC} \right)$$
(2.8)

where

$$\boldsymbol{e}_{0}(t) = i \left(\frac{2\pi\hbar}{V}\right)^{1/2} \sum_{\boldsymbol{k},\lambda} \omega_{\boldsymbol{k}}^{1/2} \hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda}(a_{\boldsymbol{k},\lambda}(0) e^{-i\omega_{\boldsymbol{k}}t} - a_{\boldsymbol{k},\lambda}^{\dagger}(0) e^{+i\omega_{\boldsymbol{k}}t})$$
(2.9)

is the free field operator, and CC stands for complex conjugate.

By using the obvious relation

$$\sum_{\lambda=1,2} \hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda} \hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda} = (\mathbf{U} - \hat{\boldsymbol{k}} \hat{\boldsymbol{k}})$$

in which **U** is the unit vector and \hat{k} is a unit vector along k and replacing $V^{-1} \Sigma_k$ by $(2\pi)^{-3} \int dk$ we find that

$$\boldsymbol{e}(t) = \boldsymbol{e}_{0}(t) + \frac{2i}{3\pi c^{3}} \int_{0}^{\omega_{\max}} \omega^{3} d\omega \int_{0}^{t} \boldsymbol{p}(t') (\mathbf{e}^{-i\omega(t-t')} - \mathbf{e}^{+i\omega(t-t')}) dt'.$$
(2.10)

We now reverse the orders of integration which is legitimate for finite ω_{\max} and use the relation

$$\int_{0}^{\omega_{\max}} \omega^{3} (e^{-i\omega x} - e^{+i\omega x}) d\omega = \frac{2}{i} \frac{d^{3}}{dx^{3}} \left(\frac{\sin \omega_{\max} x}{x} \right)$$
(2.11)

to rewrite the total field operator as

$$\boldsymbol{e}(t) = \boldsymbol{e}_{0}(t) + \frac{4}{3\pi c^{3}} \int_{0}^{t} \boldsymbol{p}(t') \frac{\mathrm{d}^{3}}{\mathrm{d}t^{3}} \left(\frac{\sin \omega_{\max}(t-t')}{t-t'} \right) \mathrm{d}t'.$$
(2.12)

In (2.12) the free field part of the total field operator reduces to $e_0(0)$ at t = 0 whilst the remaining part of the field due to dipole sources vanishes. Thus the commutation relation (2.5) between the total field operator e(t) and the matter operator $\sigma(t)$ holds at t = 0 and presumably for all t > 0: this is possible because although e(t) is linear in p(t) which does not commute with σ_x and σ_y it is actually a linear functional of p(t')for positive times t' < t. Since $e_0(t)$ evolves as a free field operator whilst the matter operators are Heisenberg operators evolving with the full Hamiltonian H the equal-time commutators of $e_0(t)$ with $\sigma(t)$ are not zero. Thus although the total field in (2.12) satisfies the commutation relations (2.5) its two parts do not.

The equation (2.12) can be integrated by parts to give

$$\boldsymbol{e}(t) = \boldsymbol{e}_0(t) + \frac{4}{3\pi c^3} \left(\boldsymbol{E}_1 + \boldsymbol{E}_2 + \boldsymbol{E}_3 + \int_0^t \ddot{\boldsymbol{p}}(t') f(t-t') \, \mathrm{d}t' \right)$$
(2.13)

in which

$$\boldsymbol{E}_{1} = -(\boldsymbol{p}(t)\ddot{f}(0) - \ddot{\boldsymbol{p}}(0)f(t))$$
(2.14a)

$$E_2 = -(\dot{p}(t)\dot{f}(0) - \dot{p}(0)\dot{f}(t))$$
(2.14b)

$$E_3 = -(\ddot{p}(t)f(0) - \ddot{p}(0)f(t))$$
(2.14c)

and

$$f(t) \equiv \sin(\omega_{\max}t)t^{-1}.$$
(2.15)

There is no reason to suppose this field breaks the commutation relations: it reduces to $e_0(0)$ at t = 0 and the commutation relations are satisfied there; since everything is well defined they will be satisfied also for all t > 0.

Trouble arises as soon as we try to take the limit as $\omega_{max} \rightarrow \infty$. In this limit

$$f(t) \to \pi \delta(t), \qquad \dot{f}(t) \to \pi \delta'(t), \qquad \dot{f}(t) \to \pi \delta''(t)$$

where $\delta''(t) = (1/2\pi) \int_{-\infty}^{\infty} (-ik)^2 e^{-ikt} dk$ etc. Thus, in this limit if it exists

$$\boldsymbol{E}_{1} = -\pi(\boldsymbol{p}(t)\delta''(0) - \boldsymbol{p}(0)\delta''(t))$$
(2.16a)

$$E_2 = -\pi(\dot{p}(t)\delta'(0) - \dot{p}(0)\delta'(t))$$
(2.16b)

$$\boldsymbol{E}_{3} = -\pi(\,\boldsymbol{\ddot{p}}(t)\delta(0) - \boldsymbol{\ddot{p}}(0)\delta(t)) \tag{2.16c}$$

and

$$\lim_{\omega_{\max}\to\infty} \left(\int_0^t \ddot{\boldsymbol{p}}(t') \frac{\sin\omega_{\max}(t-t')}{t-t'} \, \mathrm{d}t' \right) = \begin{cases} \frac{\pi}{2} \ddot{\boldsymbol{p}}(t) & t > 0\\ 0 & t = 0. \end{cases}$$
(2.17)

 E_1 , E_2 and E_3 all vanish identically at t = 0. For t > 0, E_1 and E_3 diverge. The terms in E_1 are associated with the contact term of Power and Zienau (1959) omitted in (2.1). Their longitudinal part is a self-Coulomb interaction in dipole approximation and is an artefact of that approximation. The terms in E_1 never figure in the analysis and we temporarily drop them here. The terms in E_2 vanish from the field when t > 0; they are associated with the square of the vector potential in a Hamiltonian taken outside dipole approximation. Thus in the all-mode 'limit'

$$\boldsymbol{e}(t) = \begin{cases} \boldsymbol{e}_{0}(t) + \frac{2}{3c^{3}}(\boldsymbol{\ddot{p}}(t) - \omega_{s}K_{0}\boldsymbol{\ddot{p}}(t)), & \text{if } t > 0\\ \boldsymbol{e}_{0}(t) & \text{if } t = 0. \end{cases}$$
(2.18)

and, as in I,

$$K_0 \equiv \frac{2}{\pi} \frac{c}{\omega_{\rm s}} \int_0^\infty {\rm d}k$$

Crisp and Jaynes (1969) and Stroud and Jaynes (1970) together show that K_0 diverges only as a consequence of the dipole approximation. Even within this approximation there is no difficulty at t = 0 as we noted above. However, the field in (2.18) obviously jumps at t = 0. Since $e_0(t)$ evolves smoothly as a free field operator from t = 0 and is differentiable there, whilst the remaining part of the field jumps, the total field is at best differentiable in a generalized function sense and cannot evolve smoothly as a Heisenberg operator. Since e(t) commutes with matter operators at t = 0 it cannot do so for t > 0.

An alternative is to define e(t) by (2.18) for t > 0 and as $\lim_{t \to 0_+} e(t)$ for t = 0. Since

$$\boldsymbol{e}(0_{+}) = \boldsymbol{e}_{0}(0) - \frac{2}{3c^{3}}(\omega_{s}K_{0}\ddot{\boldsymbol{p}}(0) - \ddot{\boldsymbol{p}}(0))$$
(2.19)

and $e_0(0)$ commutes whilst the remaining terms do not commute with all of σ_x , σ_y and σ_z , then if e(t) evolves from $t = 0_+$ as a Heisenberg operator, it cannot commute with the matter operators for all $t > 0_+$.

This failure of the equal-time commutation relations does not devastate the argument—apparently because it appears to be possible to carry it through for finite ω_{max} . Because this introduces functionals of p(t) we do not attempt such a programme here. Our point of view is to take ω_{max} very large but finite so that E_1 and E_2 are formally well described by (2.14*a*, *b*) for all $t \gg \omega_{max}^{-1}$. Further (2.17) will be good to order ω_{max}^{-1} for all $t \gg \omega_{max}^{-1}$ [†]. Thus we can take (2.18) as a formal definition of e(t) for t > 0 by taking ω_{max} large enough and the field operator is then a linear function of matter operators to order ω_{max}^{-1} . This definition makes the problem tractable in a formal way since it changes what would be nonlinear integro-differential operator equations to nonlinear differential operator equations which are more easily solved. Moreover, if the equal-time field-matter commutation relations (2.5) apply to (2.12), they apply to (2.18) for large enough *t*. Agarwal (private communication) has also shown that consistent approximations, more drastic than those we use here at first, can be made which preserve the commutation relations at the expense of the Heisenberg character of the operators.

[†] This is equivalent to the 'Markoffian approximation' of master equation theory. Ackerhalt *et al* (1973b) make the mistake of trying to make this approximation mode by mode for which it cannot be valid. It is here good to order ω_{max}^{-1} and is exact in the limit which is (2.17).

Finally we have to choose ω_{max} . We assume with Bethe (1947) that

$$\omega_{\rm max} = \omega_{\rm C} \equiv m_{\rm e} c^2 \hbar^{-1},$$

the Compton frequency, so that we regain his formula for the Lamb shift. For large t all the results then coincide with I and with more conventional methods.

These results do not follow from (2.18) directly. The dipole operator p(t) can be expressed in terms of positive and negative frequency part operators. We set

$$\boldsymbol{p}(t) = \hat{\boldsymbol{u}} p \sigma_{\boldsymbol{x}}(t) \equiv \hat{\boldsymbol{u}} p(\sigma_{+}(t) + \sigma_{-}(t))$$
(2.20)

where

$$\sigma_{\pm}(t) \equiv \frac{1}{2}(\sigma_{x}(t) \pm i\sigma_{y}(t)) \tag{2.21}$$

are Heisenberg operators. For free matter, $\sigma_{\pm}(t) = \sigma_{\pm}(0) e^{\pm i\omega_s t}$ and we expect that for the coupled system of matter and field

$$\sigma_{+}(t) = R_{+}(t) e^{\pm i\omega_{s}t}$$
(2.22)

where $R_{\pm}(t)$ are operators varying slowly on a time scale of order ω_s^{-1} . We can expect this when, but only when, the perturbing fields are weak and the only significantly occupied electromagnetic field modes are sharply peaked about the resonance frequency ω_s of the two-level atom. The operators (2.22) are then positive and negative frequency parts of $\sigma_x(t)$.

It is shown in an earlier paper (Bullough 1973, Appendix 2) that, with these assumptions, the field (2.18) when divided into positive and negative frequency parts by dividing σ_x as in (2.20) yields an acceptable theory of spontaneous emission[†]. However, the Lamb shift of the frequency ω_s is

$$-\frac{2}{3}\frac{p^2\omega_c^3}{c^3}K_0.$$
 (2.23)

This is not a 'dynamical shift' in the sense of the neo-classical theory (NCT) of Crisp and Jaynes (1969) and Stroud and Jaynes (1970). It does coincide with the long-time limit of that shift taken in dipole approximation, however. It disagrees with Bethe's (1947) result of low-order perturbation theory and with other perturbation theories (Saunders and Bullough 1973, Knight 1972) and it disagrees with I for the reason it appeals to the propagator **F** and not to the self-field propagator F^+ introduced there. Plainly the operator field (2.18) corresponds to the field (I, equation (2.29)) considered in the Bose theory of I § 2. The division into positive and negative frequency part fields is motivated by the Fermion theory, however, and we need to find a less arbitrary approach to this.

3. The positive and negative frequency parts of the total field operator

It is plain from the previous paragraph that e(t) must be split into mutually adjoint parts which separately contain the negative and positive frequency parts of the free field operator $e_0(t)$, preserve the commutation relations for finite ω_{max} , and preserve the character of the fields as linear combinations of single-mode operators. Only the first condition is obviously satisfied by the field just discussed.

 \dagger The argument adopts the normal ordering prescription developed in §3 and includes the free field divided as in §3. It fails only because it arbitrarily imposes the Bose property from which (2.23) follows.

The parts of the free field will be

$$\boldsymbol{e}_{0}^{(\pm)}(t) = \pm i \left(\frac{2\pi\hbar}{V}\right)^{1/2} \sum_{\boldsymbol{k},\lambda} \omega_{\boldsymbol{k}}^{1/2} \hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda} a_{\boldsymbol{k},\lambda}^{(\pm)}(0) e^{\pm i\omega_{\boldsymbol{k}}t}$$
(3.1)

where

$$a_{\mathbf{k},\lambda}^{(+)}(0) \equiv a_{\mathbf{k},\lambda}(0), \qquad a_{\mathbf{k},\lambda}^{(-)}(0) \equiv a_{\mathbf{k},\lambda}^{+}(0).$$

Therefore we define the coupled matter-field operators by

$$\boldsymbol{e}^{(\pm)}(t) = \pm i \left(\frac{2\pi\hbar}{V}\right)^{1/2} \sum_{\boldsymbol{k},\lambda} \omega_{\boldsymbol{k}}^{1/2} \hat{\boldsymbol{\epsilon}}_{\boldsymbol{k},\lambda} a_{\boldsymbol{k},\lambda}^{(\pm)}(t)$$
(3.2)

where $a_{\mathbf{k},\lambda}^{(\pm)}(t)$ evolve as Heisenberg operators. For finite $\omega_{\max} e^{(\pm)}(t)$ preserve the commutation relations with the matter operators since each $a_{\mathbf{k},\lambda}^{(\pm)}(t)$ commutes separately with them. Note that $e^{(\pm)}(t)$ and $e_0^{(\pm)}(t)$ coincide at t = 0 for finite ω_{\max} and this is consistent with (2.13).

Instead of (2.13) however, we now find

$$e^{(\pm)}(t) = e_0^{(\pm)}(t) + \frac{2}{3\pi c^3} \left(E_1^{(\pm)} + E_2^{(\pm)} + E_3^{(\pm)} + \int_0^t \ddot{p}(t') f_{\pm}(t-t') \, \mathrm{d}t' \right)$$
(3.3)

in which

$$f_{\pm}(t) = \pm i \left(\frac{e^{\pm i\omega_{\max}t} - 1}{t} \right)$$
(3.4)

and $E_1^{(\pm)}(t)$, etc are defined by analogy with (2.14). Note now that $f_{\pm}(0) = f(0) = -\frac{1}{3}\omega_{\max}^3$, $f_{\pm}(0) = f(0) = \omega_{\max}$, but $f^{\pm}(0) = \mp i\frac{1}{2}\omega_{\max}^2$. Both fields (3.3) jump at t = 0 in the formal all-mode limit as $\omega_{\max} \to \infty$ since their sum does. However, $E^{(\pm)}$ etc contain terms in $f_{\pm}(t)$ which yield principal part integral terms not necessarily vanishing for t > 0. We shall not treat these *p*-integral terms.

It is shown in the appendix that when $\omega_{\max} \rightarrow \infty$

$$\int_{0}^{t} \ddot{p}(t') f_{\pm}(t-t') dt' = \mp \frac{i\pi}{2} \ddot{p}(t) K_{1} + \pi \ddot{p}^{\pm}(t)$$
(3.5)

for all $t \gtrsim \omega_s^{-1}$. In this case

$$K_1 = \frac{2}{\pi} \ln \left| \frac{\omega_{\text{max}}}{\omega_{\text{s}}} \right|. \tag{3.6}$$

In consequence the analogue of the total field (2.18) is

$$\boldsymbol{e}^{(\pm)}(t) = \boldsymbol{e}_{0}^{(\pm)}(t) - \frac{1}{3} \left(\frac{\omega_{s}}{c^{3}} \right) K_{0} \boldsymbol{\ddot{p}} \mp \frac{iK_{1}}{3c^{3}} \boldsymbol{\ddot{p}} + \frac{2}{3c^{3}} \boldsymbol{\ddot{p}}^{(\pm)} \qquad t > 0$$
(3.7)

and the sum of $e^{(\pm)}(t)$ and $e^{(-)}(t)$ is precisely the total field of (2.18). This field deliberately ignores the contributions of $E_1^{(\pm)}(t)$ and $E_2^{(\pm)}(t)$. For t > 0 these terms add to (3.7) to give, ignoring the *p*-integrals, just

$$e^{(\pm)}(t) = e_0^{(\pm)}(t) + \frac{1}{3c^3} \left(\frac{2}{3\pi} \omega_{\max}^3 p(t) \pm \frac{i}{\pi} \omega_{\max}^2 \dot{p}(t) - \omega_s K_0 \ddot{p}(t) \mp i K_1 \ddot{p}(t) \right) + \frac{2}{3c^3} \ddot{p}^{(\pm)}(t).$$
(3.8)

These fields are essentially exact for time $t \gg \omega_s^{-1} \gg \omega_{max}^{-1}$ providing the spectrum (Fourier transform) of p(t) is peaked about $\pm \omega_s$. They are certainly not in rotating wave approximation (RWA) for example (Bullough 1973).

Note that since the two-level restriction nowhere enters into the argument used to derive the fields $e^{\pm}(t)$ and the total field e(t) these fields are also valid for a single multilevel atom and also for the super-radiant problem of N atoms on one site provided p(t) is now the total dipole operator for the system and the definitions of K_0 and K_1 are appropriately extended.

4. The Bloch equations for the two-level atom

Using the matter operator commutation relations (2.4) and Heisenberg's equations of motion we derive the Bloch equation for the two-level atom. These are[†]

$$\dot{\sigma}_x = -\omega_s \sigma_y \tag{4.1a}$$

$$\dot{\sigma}_{y} = +\omega_{s}\sigma_{x} + 2p\hbar^{-1}(e^{(-)}\sigma_{z} + \sigma_{z}e^{(+)})$$
(4.1b)

$$\dot{\sigma}_{z} = -2p\hbar^{-1}(e^{(-)}\sigma_{y} + \sigma_{y}e^{(+)}).$$
(4.1c)

The fields $e^{(\pm)}(t)$ are placed in normal order with respect to the matter operators $\sigma(t)$, that is $e^{(-)}(t)$ is placed to the left and $e^{(+)}(t)$ to the right of these operators. This offers the computational advantage that for finite ω_{\max} the operators $e_0^{(\pm)}(t)$ inside the expectation values for such operator products can be simply evaluated by expressing the initial state vector $|\cdots\rangle$ at t = 0 as a combination of free matter and free field states. In the limit as $\omega_{\max} \rightarrow \infty$ the fields $e^{(\pm)}(t)$ do not commute with the $\sigma(t)$ and we need to choose the order of field and matter operators. We are free to choose the normal order and call this the 'normal ordering prescription'.

Now we take the cut-off ω_{\max} as the Compton frequency ω_c . Thus K_1 is small. We suppose the initial state of the field is such that excited modes are 'resonant'; such modes are resonant if their spectrum has a width $\Delta \omega \ll \omega_s$ clustered about ω_s . The fields are also 'weak' if the expectation values $\langle \cdots | 2p\hbar^{-1}e_0^{(\mp)} | \cdots \rangle$ are small compared with ω_s .

The first two equations of (4.1) imply

$$\ddot{\sigma}_{x} = -\omega_{s}^{2}\sigma_{x} - 2p\hbar^{-1}\omega_{s}(e^{(-)}\sigma_{z} + \sigma_{z}e^{(+)}).$$
(4.2)

If the driving fields are both resonant and weak and if we ignore the point that K_0 is actually large, (4.2) shows that we can replace $\dot{\sigma}_x$ by $-\omega_s^2 \sigma_x$ to neglect of terms of order $\Delta \omega \omega_s^{-1}$, $2p\hbar^{-1} \langle |e_0^{(\mp)}| \rangle \omega_s^{-1}$ and $\Gamma_0 \omega_s^{-1}$, where $\Gamma_0 = \frac{4}{3} (\omega_s/c)^3 p^2/\hbar$ is the Einstein A coefficient. Under these conditions equations (2.22) apply and $R_{\pm}(t)$ are slowly varying operators. Thus the approximation which allows us to write $\dot{\sigma}_x = -\omega_s^2 \sigma_x$ is the slowly varying amplitude approximation (sva).

Note that $\ddot{\sigma}_x = -\omega_s^2 \sigma_x$ means neglect of a power series in, in particular, $\Gamma_0 \omega_s^{-1}$ and hence of a power series in e^2 . This restricts the results to ones equivalent to those at first order in e^2 in perturbation theory, but the theory remains a dynamical one valid for all times greater than or equal to ω_s^{-1} . Note this series also contains powers of K_0 . Thus the mass renormalization problem is ducked and can be only treated at order equivalent to order e^2 in perturbation theory. This problem could apparently be solved to all orders if K_0 could be directly if formally eliminated as a mass term from the equations (4.1) since these with (3.7) constitute an almost 'exact' system of equations for $t \ge \omega_s^{-1} \ge \omega_{max}^{-1}$. We have not solved the problem in this form.

† We use $pe^{(\mp)}$ for $p\hat{u} \cdot e^{(\mp)}$.

If $\ddot{\sigma}_x = -\omega_s^2 \sigma_x$, so that terms of the orders stated are neglected, (3.7) is[†]

$$\boldsymbol{e}^{(\pm)}(t) = \boldsymbol{e}_{0}^{(\pm)}(t) + \frac{1}{3} \left(\frac{\omega_{s}}{c}\right)^{3} \boldsymbol{\hat{u}} p(K_{0}\sigma_{x} \mp iK_{1}\sigma_{y}) + \frac{2}{3} \left(\frac{\omega}{c}\right)^{3} \boldsymbol{\hat{u}} p\sigma_{y}^{(\pm)}(t).$$
(4.3)

This field neglects terms in $E_1^{(\pm)}$ and $E_2^{(\pm)}$. If these terms are included they change the field to

$$e^{(\pm)}(t) = e_{0}^{(\pm)}(t) + \frac{1}{3} \left(\frac{\omega_{s}}{c}\right)^{3} \hat{u} p \left[\left(K_{0} + \frac{2}{3\pi} \omega_{s}^{-3} \omega_{max}^{3} \right) \sigma_{x}(t) \right. \\ \left. \left. \left. \left. \left(K_{1} + \frac{1}{\pi} \omega_{s}^{-2} \omega_{max}^{2} \right) \sigma_{y}(t) \right] + \frac{2}{3} \left(\frac{\omega_{s}}{c} \right)^{3} \hat{u} p \sigma_{y}^{(\pm)}(t) \right] \right] \right]$$

$$(4.4)$$

where it is now necessary to assume that $\omega_s^{-3}\omega_{max}^3$ and $\omega_s^{-2}\omega_{max}^2$ as well as K_0 are small so that $\ddot{\sigma}_x = -\omega_s^2 \sigma_x$. Again we expect renormalization theory 'valid' only to order e^2 although it is possible to do better than this with the term in ω_{max}^3 by including contact terms in the Hamiltonian (2.1) as we will see below.

In the rest of this section we consider, for simplicity, the spontaneous emission of a single two-level atom. The effects of coherent and incoherent fields on the two-level atom will be delayed to later papers; the following discussion is essential for an understanding of these more complex effects of fully quantized fields on the two-level atom. If the field (4.3) is used in the Bloch equations (4.1), use of the commutation relations (2.4) reduces these equations to

$$\dot{\sigma}_x = -\omega_s \sigma_y \tag{4.5a}$$

$$\dot{\sigma}_{y} = \omega_{s}\sigma_{x} - \Gamma_{0}\sigma_{y} - \Gamma_{0}K_{1}\sigma_{x} + 2p\hbar^{-1}(e_{0}^{(-)}\sigma_{z} + \sigma_{z}e_{0}^{(+)})$$
(4.5b)

$$\dot{\sigma}_{z} = -\Gamma_{0}(1+\sigma_{z}) - 2p\hbar^{-1}(e_{0}^{(-)}\sigma_{y} + \sigma_{y}e_{0}^{(+)}).$$
(4.5c)

Since at t = 0 the initial state $|\cdots\rangle$ is a product of the excited state and the no-photon state we can drop the free field operators $e_0^{(\pm)}(t)$ from these equations. Hence we obtain from the two equations (4.5*a*, *b*) the analogue of (4.2) as

$$\dot{\sigma}_x + \Gamma_0 \dot{\sigma}_x + (\omega_s^2 - K_1 \omega_s \Gamma_0) \sigma_x = 0.$$
(4.6)

This is an oscillator with damping constant Γ_0 and natural frequency $(\omega_s^2 - K_1 \omega_s \Gamma_0)^{1/2}$. Thus the Lamb Shift of the level spacing is

$$\hbar[(\omega_{\rm s}^2 - K_1 \omega_{\rm s} \Gamma_0)^{1/2} - \omega_{\rm s}] \simeq -\frac{1}{2} \hbar K_1 \Gamma_0$$
(4.7)

where

$$-\frac{1}{2}K_{1}\Gamma_{0} = -\frac{4p^{2}\omega_{s}^{3}}{3\pi c^{3}}\ln\left(\frac{\omega_{\max}}{\omega_{s}}\right).$$

$$(4.8)$$

If we choose $\omega_{\max} = \omega_C \equiv m_e c^2 \hbar^{-1}$ this shift of the level spacing is precisely Δ , twice the Bethe shift of each level separately, in agreement with I[‡]. If we define $P(t) = p \langle \dots | \sigma_x(t) | \dots \rangle$ we see equation (4.6) is equivalent to a Lorentz damped oscillator with inclusion of the Lamb shift.

[†] If the exciting modes are well off resonance and are grouped about frequency ω , this frequency replaces ω_s in (4.3): if the exciting fields are not weak, their effect must be calculated by working from (3.7) rather than (4.3) (likewise (4.4) which follows applies only to weak resonant driving fields). Weak fields can still be as much as 10³ cgs units corresponding to powers of gigawatts cm⁻²: the frequencies $2ph^{-1}\langle \ldots | e_0^{(\mp)} | \ldots \rangle \lesssim 10^{12}$ Hz. ‡ Compare also Ackerhalt *et al* (1973a) and Bullough (1973).

We have derived equations (4.5) using the fields (4.3). The more complete fields (4.4) introduce quadratic and cubic divergence terms. Then a comparison between these two fields shows that the quadratically divergent term is associated with K_1 whilst the cubically divergent term is associated with K_0 and goes out with it. This is a feature of the two-level atom restriction.

We should point out that the cubic divergence vanishes in any case. Power and Zienau (1959) show that the Hamiltonian (2.1) which is taken in dipole approximation must be corrected by the contact term

$$H_{\text{contact}} = 2\pi \int (\boldsymbol{p}(\boldsymbol{x}))^2 \, \mathrm{d}\boldsymbol{x}. \tag{4.9}$$

For the dipole density p(x) we take

$$\boldsymbol{p}(\boldsymbol{x}) = \hat{\boldsymbol{u}}\sigma_{\boldsymbol{x}}\,\delta(\boldsymbol{x}-\boldsymbol{x}_0) \tag{4.10}$$

where x_0 is the site of the single two-level atom. Then

$$p^{2}(\mathbf{x}) = p^{2} \sigma_{\mathbf{x}}^{2} \delta(\mathbf{0}) \delta(\mathbf{x} - \mathbf{x}_{0}) = p^{2} \delta(\mathbf{0}) \delta(\mathbf{x} - \mathbf{x}_{0}) I$$
(4.11)

where we have used the operator relation $\sigma_x^2 = I$, the identity operator. Thus H_{contact} does not change the equations of motion in this case. Then the tranverse part of H_{contact} is

$$\frac{4\pi}{3}p^2\delta(\mathbf{0}) = \frac{2p^2}{3\pi}\int_0^{\omega_{\text{max}}} k^2 \,\mathrm{d}k.$$

For the two-level atom this energy shift is to be associated with K_0 in (4.4) and goes out with it in this case. In the cases of the multi-level atom and of N atoms on the same site we cannot use the constant of motion $\sigma_x^2 = I$. In these cases the transverse part of the contact term figures in the equations of motion and, up to e^2 order in perturbation theory, is just sufficient to remove the cubic divergence from the theory. The linear divergence K_0 remains in the equations of motion. We are therefore justified in systematically dropping the contact term from H and ignoring the cubic divergences where these emerge later in the argument.

Since the quadratically divergent term is not eliminated from the shift of the level spacing in the theory of the two-level atom it may be said to be this that breaks the equal-time matter-field commutation relations. Note however that this term vanishes from the total field operator since the fields (3.8) sum to

$$\boldsymbol{e}(t) = \boldsymbol{e}_{0}(t) + \frac{2}{3c^{3}} \left(\frac{2}{3\pi} \omega_{\max}^{3} \boldsymbol{p}(t) - \omega_{s} K_{0} \, \boldsymbol{\ddot{p}}(t) \right) + \frac{2}{3c^{3}} \, \boldsymbol{\ddot{p}}(t).$$
(4.12)

This field contains K_0 and what more generally is the spurious contact contribution and breaks the equal-time matter-field commutation relations (2.5). Thus the theory is internally inconsistent in the all-mode limit. For this reason a number of alternative fields and ordering prescriptions were examined in Bullough (1973): none displayed the elegance, simplicity and complete agreement with previous work exhibited by the fields (3.8) interpreted with the normal ordering prescription in e^2 approximation. Presumably this is because for finite ω_{max} the theory can be carried through consistently and exactly—although at order e^2 (convergent) mass terms would need to be eliminated in the usual way. The normal ordering prescription facilitates evaluation of the free field terms whether the problem can be formulated consistently or not: in a later paper we will show that all field-dependent quantities can be evaluated this way again in agreement with order e^2 perturbation theory.

We can now comment on the status of the neo-classical theory (NCT) of Jaynes and co-workers (Jaynes and Cummings 1963, Crisp and Jaynes 1969, Stroud and Jaynes 1970, Jaynes 1973). The NCT is a reaction field theory: it can always be obtained from a quantal theory by replacing the total field operator, including all self- and reaction-field parts, by its expectation value. Two consequences follow: first normal ordering is irrelevant so division of the field into negative and positive frequency parts is also. Then only the total field figures in the theory and only K_0 figures in the level shift. Since the transverse part of the contact term in H eliminates the cubic divergence, whilst Crisp and Jaynes (1969) show that K_0 is actually finite in the all-mode limit outside dipole approximation, and since the quadratic divergence does not appear in the total field, the NCT is a finite theory.

This feature is a feature of the Bose theory of I for exactly the same reasons. However the second result implicit in the NCT is that products of matter operators are decorrelated so that the theory is intrinsically nonlinear: indeed the expectation values of equations (4.1) become the nonlinear *c*-number equations used by Jaynes. Despite the internal inconsistency of the non-relativistic quantum theory of self- and reaction-fields developed in this paper the initial postulates of the theory appeal to us more than the ad hoc definitions of the field in the NCT: experiment also seems to prefer the quantal theory (Gibbs 1973, Wessner et al 1973). One final summarizing comment on the quantal theory: although the fields (4.4) contain terms in ω_{\max}^3 , ω_{\max}^2 and ω_{\max} , the first is always eliminated by the contact terms in the original Hamiltonian taken in the dipole approximation as we showed. Then in the particular case of the two-level atom the third term in $\omega_{\rm max}$ does not figure in the equations of motion (4.5) but the second does. In contrast in the case of the multi-level atom the second can be eliminated by the sum rule for oscillator strengths at the order e^2 of the calculation but the second term in ω_{max} now remains. It can then be identified with Bethe's kinetic mass renormalization. We have not been able to solve the mass renormalization problem at any higher order in e^2 and the quantal theory remains a divergent theory.

5. The spectrum of spontaneous emission

We calculate the emission spectrum of a single atom in the case when the initial state $|\cdots\rangle$ is a product of the excited matter state $|s\rangle$ and the photon vacuum state. Thus we can drop the free fields $e_0^{(\pm)}(t)$ from equations (4.5*a*, *b*) and rewrite these as

$$\dot{\sigma}_{\pm} + \frac{1}{2}\Gamma_0(1 \pm iK_1)\sigma_{\pm} - \frac{1}{2}\Gamma_0(1 \mp iK_1)\sigma_{\mp} \mp i\omega_s\sigma_{\pm} = 0.$$
(5.1)

The first equation, for example, integrates to

$$\sigma_{+}(t) = \sigma_{+}(0) e^{i\omega_{s}t} e^{-\frac{1}{2}\Gamma_{0}t} + \frac{1}{2}\Gamma_{0}(1 - iK_{1}) e^{+i\omega_{s}t} e^{-\frac{1}{2}\Gamma_{0}t} \int_{0}^{t} \sigma_{-}(t') e^{-i\omega_{s}t'} e^{+\frac{1}{2}\Gamma_{0}t'} dt'$$
(5.2)

in which ω'_s is the resonance frequency with total Lamb shift

$$\omega'_{\rm s} \equiv \omega_{\rm s} - \frac{1}{2} \Gamma_0 K_1 \tag{5.3}$$

and we have agreed to ignore the correction $-\pi^{-1}\omega_s^{-2}$ to K_1 . Note that σ_+ couples to σ_- and vice versa. However by successive iteration it is clear that the corrections oscillate at frequency $2\omega_s$ approximately under the integral sign. These terms may be dropped. This approximation is commonly called a rotating wave approximation (RWA) and it is the first time that such an approximation has been used in the theory. Thus we may take

$$\sigma_{+}(t) = \sigma_{+}(0) e^{-\frac{1}{2}\Gamma_{0}t} e^{i\omega_{s}t}.$$
(5.4)

We now calculate the autocorrelation function

$$R(t, t') \equiv \frac{1}{2} \langle \dots | \sigma_{+}(t) \sigma_{-}(t') + \sigma_{+}(t') \sigma_{-}(t) | \dots \rangle \rangle$$

$$\equiv \langle \dots | \sigma_{+}(0) \sigma_{-}(0) | \dots \rangle e^{-\frac{1}{2} \Gamma_{0}(t+t')} \cos[\omega_{s}'(t-t')].$$
(5.5)

which is symmetric in (t, t'). We note however that it can be written as

$$R(t, t') \equiv \langle \dots | \sigma_{+}(t') \sigma_{-}(t') | \dots \rangle e^{-\frac{1}{2}\Gamma_{0}(t-t')} \cos[\omega'_{s}(t-t')]$$

$$\equiv \rho_{ss}(t') e^{-\frac{1}{2}\Gamma_{0}(t-t')} \cos \omega'_{s}(t-t').$$
(5.6)

These results exemplify the quantum-mechanical regression theorem (Lax 1968): $\rho_{ss}(t')$ is the occupation number of the upper state at time t' and takes the form

$$\rho_{\rm ss}(t') = e^{-\Gamma_0 t'}.\tag{5.7}$$

In a system of many weakly interacting atoms in a steady state the occupation numbers $\rho_{ss}(t')$ can be averaged over all initial states t' and will be independent of t'. Since t' is chosen as the initial time, $\tau = t - t' \ge 0$. The power spectrum is therefore

$$\frac{\langle \rho_{ss}(t') \rangle_{av}}{\pi} \int_{0}^{\infty} e^{-\frac{1}{2}\Gamma_{0}\tau} \cos \omega_{s}'\tau \cos \omega\tau \,d\tau$$
$$= \frac{\langle \rho_{ss}(t') \rangle_{av}}{2\pi} \left(\frac{\Gamma_{0}}{(\omega_{s}' + \omega)^{2} + \frac{1}{4}\Gamma_{0}^{2}} + \frac{\Gamma_{0}}{(\omega_{s}' - \omega)^{2} + \frac{1}{4}\Gamma_{0}^{2}} \right).$$
(5.8)

Since the negative frequency part is negligible for $\omega \simeq \omega'_s$ the spectrum is Lorentzian and peaked at ω'_s as expected. The frequency ω'_s is shifted from ω_s by twice the Bethe level shift: this result completely solves a problem which could only be treated very artificially by other methods (Kroll 1965). In other respects the spectrum agrees with that obtained by Weisskopf and Wigner (1930) once their spectrum is renormalized[†].

Note that the expectation values of σ_+ and σ_- vanish if the initial state is $|s\rangle$ and the dipole moment

$$p\langle \cdots | \sigma_{+}(t) + \sigma_{-}(t) | \cdots \rangle = p\langle \cdots | \sigma_{x} | \cdots \rangle$$
(5.9)

vanishes throughout the motion. Thus radiation takes place through the autocorrelation function, and not through the dipole moment as in classical theories.

[†] The Weisskopf-Wigner spectrum contains ω in the numerator which must be replaced by ω_s : otherwise the integrated spectrum diverges logarithmically.

6. Conclusions

The results of this section support the view that the self-field theory developed in this paper is an applicable theory despite its internal inconsistencies.

We shall consider in further papers the absorption, emission and radiative level shifts in the case of a single two-level atom in 'weak' imposed coherent and incoherent fields using the self-field theory of this paper. We show later how the operator field theory can be applied with equal apparent success to multi-level single-atom problems and to many-atom problems.

Appendix

We here derive the result (3.5):

$$\int_{0}^{t} \ddot{p}(t') f_{\pm}(t-t') dt' = \mp i \frac{1}{2} \pi \ddot{p}(t) K_{1} + \pi \ddot{p}^{(\pm)}(t)$$
(3.5)

for all $t \gg \omega_s^{-1}$. Here $f_+(t)$ is given by (3.4):

$$f_{\pm}(t) \equiv \pm i \frac{e^{\mp i\omega_{max}t} - 1}{t}$$
(3.4)

and K_1 is given by (3.6). We have

$$\int_{0}^{t} \ddot{p}(t') f_{\pm}(t-t') dt' = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk p(k) (-ik)^{3} \int_{0}^{\omega_{\max}} \int_{0}^{t} e^{\mp i\omega(t-t') - ikt'} dt' d\omega$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk p(k) (-ik)^{3} \int_{0}^{\omega_{\max}} d\omega \frac{e^{-ikt} (1 \mp e^{\mp i(\omega \mp k)t})}{\pm i(\omega \mp k)}$$

$$= \mp \frac{i}{2\pi} \int_{-\infty}^{\infty} dk p(k) (-ik)^{3} e^{-ikt} \ln\left(\frac{\omega_{\max} \mp k}{|k|}\right)$$

$$\pm \frac{i}{2\pi} \int_{-\infty}^{\infty} ak p(k) (-ik)^{3} e^{-ikt} \int_{0}^{\omega_{\max}} \frac{e^{\mp i(\omega \mp k)t}}{\omega \mp k} d\omega \qquad (A.1)$$

$$\approx \mp i \ddot{p}(t) \ln \frac{\omega_{\max}}{\omega_{s}}$$

$$\pm \frac{\mathrm{i}}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k p(k) (-\mathrm{i}k)^3 \,\mathrm{e}^{-\mathrm{i}kt} \int_{0}^{\omega_{\max}} \frac{\mathrm{e}^{\pm\mathrm{i}(\omega\pm k)t}}{\omega\pm k} \,\mathrm{d}\omega. \tag{A.2}$$

We assume that p(k) is peaked about $\pm \omega_s$ where $0 < \omega_s \ll \omega_{max}$ and have used

$$\ln \frac{\omega_{\max} - \omega_s}{\omega_s} \simeq \ln \frac{\omega_{\max}}{\omega_s}.$$

Next

$$\int_{0}^{\omega_{\max}} \frac{e^{\mp i(\omega \mp k)t}}{\omega \mp k} d\omega = \int_{\mp kt}^{(\omega_{\max} \mp k)t} \frac{e^{\mp iu}}{u} du \simeq \int_{\mp kt}^{\infty} \frac{e^{\mp iu}}{u} du \qquad (t > 0) \quad (A.3)$$

for $\omega_{\text{max}} \gg |k|$. This is approximately

$$\int_{\mp kt}^{\infty} \frac{e^{\mp iu}}{u} du \simeq \begin{cases} -i\pi, & k > 0\\ 0, & k < 0 \end{cases} \text{ the case } (-) \\ 0, & k > 0\\ +i\pi, & k < 0 \end{cases} \text{ the case } (+)$$
(A.4)

for all times $t \gg |k|^{-1}$. Then (A.2) reduces to approximately

$$-i\ddot{p}(t)\ln\frac{\omega_{\max}}{\omega_s} + \frac{i(-i\pi)}{2\pi} \int_0^\infty p(k)(-ik)^3 e^{-ikt} dk \qquad (case (-))$$

$$+i\ddot{p}(t)\ln\frac{\omega_{\max}}{\omega_{s}} - \frac{i(i\pi)}{2\pi} \int_{-\infty}^{0} p(k)(-ik)^{3} e^{-ikt} dk \qquad (case (+)) \qquad (A.5)$$

for all times $t \gg \omega_s^{-1}$. This is just the result (3.5), namely

$$\mp \frac{i\pi}{2} \ddot{p}(t) \ln \frac{\omega_{\max}}{\omega_{s}} + \pi \ddot{p}^{(\pm)}(t).$$
(3.5)

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