Semiclassical Random Electrodynamics: Spontaneous Emission and the Lamb Shift

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It is often remarked that an explanation of spontaneous emission and the Lamb shift requires quantization of the electromagnetic field. Here, these two quantities are derived in a semiclassical formalism by use of second-order perturbation theory. The purpose of this report is not to argue the validity of QED but rather to develop a semiclassical approximation to QED that may nonetheless have certain computational advantages over QED. To this end, the vacuum of QED is simulated with a classical zero-point field (ZPF), and as a consequence, the resulting theory is entitled semiclassical random electrodynamics (SRED). In the theory, the atom is coupled to the ZPF and to its own radiation-reaction field through an electric dipole interaction. These two interactions add to produce exponential decay of excited states while they cancel each other to prevent spontaneous excitation of the ground state; the Lamb shift appears in the theory as an ac Stark shift induced by the ZPF. The spontaneous decay rate of an excited-state derived in SRED is equal to the Einstein A coefficient for that state, and the Lamb shift agrees with that of nonrelativistic QED. Moreover, SRED is shown to be useful for the numerical simulation of spontaneous decay.
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1. INTRODUCTION

Though few would argue that quantum electrodynamics is an accurate description of nature, the semiclassical theory of field–atom interactions still holds an important place in modern physics. One need only consider the Bloch equations and their utility in quantum optics and magnetic resonance to appreciate the vitality of semiclassical electrodynamics. Notwithstanding this utility, a failing of traditional semiclassical electrodynamics has been its inability to predict accurately spontaneous emission from first principles. There is nonetheless a feeling among many that semiclassical electrodynamics ought to be more successful in this regard; after all, QED indicates that vacuum fluctuations and radiation reaction are inextricably linked (and therefore that spontaneous decay can be interpreted as an effect driven by radiation reaction) and radiation reaction is a feature of classical electrodynamics.

Beyond the issue of classical field theory’s intrinsic capabilities, there are pragmatic reasons for pursuing a semiclassical description of spontaneous emission. Typically, spontaneous decay is incorporated into the classical theories of quantum optics through an exponential decay rate for atomic density matrix elements. However, there are processes such as quantum jumps and radiative decay in photonic bandgaps for which this approach is inappropriate. Although valid and successful theoretical methods exist for describing processes, their semiclassical interpretation might nevertheless lack utility. In this regard, the present work is meant as a step toward extending the reach of semiclassical methods to a broader class of radiative phenomena.

To this end, it is worth noting that no matter how one interprets the cause of spontaneous decay in QED, the vacuum plays a significant role. Consequently, if a semiclassical theory is to be successful in describing this phenomenon, then vacuum fluctuations should somehow appear in the theory. Here the vacuum of QED is simulated with a classical zero-point field (ZPF), and the consequences of this ZPF in semiclassical electrodynamics are explored. For clarity, the resulting theory is titled semiclassical random electrodynamics (SRED). I wish to state explicitly that I make no claims for SRED as a rival to QED; the present experimental situation provides no imperative for such a rival. If anything, low-to-high-energy experiments argue forcefully for the validity of quantized fields. Rather, SRED should be viewed as a semiclassical approximation to QED, which may nevertheless have computational advantages over QED with regard to the investigation of specific radiative problems. Additionally, SRED may prove useful as a touchstone for semiclassical approximations to quantum gravity.

In essence, SRED should be viewed as the semiclassical extension of what has come to be called stochastic electrodynamics (SED). In SED, one often approaches radiative problems through the Braffort–Marshall equation, a generalization of the Abraham–Lorentz equation of classical electrodynamics that includes the ZPF. The resultant theory thereby contains a fluctuating vacuum field along with the atom’s radiation-reaction field, and SED has been quite successful in accounting for various radiative processes, in particular, spontaneous emission and the Lamb shift. Alternatively, SRED is truly semiclassical in that the atom is described quantum mechanically in terms of its wave function, while the ZPF and the radiation-reaction fields are considered perturbations on the wave function’s evolution. As a consequence, one of the main difficulties for SRED that differentiates it from SED concerns the identification of a radiation-reaction operator for inclusion in the Schrödinger equation.

In Section 2 of this paper a quantum-mechanical operator for an atom’s radiation-reaction field is constructed by use of classical electrodynamics and operator hermiticity as guides. Then, in Section 3, the ZPF is described along with its electric dipole interaction with an atomic system. In Section 4 the influence of the ZPF and the radiation-reaction field on atomic state evolution are explored up to second order in perturbation theory. One of the major problems with standard semiclassical electrodynamics has always been its inability to obtain spontaneous decay without spontaneous excitation of the ground state. The analysis of Section 4 shows that, for an excited atomic eigenstate |m⟩, the average electric dipole interactions associated with the ZPF and the radiation-reaction field add to produce exponential decay of |m⟩, whereas they cancel to prevent spontaneous excitation of the ground state. The numerical value for the spontaneous decay rate obtained in SRED equals that of QED, and SRED predicts a radiative level shift for |m⟩ in agreement with the nonrelativistic Lamb shift of QED. The paper concludes with Section 5, in which a numerical method for applying SRED to more-general problems of radiative decay is discussed.

2. RADIATION REACTION

Classically, when an electrical charge accelerates it emits a field that acts back on the charge. This field is called the radiation-reaction field, E_{RR}, and in nonrelativistic, classical electrodynamics it is simply related to the rate at which the charge’s acceleration is changing:

$$E_{RR} = \frac{2e}{3c^3} \sigma_3^\alpha \tau = \frac{2}{3c^3} \sigma_3^\alpha \mu,$$

where $\mu$ is the electric dipole moment. As simple as this description seems, radiation reaction presents many thorny problems in classical electrodynamics. For example, in the Abraham–Lorentz derivation of Eq. (1) an electromagnetic mass enters the problem and becomes infinite for a point particle such as the electron. Additionally, radiation reaction in classical electrodynamics can lead to preacceleration, that is, acceleration of a charged particle before the application of any force. Here we shall not consider such problems but rather, in the spirit of Series, use Eq. (1) as a guide in the construction of an atomic operator whose expectation value is reminiscent of the classical radiation reaction field.

As a first step in transforming Eq. (1) into such an operator, it should be recognized that both $\mu$ and $\sigma_3^\alpha$ need to take on atomic operator characteristics. Inasmuch as $\mu$
is already a quantum-mechanical operator, the task is to define an atomic operator to represent the temporal derivative. To this end, we take advantage of the Schrödinger equation for the unperturbed wave function and the relationship that it provides between \( \dot{\varphi} \) and the unperturbed Hamiltonian. There is, however, some ambiguity in this relationship, as we can replace \( \dot{\varphi} \) with the Hamiltonian as it appears in the Schrödinger equation for the atomic wave function or with the Hamiltonian as it appears in the Schrödinger equation for the conjugate atomic wave function:

\[
i \hbar \dot{\varphi} \psi = \hat{H}_0 \psi = \frac{i\hbar}{\epsilon} \frac{\partial \hat{H}_0}{\partial \epsilon}, \quad (2a)
\]

\[-i \hbar \dot{\psi} \varphi = \langle \psi | \hat{H}_0 | \varphi \rangle = \frac{i\hbar}{\epsilon} \frac{\partial \langle \psi | \hat{H}_0 | \varphi \rangle}{\partial \epsilon}. \quad (2b)
\]

A proper description of spontaneous emission in SRED requires the latter replacement (i.e., Eq. (2b)) because the alternative choice leads to spontaneous excitation of the atomic ground state. Although it would lead us too far astray to speculate here on the implications of this choice, it is intriguing to recognize a possible connection to Wheeler's and Feynman's absorber theory, in which the seat of radiation reaction lies in fields that are traveling backward in time from distant absorbers.

Taking Eq. (2b) as an operator equivalent for \( \dot{\varphi} \) and maintaining the classical ordering of \( \hbar^2 \) and \( \mu \), one might attempt to define \( E_{RR} \) as \((-2i/3\hbar c^3)\hat{H}_0^2\mu\). Unfortunately, \( E_{RR} \) is then not Hermitian. However, if this expression for \( E_{RR} \) is averaged with its Hermitian conjugate, a Hermitian operator can be created. Thus we define the radiation-reaction field operator as

\[
E_{RR} = -\frac{i}{3\hbar c^3} (\hat{H}_0^2 \hat{\mu} - \hat{\mu} \hat{H}_0^2).
\]

For an atomic system described by the wave function \( |\varphi\rangle \) the expectation value of \( E_{RR} \) obtained from Eq. (3) is

\[
\langle \varphi | E_{RR} | \varphi \rangle = -\frac{i}{3\hbar c^3} \sum_n \langle \varphi | \hat{H}_0^2 | n \rangle \langle n | \hat{\mu} | \varphi \rangle - \langle \varphi | \hat{\mu} | n \rangle \langle n | \hat{H}_0^2 | \varphi \rangle,
\]

(4)

where \( \{n\} \) are eigenstates of the unperturbed Hamiltonian. If \( |\varphi\rangle \) corresponds to one of these eigenstates, for example \( |m\rangle \), then it is straightforward to show that \( \langle m | E_{RR} | m \rangle = 0 \). Thus atoms in eigenstates of the unperturbed Hamiltonian do not emit a radiation-reaction field. Alternatively, if \( |\varphi\rangle \) corresponds to a superposition of eigenstates that can be coupled by an electric dipole interaction, for example \( |\varphi\rangle = (1/\sqrt{2})(|1\rangle \exp(-i\omega_1 t) \pm |2\rangle \exp(-i\omega_2 t)) \), then under the assumption that

\[
|\omega_2| > \sqrt{3} |\omega_1|,
\]

\[
|\omega_2| = \omega_2 = \omega_1 - \omega_1
\]

(e.g., \(|1\rangle \) is the ground state so that \( \omega_1 = 0 \)), the expectation value for the radiation-reaction field becomes

\[
\langle \varphi | E_{RR} | \varphi \rangle = \frac{|\mu_{21}|^2 \omega_2^3}{3\epsilon} \sin(\omega_2 t + \theta), \quad (5b)
\]

where \( \mu_{21} = |\mu_{21}|e^{i\theta} \). This is essentially the classical expression for an oscillating dipole's radiation-reaction field, and it indicates that radiation-reaction fields arise when atoms are in superposition states of the unperturbed Hamiltonian. Thus Eq. (3) can be taken as a reasonable quantum-mechanical operator for the radiation-reaction field.

Although it is to be noted that Eq. (5b) is half of the magnitude of the classical value, it should also be recognized that \( E_{RR} \) is not gauge invariant because of its dependence on \( \hat{H}_0 \). Thus the radiation-reaction field operator of Eq. (3) is simply a calculational tool, not a true physical quantity. Consequently, any rigorous comparison between the present quantum-mechanical version of the radiation-reaction field and its classical analog must be treated cautiously.

For future reference we note that if \( V^{RR} \) is defined as the perturbation of the atom that is due to a dipole coupling with its radiation-reaction field; then Eq. (5) yields

\[
V^{RR} = -\mu \cdot E_{RR} = -\frac{i}{3\hbar c^3} (\mu \cdot \hat{H}_0^2 \mu - \mu \cdot \hat{\mu} \hat{H}_0^2).
\]

(6)

3. CLASSICAL ZERO-POINT FIELD

As outlined by Boyer, Maxwell's equations are valid for a variety of boundary conditions. Standard classical electrodynamics arises when the boundary conditions are chosen such that the fields in vacuum are zero, and only retarded fields are allowed. Random electrodynamics arises when the choice of boundary conditions consists of random electromagnetic radiation with a Lorentz invariant spectrum (i.e., the classical ZPF), and again only retarded fields are considered. Whereas the "proper" choice for boundary conditions will often lead to debate, it should be noted that according to Boyer "a consistently classical treatment of thermal radiation leads to the natural introduction of temperature-independent fluctuating radiation in the universe." Here, questions regarding the value of various boundary conditions for classical electrodynamics will be ignored. We simply consider an atom enclosed in a large conducting box of length \( L \), filled with a classical ZPF, as a reasonable approximation to an atom interacting with the vacuum of QED. The ZPF vector potential \( A_0 \) within the box can then be written as a modal expansion of random plane waves:

\[
A_0 = L^{-3/2} \sum_{k_\parallel} \epsilon_{k_\parallel} \langle c_{k_\parallel} \exp[i(k \cdot r - \omega_0 t)]
\]

\[
+ \epsilon_{k_\parallel}^* \exp[-i(k \cdot r - \omega_0 t)].
\]

(7)

Here \( \epsilon_{k_\parallel} \) is a modal polarization vector, \( c_{k_\parallel} \) is a random complex amplitude for the wave, \( k_\parallel = 2\pi n/L \) (\( n \), \( = 0, \pm 1, \pm 2, ... \)), and
\[ \mathbf{k} \cdot \mathbf{k} = \left( \frac{2\pi}{L} \right)^2 [n_x^2 + n_y^2 + n_z^2] = \left( \frac{\omega_k}{c} \right)^2, \quad (8) \]

where the modal index \( s \) corresponds to the triplet of numbers \([n_x, n_y, n_z]\). Taking the derivative of Eq. (7) and replacing the sum over wave vectors by a sum over modes, we get for the zero-point electric field

\[
E_0 = \frac{1}{\sqrt{2} \mathcal{V}} \sum_{s_k} \left[ \hat{e}_{s_k} \exp [i(\mathbf{k}_s \cdot \mathbf{r} - \omega_k t)] + i \omega_c \hat{e}_{s_k} \exp [-i(\mathbf{k}_s \cdot \mathbf{r} - \omega_k t)] \right].
\]

(9)

The complex modal amplitudes can be written in terms of a scale factor \( c_{s_k} \) and a zero-mean complex random variable \( z_{s_k} \):

\[ c_{s_k} = c_{s_k} z_{s_k}. \]

Then, expressing \( z_{s_k} \) in terms of two independent, unit-variance, real-valued random variables \( u_{s_k} \) and \( v_{s_k} \) with zero mean such that

\[ \mathbb{E} [u_{s_k} v_{s_k}] = \mathbb{E} [u_{s_k} u_{s_k} v_{s_k}] = \delta_{s_k} \delta_{s_k}, \]

we have

\[ z_{s_k} = \frac{1}{\sqrt{2}} (u_{s_k} - i v_{s_k}), \quad (10a) \]

\[ \mathbb{E} [z_{s_k} z_{s_k}^*] = \delta_{s_k} \delta_{s_k}, \quad (10b) \]

\[ \mathbb{E} [z_{s_k} z_{s_k}^*] = \mathbb{E} [z_{s_k} z_{s_k}^*] = 0, \quad (10c) \]

where \( \mathbb{E} [\cdot] \) indicates an ensemble average.

To evaluate the scale factor one can use Eqs. (9) and (10) to show that

\[ U_0 = \frac{1}{4\pi} \int \mathbb{E} [E_0]^2 d^3 r = \sum_{s_k} \frac{(\omega_c c_{s_k})^2}{2 \pi c^2}. \quad (11) \]

Lorentz invariance of the ZPF spectrum requires that the energy of each mode be proportional to \( \omega_k \). Consequently, the scale factor must be inversely proportional to \( \sqrt{\omega_k} \), and for agreement with the experimental results for blackbody radiation the proportionality constant must be related to Planck's constant \( h \). In this way it can be shown that

\[ c_{s_k} = \left( \frac{\pi \hbar / L^3}{\mathcal{V}} \right) \Rightarrow U_0 = \sum_{s_k} \frac{\hbar \omega_k}{2}. \quad (12) \]

With the aid of Eqs. (10a) and (12), the electric field vector of the ZPF now becomes

\[
E_0 = \left[ (2\pi L^3)^{1/2} \sum_{s_k} \hat{e}_{s_k} \sqrt{\omega_k} u_{s_k} \exp [i(\mathbf{k}_s \cdot \mathbf{r} - \omega_k t)] \right.
+ (2\pi L^3)^{1/2} \sum_{s_k} \hat{e}_{s_k} \sqrt{\omega_k} v_{s_k} \cos (\omega_k t)
- u_{s_k} \sin (\omega_k t)]
\]

\[
= \left[ (2\pi L^3)^{1/2} \sum_{s_k} \hat{e}_{s_k} \sqrt{\omega_k} e_{s_k} \exp [i(\mathbf{k}_s \cdot \mathbf{r} - \omega_k t)] \right.
- u_{s_k} \sin (\omega_k t)]
\]

(13)

Note that this expression for the ZPF is equivalent to that recently discussed by Ibison and Haisen.25

To explore the interaction of the ZPF with a quantum system we consider an atom conveniently placed at the origin of the coordinate system and make the dipole approximation (i.e., for the modes of interest, \( \mathbf{k}_s \cdot \mathbf{r} \ll 1 \)). Then, in the vicinity of the atom,

\[ E_0 = \left[ (2\pi h / L^3)^{1/2} \sum_{s_k} \hat{e}_{s_k} \sqrt{\omega_k} [e_{s_k} \cos (\omega_k t)
+ u_{s_k} \sin (\omega_k t)] \right. \]

\[ + \left. u_{s_k} \sin (\omega_k t)] \right. \]

(14a)

or, equivalently,

\[ E_0 = \left[ (2\pi h / L^3)^{1/2} \sum_{s_k} \hat{e}_{s_k} \sqrt{\omega_k} [e_{s_k} \exp (i \omega_k t)
- u_{s_k} \sin (\omega_k t)] \right. \]

\[ - \left. u_{s_k} \sin (\omega_k t)] \right. \]

(14b)

Defining \( V^0 \) as the perturbation of the atom owing to dipole coupling with the ZPF, we have

\[ V^0(t) = -\mathbf{\mu} \cdot E_0 = -i[(\pi h / L^3)^{1/2} \sum_{s_k} \mathbf{\mu} \cdot \hat{e}_{s_k}
\]

\[ \times \sqrt{\omega_k} [e_{s_k} \exp (i \omega_k t) - u_{s_k} \sin (\omega_k t)]]. \]

(15)

Later we shall have need for \( \mathbb{E} [V^0_{mn}(t)] \) as well as for \( \mathbb{E} [V^0_{mn}(t) V^0_{mp}(t')] \), where \( V^0_{mn} \) is defined as \( (m|V^0|n) \).

Clearly, from the mean-zero characteristic of \( e_{s_k} \),

\[ \mathbb{E} [V^0_{mn}(t)] = 0. \]

(16)

Computing the second-order correlation function for the perturbation yields

\[ \mathbb{E} [V^0_{mn}(t) V^0_{mp}(t')] \]

\[ = -\frac{\pi h}{L^3} \sum_{s_k} \mathbb{E} [e_{s_k} \exp (i \omega_k t) - u_{s_k} \sin (\omega_k t)] \times \mathbb{E} [e_{s_k} \exp (i \omega_k t) - u_{s_k} \sin (\omega_k t)] \]

\[ \times \left[ \exp [-i \omega_k (t - t')] - \exp [i \omega_k (t - t')] \right] \]

(17)

Multiplying out the terms in the ensemble average and employing Eqs. (10) yields

\[ \mathbb{E} [V^0_{mn}(t) V^0_{mp}(t')] \]

\[ = \frac{\pi h}{L^3} \sum_{s_k} \mathbb{E} [e_{s_k} \exp (i \omega_k t) - u_{s_k} \sin (\omega_k t)] \times \mathbb{E} [e_{s_k} \exp (i \omega_k t) - u_{s_k} \sin (\omega_k t)] \]

\[ \times \exp [-i \omega_k (t - t')] + \exp [i \omega_k (t - t')] \]

(18)

or

\[ \mathbb{E} [V^0_{mn}(t) V^0_{mp}(t')] \]

\[ = \frac{\pi h}{L^3} \sum_{s_k} \mathbb{E} [e_{s_k} \exp (i \omega_k t) - u_{s_k} \sin (\omega_k t)] \times \left[ \exp [-i \omega_k (t - t')] + \exp [i \omega_k (t - t')] \right] \]

(19)

4. PERTURBATION THEORY

A. Evolution of the Wave Function

We now consider the Schrödinger equation for an atom in the presence of the ZPF and the radiation-reaction field,

\[ i \hbar \frac{\partial |\Psi\rangle}{\partial t} = [H_0 + V_R R + V^0(t)] |\Psi\rangle, \]

(20)

and expand the atom's wave function in terms of the unperturbed basis wave functions:
\[ |\psi\rangle = \sum_n a_n(t) |n\rangle \exp(-i \omega_n t). \] (21)

Then in standard fashion we obtain an equation for the expansion coefficients:
\[ \dot{a}_n(t) = -\frac{i}{\hbar} \sum_j \left[ \langle n | V_{n}^{t} | j \rangle \right] a_j(t) \exp(i \omega_j t), \] (22)

where \( \omega_{nj} = \omega_n - \omega_j \). Integrating and defining \( a_n^0 \) as \( a_n(0) \), we can also write Eq. (22) as
\[ a_n(t) = a_n^0 - \frac{i}{\hbar} \int_0^t \left[ V_{nj}^{RR} + V_{nj}^0(t') \right] a_j(t') \exp(i \omega_{nj} t') dt'. \] (23)

B. Wave-Function Evolution Owing to Radiation Reaction

Defining the first term on the right-hand side of Eq. (22) as \( a_n^{RR}(t) \), we have, after substituting from Eq. (6),
\[ \dot{a}_n^{RR}(t) = \frac{1}{3 \hbar c^3} \sum_j a_j(t) \times \langle n | (\mu \cdot H_0^3 \mu - \mu \cdot \mu H_0^3) | j \rangle \exp(i \omega_{nj} t). \] (24)

Note that the radiation-reaction field forces an orientation on the atom’s dipole moment. Taking an ensemble average of Eq. (24) over the ZPF, and defining \( b_n(t) \) as \( \mathcal{E}[a_n(t)] \), yields
\[ \dot{b}_n^{RR}(t) = \frac{1}{3 \hbar c^3} \sum_{np} b_j(t) \mu_{np} (p | H_0^3 | q) \mu_{qj} - \mu_{np} \mu_{pq} (q | H_0^3 | j) \exp(i \omega_{np} t). \] (25)

or, when the Hamiltonian terms are evaluated,
\[ \dot{b}_n^{RR}(t) = \frac{1}{3 \hbar c^3} \sum_{np} b_j(t) \mu_{np} \mu_{pj} (\omega_p^3 - \omega_n^3) \exp(i \omega_{np} t). \] (26)

We now ignore the rapidly rotating terms in Eq. (26) [i.e., \( \exp(i \omega_{np} t) \rightarrow 1 \)] and recognize that the sum in Eq. (26) will be dominated by those states \( |p\rangle \) that best satisfy the validity condition for the radiation-reaction field operator, inequality (5a). Thus we approximate \( (\omega_p^3 - \omega_n^3) \) with \( \omega_{np}^3 \) and obtain
\[ \dot{b}_n^{RR}(t) = \frac{\dot{b}_n(t)}{3 \hbar c^3} \sum_p |\mu_{np}|^2 \omega_{np}^3. \] (27)

C. Wave-Function Evolution Owing To The Zero-Point Field

We now define the second term on the right-hand side of Eq. (22) as \( \dot{a}_n^{ZPF}(t) \):
\[ \dot{a}_n^{ZPF} = -\frac{i}{\hbar} \sum_j V_{nj}^0(t) a_j(t) \exp(i \omega_j t), \] (28)

and substituting from Eq. (23) yields
\[ \dot{a}_n^{ZPF}(t) = -\frac{i}{\hbar} \sum_n V_{mn}^0(t) \exp(i \omega_{mn} t) \times \left[ a_n^0 - \frac{i}{\hbar} \sum_j V_{nj}^{RR} a_j(t) \right] \times \exp(i \omega_{nj} t) dt'. \] (29)

We can now ensemble average Eq. (29) over the ZPF, so that
\[ \dot{b}_n^{ZPF}(t) = -\frac{1}{\hbar^2} \sum_{nj} \exp(i \omega_{mn} t) \times \int_0^t \langle V_{mn}^0(t) V_{nj}^0(t') \rangle b_j(t') \exp(i \omega_{nj} t') dt'. \] (30)

In writing Eq. (30) we have taken advantage of the fact that causality requires \( a_j(t') \) to be independent of \( V_{mn}^0(t) \) for \( t' < t \), and we have assumed that the evolution of the ZPF is unrelated to the atom’s dynamics. Thus we conclude that \( a_j(t') \) and \( V_{mn}^0(t) \) are independent of each other for \( t' < t \). Moreover, inasmuch as the ZPF perturbation is weak in the limit of a large volume enclosure, to second order in perturbation theory we may make a decorrelation approximation between \( V_{nj}^0(t') \) and \( a_j(t') \) [i.e., the ZPF correlation time is much less than \( \hbar^{-1} V_{nj}^0(t')^{-1} \)]. In this way we obtain
\[ \langle V_{mn}^0(t) V_{nj}^0(t') \rangle = \langle V_{mn}^0(t) \rangle \langle V_{nj}^0(t') \rangle \langle a_j(t') \rangle \]
\[ = \langle V_{mn}^0(t) V_{nj}^0(t') \rangle b_j(t'). \] (31)

To second order in perturbation theory we approximate \( b_j(t') \) with its value at \( t \) and substitute for the correlation function from Eq. (19). Equation (30) then becomes
\[ \dot{b}_n^{ZPF}(t) = \frac{\pi}{\hbar^2} \sum_{nj} b_j(t) \exp(i \omega_{mn} t) \times \int_0^t \left[ \sum_{n'j} \omega_{n'n} (m | \mu \cdot \hat{e}_{n'n} | n') (n | \mu \cdot \hat{e}_{n'n} | j) \right] \times \left[ \exp[-i \omega_{n'}(t - t')] + \exp[i \omega_{n'}(t - t')] \right] \times \exp(i \omega_{nj} t') dt'. \] (32)

As we discussed above, the dipole moment of the atom is aligned along the direction of the radiation-reaction field. We define this orientation as the \( z \) axis of the coordinate system
\[ \sum_k \hat{e}_{nk} \hat{e}_{nk} = 1 - \frac{k_z}{|k|^2}, \] (33)
so Eq. (32) becomes
\[ \dot{b}_m^{\text{ZPF}}(t) = -\frac{\pi}{\hbar L^2} \sum_{nj} b_j(t) \exp(i\omega_{mn}t) \mu_{mn}\mu_{nj} \]
\[ \times \left[ \int_0^t \left( \sum_{r} \omega_r \sin^2(\theta_r) \exp(-i\omega_r(t-t')) \right) \right. \]
\[ + \left. \exp(i\omega_r(t-t')) \right] \exp(i\omega_{nj}t') dt'. \]  
(34)

where $\theta_r$ is the polar angle between the wave vector for the $r$th mode and the $z$ axis as defined by the radiation-reaction field. If we now allow the volume of the box enclosing the atom to go to infinity,
\[ \sum_{i} = \frac{L^3}{8\pi^3} \int d^3k, \]  
(35)
Eq. (34) becomes
\[ \dot{b}_m^{\text{ZPF}}(t) = -\frac{1}{3\pi\hbar c^2} \sum_{nj} b_j(t) \exp(i\omega_{mn}t) \mu_{mn}\mu_{nj} \]
\[ \times \left[ \int_0^t \left( \int_0^\infty \int_0^{2\pi} \omega^3 \left[ \exp(-i\omega(t-t')) \right. \right. \right. \]
\[ + \exp(i\omega(t-t')) \left. \right] \sin^3(\theta)d\theta d\phi d\omega \right. \]
\[ \left. \times \exp(i\omega_{nj}t') \right] dt'. \]  
(36)

Integrating over $\theta$ and $\phi$ then yields
\[ \dot{b}_m^{\text{ZPF}}(t) = -\frac{1}{3\pi\hbar c^2} \sum_{nj} b_j(t) \exp(i\omega_{mn}t) \mu_{mn}\mu_{nj} \]
\[ \times \left[ \int_0^t \left( \int_0^\infty \omega^3 \left[ \exp(-i\omega(t-t')) \right. \right. \right. \]
\[ + \exp(i\omega(t-t')) \left. \right] d\omega \right] \exp(i\omega_{nj}t') dt'. \]  
(37)

Integrating over $\omega$, \[ \int_0^\infty \omega^3 \exp(-i\omega(t-t')) d\omega = \frac{\pi \omega^3}{6} \exp(-i\omega(t-t')) d\omega, \]  
(38a)

or, when we rearrange the orders of integration,
\[ \dot{b}_m^{\text{ZPF}}(t) = -\frac{1}{3\pi\hbar c^2} \sum_{nj} b_j(t) \exp(i\omega_{mn}t) \mu_{mn}\mu_{nj} \]
\[ \times \left[ \int_0^\infty \omega^3 \left[ \exp(-i\omega t) \right. \right. \right. \]
\[ \left. \int_0^t \exp(i(\omega + \omega_{nj})t') dt' \right] d\omega, \]  
(38b)

\[ \dot{b}_m^{\text{ZPF}}(t) = -\frac{1}{3\pi\hbar c^2} \sum_{nj} b_j(t) \exp(i\omega_{mn}t) \mu_{mn}\mu_{nj} \]  

\[ \times \exp(i\omega_{mn}t) \mu_{mn}\mu_{nj} \]  

\[ \text{Int}(1) = \lim_{\omega \to 0} \int_0^\infty \omega^3 \exp(-i\omega t) \]  
\[ \times \left[ \int_0^t \exp(at' + i(\omega + \omega_{nj})t') dt' \right] \]  
\[ \times \int_0^\infty d\omega = \frac{\pi \omega^3}{6} \exp(-i\omega(t-t')) d\omega, \]  
(39)

which on integration with respect to the temporal variable yields
\[ \text{Int}(1) = \lim_{\omega \to 0} \left[ \exp[(a + i\omega) t)] \int_0^\infty \frac{\omega^3 d\omega}{a + i(\omega + \omega_{nj})} \right. \]
\[ - \left. \int_0^\infty \frac{\omega^3 \exp(-i\omega t) d\omega}{a + i(\omega + \omega_{nj})} \right]. \]  
(40)

Note that both integrals will be dominated by large $\omega$. However, in the second integral these terms oscillate rapidly and quickly average to zero. Thus
\[ \text{Int}(1) = \lim_{\omega \to 0} \left[ \exp[(a + i\omega) t)] \right. \]
\[ \times \int_0^\infty \frac{\omega^3 d\omega}{a^2 + (\omega + \omega_{nj})^2}. \]  
(41)

As discussed by Heitler,27 the limit of the real term yields a Dirac delta function, whereas that of the imaginary term can be expressed in terms of a principal value:
\[ \text{Int}(1) = \exp(i\omega_{nj} t) \left[ \pi \int_0^\infty \omega^3 \delta(\omega + \omega_{nj}) d\omega \right. \]
\[ \left. - i\beta \int_0^\infty \frac{\omega^3 d\omega}{(\omega + \omega_{nj})^2}. \right] \]  
(42)

In a similar fashion the second integral is evaluated and yields
\[ \text{Int}(2) = \exp(i\omega_{nj} t) \left[ \pi \int_0^\infty \omega^3 \delta(\omega - \omega_{nj}) d\omega \right. \]
\[ \left. + i\beta \int_0^\infty \frac{\omega^3 d\omega}{(\omega - \omega_{nj})^2}. \right] \]  
(43)

Combining Eqs. (42) and (43) in Eq. (38b), we get
\[ \dot{b}_m^{\text{ZPF}}(t) = -\frac{1}{3\pi\hbar c^2} \sum_{nj} b_j(t) \exp(i\omega_{mn}t) \mu_{mn}\mu_{nj} \]
\[ \times \left[ \int_0^\infty \omega^3 \delta(\omega + \omega_{nj}) + \delta(\omega - \omega_{nj}) \right] d\omega \]
\[ - i\Delta, \]  
(44)

where the imaginary term is defined as
\[ \Delta = \frac{1}{3\pi\hbar c^2} \sum_{nj} b_j(t) \exp(i\omega_{mn}t) \mu_{mn}\mu_{nj} \]
\[ \times \left[ \int_0^\infty \left[ \frac{\omega^3}{\omega - \omega_{nj}} - \frac{\omega^3}{\omega + \omega_{nj}} \right] d\omega \right]. \]  
(45)
and leads to a radiative level shift induced by the ZPF.

Recognizing that the rapidly oscillating terms in Eqs. (44) and (45) quickly average to zero, we have

\[
\hat{b}_{\text{ZPF}}(t) = -\frac{b_{\text{m}}(t)}{3\hbar c^2} \sum_n |\mu_{mn}|^2 \int_0^\infty \omega^3 \delta(\omega - \omega_{nm}) d\omega \\
+ \int_0^\infty \frac{\omega^2 \delta(\omega - \omega_{nm}) d\omega}{\omega^2 - \omega_{nm}^2} - i b_{\text{m}}(t) \Delta',
\]

(46a)

where

\[
\Delta' = \frac{2}{3 \pi \hbar c^2} \sum_n \omega_{nm} |\mu_{mn}|^2 \int_0^\infty \frac{\omega^3 d\omega}{\omega^2 - \omega_{nm}^2}.
\]

(46b)

Note that in Eq. (46a) the integrals are only over positive values of \(\omega\). Thus, depending on the energetic relationship between |\(n\rangle\) and |\(m\rangle\), the delta functions will cause only one of the two integrals to be nonzero. Thus

\[
\hat{b}_{\text{ZPF}}(t) = -\frac{b_{\text{m}}(t)}{3\hbar c^2} \sum_n |\mu_{mn}|^2 \begin{cases} \\
\omega_{nm}^3 & \omega_m > \omega_n \\
-\omega_{nm}^3 & \omega_n > \omega_m
\end{cases}

- i b_{\text{m}}(t) \Delta'.
\]

(47)

D. Spontaneous Decay

Combining Eqs. (47) and (27), and ignoring the radiative level shift term for the moment as this has no influence on decay, we find for the evolution of the eigenfunction coefficients that

\[
\hat{b}_{\text{m}}(t) = -\frac{b_{\text{m}}(t)}{3\hbar c^2} \\
\times \sum_n |\mu_{mn}|^2 \begin{cases} \\
\omega_{nm}^3 & \omega_m > \omega_n \\
-\omega_{nm}^3 & \omega_n > \omega_m
\end{cases},
\]

(48a)

or

\[
\hat{b}_{\text{m}}(t) = -\frac{2b_{\text{m}}(t)}{3\hbar c^2} \sum_{n<m} |\mu_{mn}|^2 \omega_{nm}^3.
\]

(48b)

Defining \(P_m\) as the probability for finding the atom in the excited state |\(m\rangle\) (i.e., |\(b_{\text{m}}|^2\)), we obtain an exponential decay equation for this probability:

\[
\frac{dP_m}{dt} = -\Gamma_m P_m,
\]

(49a)

where

\[
\Gamma_m = \frac{4}{3 \pi \hbar c^2} \sum_{n<m} |\mu_{mn}|^2 \omega_{nm}^3.
\]

(49)

This, of course, is just the Einstein A coefficient for the spontaneous decay rate of |\(m\rangle\). Note that if we define \(1\) as the atomic ground state, then \(\Gamma_1\) is identically zero because there are no states of lower energy. Essentially, in SRED excited states decay exponentially because the radiation reaction and vacuum pathways add constructively. Spontaneous excitation of the ground state does not occur, because in that case these two pathways would interfere destructively. Although many authors have recognized this interference between radiation reaction and the vacuum in QED, here we find it again in the context of a semiclassical description of spontaneous decay.

E. Lamb Shift

Returning now to the radiative level shift described by Eq. (46b), we note that the integral is strongly influenced by the very high-frequency ZPF modes:

\[
\Delta' = \frac{2}{3 \pi \hbar c^2} \sum_n \omega_{nm} |\mu_{mn}|^2 \int_0^\infty \omega d\omega = \Delta_0.
\]

(50)

Employing the Thomas–Reiche–Kuhn sum rule \(^{28}\) and remembering that \(|\mu_{mn}| = e|x_m|^2\), we can rewrite relation (50) as

\[
\hbar \Delta_0 = \int \frac{\hbar e^2}{3 \pi m^2 n^3} \frac{d\omega}{\omega}. \quad (51)
\]

This, however, is just the average value of the interaction energy between a free electron and the z component of the ZPF, as can easily be shown from Eqs. (7) and (33) and expression (35):

\[
\hbar \Delta_0 = \frac{1}{2} \int_0^\infty \frac{e^2}{2mc^2} (|\Delta_0|^2) d\omega.
\]

(52)

Because this energy is the same for all levels, it does not give rise to an observable shift and so should be subtracted from the shift of Eq. (46b). Of course this subtraction is just the well-known mass renormalization of QED.12,29

The observable radiative level shift in SRED is thus

\[
\Delta = \frac{2}{3 \pi \hbar c^2} \sum_n \omega_{nm} |\mu_{mn}|^2 \int_0^\infty \frac{\omega d\omega}{\omega^2 - \omega_{nm}^2},
\]

(53)

and, when the integral is evaluated with a high-frequency cutoff of \(mc^2/\hbar\), the result is the standard Lamb-shift formula of nonrelativistic QED:

\[
\Delta = \frac{2}{3 \pi \hbar c^2} \sum_n \omega_{nm} |\mu_{mn}|^2 \ln \left( \frac{m^2}{|E_n - E_m|} \right). \quad (54)
\]

In SRED, as can be argued in QED,12 the Lamb shift is seen as an ac Stark shift of an atomic-energy level induced by the ZPF.30

5. NUMERICAL SIMULATION OF SPONTANEOUS DECAY

One of the attractive features of SRED with regard to computation concerns the representation of the vacuum as an easily simulated classical ZPF. A potential utility of SRED may therefore reside in the numerical simulation of spontaneous decay in an arbitrary vacuum (e.g., a cavity).31 Unfortunately, the description of spontaneous decay in SRED as formulated above requires an expres-
sion for radiation reaction, and in an arbitrary vacuum it may be difficult to arrive at a workable operator representation of radiation reaction for inclusion in the Schrödinger equation. To circumvent this problem, in this section we appeal to the fluctuation-dissipation theorem in order to remove the explicit reference to radiation reaction from the equations that describe a wave function's evolution. As will be shown below, for the vacuum of free space the procedure provides an accurate numerical simulation of the sodium $3p_{10}$ state's radiative decay.

For simplicity we consider the case of a two-level atom, where $\mathcal{E}_1 = 0$ and $\mathcal{E}_2 = \hbar \omega_{21}$, and we take advantage of the wave function's normalization to write $|a_2|^2 = 1 - |a_1|^2$. Thus with regard to spontaneous decay we need only consider a second-order perturbation solution to

\begin{equation}
\dot{a}_2 = \dot{a}_2^{\text{RR}} + \dot{a}_2^{\text{ZPF}}.
\end{equation}

(55)

As the previous analysis demonstrates, if Eq. (55) were to be averaged over the vacuum field then each term on the right-hand-side would contribute equally to the decay of $a_2$; that is,

\begin{equation}
\text{Re}(\dot{a}_2^{\text{RR}}) = \text{Re}(\dot{a}_2^{\text{ZPF}}) = -\frac{A}{4} (a_2(t)).
\end{equation}

(56)

As many authors have stated, this equality is to be interpreted as a manifestation of the fluctuation-dissipation theorem\textsuperscript{32} that is, the wave function's evolution as a result of radiation reaction corresponds to the atom's dissipative response to the random fluctuating force of the vacuum field. Physically, then, Eq. (56) would suggest that radiation reaction can be eliminated from perturbation theory by the replacement of terms that correspond to radiation reaction with terms that correspond to the vacuum field, so long as there is a proper accounting of each term's relative sign. Following this procedure for Eq. (55), we obtain $\dot{a}_2 = 2a_2^{\text{ZPF}}$ or, using Eq. (29),

\begin{align}
\dot{a}_2(t) &= \frac{2i}{\hbar} \mu_{21} \dot{\mathcal{E}}_2 \cdot \mathbf{E}_0(t) \exp(i \omega_{21} t) \\
&\times \left[ a_1^* \frac{1}{\hbar} \int_0^{t'} \left[ a_1 \dot{\mathcal{E}}_2 \cdot \mathbf{E}_0(t') \right] \exp(-i \omega_{21} t') dt' \right].
\end{align}

(57)

As our interest is in the atom's spontaneous decay, we can perform a coarse-grain averaging of Eq. (57) over a time scale $\tau$ that is long compared with the correlation time of the vacuum field but short compared with the wave function's evolution. Then, with

\begin{equation}
(Y(t))_\tau = \frac{1}{\tau} \int_{t-\tau/2}^{t+\tau/2} Y(t) dt',
\end{equation}

(58)

Eq. (57) becomes

\begin{equation}
\dot{a}_2(t) = -\frac{2|\mu_{21}|^2}{\hbar^2} \int_0^t (\exp(i \omega_{21} t') \dot{\mathcal{E}}_2 \cdot \mathbf{E}_0(t')) \dot{a}_2(t') dt',
\end{equation}

(59)

Substituting for $\epsilon_\delta \cdot \mathbf{E}_0(t)$ from Eq. (15), defining $\delta_\sigma$ as $\omega_{\sigma} - \omega_{21}$, and ignoring the rapidly rotating terms of $\omega_{\sigma} + \omega_{21}$, we obtain

\begin{align}
\dot{a}_2(t) &= \frac{2 \pi |\mu_{21}|^2}{\hbar L^3} \sum_{\delta_\sigma \neq 0} \left[ z_{\sigma \lambda} z_{\rho \lambda}^* \sqrt{\omega_{\sigma} \omega_{\rho}} \left( \epsilon_{\sigma \lambda} \cdot \epsilon_{\rho \lambda} \right) \right] \\
&\times \int_0^t (\exp(-i \delta_\sigma t') \exp(i \delta_\rho t'), a_2(t')) dt'.
\end{align}

(60)

Because of the independent nature of the $z_{\sigma \lambda}$, as the vacuum field mode spacing $\Delta \omega$ decreases we expect that

\begin{equation}
\lim_{\Delta \omega \to 0} \sum_{\delta_\sigma} z_{\sigma \lambda}^* z_{\rho \lambda} = |z_{\sigma \lambda}|^2 \delta_\sigma \delta_\rho.
\end{equation}

(61)

Thus the sum over vacuum field modes in Eq. (60) can be approximated with

\begin{align}
\dot{a}_2(t) &= -\frac{2 \pi |\mu_{21}|^2}{\hbar L^3} \sum_{\delta_\sigma} \left[ |z_{\sigma \lambda}|^2 \omega_{\delta_\sigma} \right] \\
&\times \int_0^t (\exp(-i \delta_\sigma t - t'), a_2(t')) dt'.
\end{align}

(62)

Making the second-order perturbation theory replacement of $a_2(t')$ with $a_2(t')$ on the right-hand side of relation (62) and evaluating the integral then yield

\begin{align}
\dot{a}_2(t) &= -\frac{2 \pi |\mu_{21}|^2}{\hbar L^3} a_2(t) \sum_{\delta_\rho} \left[ |z_{\rho \lambda}|^2 \omega_{\delta_\rho} \right] \\
&\times \left[ 1 - \exp(-i \delta_\rho t) \right].
\end{align}

(63)

For the purposes of computational convenience we now set $|z_{\sigma \lambda}|^2 = |z_{\rho \lambda}|^2$, recognizing that doing so should have little effect on a numerical simulation of spontaneous decay so long as the number of modes used in the computation is large. The sum of polarization terms in Eq. (63) can now be easily handled as in Eq. (33) and then averaged over $4\pi$ steradians, so that

\begin{align}
\dot{a}_2(t) &= \frac{4 \pi |\mu_{21}|^2}{3 \hbar L^3} a_2(t) \sum_{\delta_\rho} \left[ |z_{\rho \lambda}|^2 \omega_{\delta_\rho} \right] \\
&\times \left[ 1 - \exp(-i \delta_\rho t) \right].
\end{align}

(64)

We can further simplify Eq. (64) by recognizing that the volume of the vacuum under consideration, $L^3$, is proportional to the vacuum field mode spacing (i.e., $L^3 = 2 \pi^2 \hbar^3 / (\omega^2 \Delta \omega)$), so that

\begin{align}
\dot{a}_2(t) &= -\frac{2 |\mu_{21}|^2 |z_{\rho \lambda}|^2 \Delta \omega}{3 \pi \hbar^3} a_2(t) \left[ |z_{\rho \lambda}|^2 \omega_{21} t \\
&+ \sum_{\delta_\rho} \left[ |z_{\rho \lambda}|^2 \omega_{\delta_\rho} \right] \left[ 1 - \exp(-i \delta_\rho t) \right] \right].
\end{align}

(65)

where the prime on the summation indicates that the $\delta_\rho = 0$ term has been removed.

Finally, integrating Eq. (65) yields
\[ \ln \left[ \frac{\alpha_2(t)}{\alpha_2(0)} \right] = -\kappa \left[ |x_0|^2 \omega_2 t^2 \right] + \sum_s \left( |z_s|^2 \left( \frac{\alpha_s}{\delta^2_s} \right) \right) \left( 1 - \cos(\delta_s t) \right) + \left( \frac{i \alpha_s}{\delta^2_s} \left[ \sin(\delta_s t) - \delta_s t \right] \right) \]

where

\[ \kappa = \frac{2|\mu_{21}|^2 \omega_2 \Delta \omega}{3 \pi \hbar c^3} \]  

Again, with \( P_2(t) \) defined as the probability of finding the atom in the excited state, Eq. (66) results in

\[ P_2(t) = P_2(0) \exp \left( -\kappa |x_0|^2 \omega_2 t^2 - 2\kappa \sum_s \left( |z_s|^2 \left( \frac{\alpha_s}{\delta^2_s} \right) \right) \right) \times \left( 1 - \cos(\delta_s t) \right) \]  

Fig. 1. Numerical simulation of the sodium \( 3^2P_{1/2} \) state's spontaneous decay using SRED: squares, mode spacing of 100 kHz; circles, mode spacing of 10 kHz; diamonds, mode spacing of 1 kHz. For comparison, the solid curve corresponds to exponential decay given the \( 3^2P_{1/2} \) state's 17.0-ns lifetime.

To test the validity of this semiclassical procedure for numerically simulating spontaneous emission we can apply Eq. (68) to the decay of sodium's first excited state at 589.6 nm (i.e., \( 3^2P_{1/2} \rightarrow 3^2S_{1/2} \)). The \( 3^2P_{1/2} \) state lifetime is 17.0 ns,\(^{34}\) yielding an electric dipole moment for this transition of \( 2.07 \times 10^{-29} \) C m.\(^{35}\) Figure 1 shows \( P_2(t) \) computed from Eq. (68) for three values of the mode spacing (i.e., 100, 10, and 1 kHz).\(^{36}\) The range of modes employed in the summation of Eq. (68) was limited to \( \pm 10 \) GHz, which corresponds to a correlation time for the simulated vacuum field of \( \sim 0.01 \) ns. Clearly, as the mode spacing approaches zero the decay of \( P_2(t) \) becomes exponential to high precision, and the numerically simulated rate of decay corresponds to a 17-ns lifetime.

6. SUMMARY

The Einstein \( A \) coefficient for spontaneous decay has been derived by use of second-order perturbation theory in a completely semiclassical formalism with (1) the assumption of a classical ZPF and (2) a Hermitian operator for the atom's radiation-reaction field. Additionally, the semiclassical theory has yielded the Lamb shift, which appears as an ac Stark shift induced by the ZPF. Although these results are intriguing in their own right, the primary motivation for developing SRED is for its use as a tool in computer simulations of spontaneous decay under various conditions. It was therefore demonstrated that SRED has the potential to simulate spontaneous decay in arbitrary vacuum fields once the modal composition of the vacuum field is specified.

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REFERENCES AND NOTES


14. It is worth mentioning here that (as was pointed out by Eberly) when a classical Lagrangian for the field–atom system is supplemented by the assumption of stochastic, homogeneous solutions, a description of the field–atom interaction is obtained that "...does not differ from QED at all in its second-order predictions of decay rates and level shifts." See J. H. Eberly, "Unified view of spontaneous emission in several theories of radiation," in Foundations of Radiation Theory and Quantum Electrodynamics, A. O. Barut, ed. (Plenum, New York, 1980).


22. Physically, in SRED the missing factor of 2 in Eq. (5b) is to be attributed to an explicit role for the vacuum field in describing an oscillating dipole's dynamics.


30. It should at least be mentioned in passing that the connection between the Lamb shift and the ac Stark shift goes back to some of the first ac Stark shift investigations. See, for example, S. Pancharatnam, "Light shifts in semiclassical dispersion theory," J. Opt. Soc. Am. 56, 1636 (1966), and references therein.


36. The computation first simulated each mode of the ZPF over the ~100-nsec simulation time (Δt_{sim} ~ 1 ns) and then summed over modes. For the case of Δ = 10 kHz the entire simulation of P(t)'s required only 4 min. on a 130-MHz Pentium computer.
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