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Power operator, effective Hamiltonian and AC Poynting splitting

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Abstract. The concept of the effective Hamiltonian is introduced and the first- and second-order perturbative solutions are obtained for a non-degenerate system. By solving the first-order effective Schrödinger equation, we derive the AC Poynting splitting for the *exact* field. In the long wavelength approximation, the AC Poynting splitting is shown to reduce to the AC Stark splitting if the electric dipole dominates and to the AC Zeeman splitting if the magnetic dipole dominates. For the quantised electromagnetic fields, it is found that the effective Hamiltonian approach does not distinguish between (i) the conventional quantisation of the vector potential and (ii) the quantisation of the fields directly.

1. Introduction

With the availability of the coherent laser radiation, atomic and molecular physics has taken a new dimension. In the strong-field resonance phenomena where a laser field is tuned to near-resonance with two atomic energy states, the conventional (weak-field) time-dependent perturbation theory is no longer adequate to give sufficiently detailed information, and the descriptions are now dominated by the Rabi frequency, AC Stark splitting, detuning and so on. For a recent review of the importance of the Rabi frequency in the matter–strong-field interactions, see e.g. Knight and Milonni (1980).

Accompanying this new and exciting field of physics is an old problem that demands immediate attention. The problem in question is gauge invariance in quantum mechanics. The urgency of this problem is illustrated in a statement in the textbook on laser physics by Sargent *et al* (1977, pp 15–6) where these authors state: 'We note that the interaction Hamiltonian $\mathscr{H}_1 = em^{-1}\boldsymbol{A}\cdot\boldsymbol{p}$ is not as accurate as equation (6) $[-e\boldsymbol{E}(\boldsymbol{R}, t)\cdot\boldsymbol{r}]$ in the dipole approximation (does not include the A^2 term) and can lead to incorrect results'. This conclusion is a direct consequence of the construction of the Rabi flopping frequency from the matrix elements of the 'interaction Hamiltonians': that the Rabi frequency for one form of the 'interaction Hamiltonian' simply differs from that for another form of 'interaction Hamiltonian' when the detuning does not vanish (i.e. not on resonance).

The above statement has its origin in Lamb's shift measurements (Lamb 1952, see also Scully and Lamb 1967). Since Lamb's (1952) paper, there has been considerable interest (and disagreement) among those who have tried to understand the

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fundamental mechanism by which charged matter interacts with electromagnetic fields, classical or quantised (e.g. Fried 1973, Power and Zienau 1959, Yang 1976, 1982a, Shirokov 1981). As Shirokov (1981) has pointed out very clearly, those who have shown the 'complete equivalence' of $\boldsymbol{A}\cdot\boldsymbol{p}$ and $\boldsymbol{r}\cdot\boldsymbol{E}$ have based their argument on the gauge invariance of the S-matrix, defined to be $U(t_i, t_f)$ with $t_i = -\infty$ and $t_f = +\infty$ where U is an evolution operator. He further observes that *not* all physical processes can be described by the S-matrix formalism. As this author has pointed out (Yang 1982a), the evolution operators $U(t_i, t_f)$ are gauge dependent for any *finite* times t_i and t_f.

So far, the only way to avoid the gauge problem in the strong-field interaction has been to use the $-e\boldsymbol{r}\cdot\boldsymbol{E}(\boldsymbol{0}, t)$ exclusively in the dipole approximation (e.g. Sargent *et al* 1977, Knight and Milonni 1980, Dalton 1982, Radmore and Knight 1982), simply because of its explicit dependence on the physically measurable quantity $\boldsymbol{E}$. Although the dipole approximation is apparently adequate for the moment, a deeper theoretical question remains: how can the fields be treated exactly instead of just being in the dipole approximation?

The purpose of this paper is to propose a method by which the electromagnetic fields can be treated exactly and in a gauge-invariant manner. We will present a particular formulation based on the classical Poynting theorem and the conservation of energy (e.g. Jackson 1975, pp 236–41), in which, for example, the dynamic AC Stark splitting will be replaced by the AC Poynting splitting that reduces to the former when the electric dipole approximation on the fields is made. Our basic idea is to introduce the *effective* Hamiltonian and wavefunction with the characteristics that they both are gauge invariant and are in a one-to-one correspondence to a given field situation. These two properties are absent in the ordinary Hamiltonians and wavefunctions which are gauge dependent and hence do not have the one-to-one correspondence property with the fields (e.g. Cohen-Tannoudji *et al* 1977).

Of course, the effective Hamiltonian and wavefunction are derived from the ordinary Hamiltonians and wavefunctions through the Schrödinger equations. What is needed in between is the gauge-invariant formulation of quantum mechanics (Yang 1976, 1982a,b, Cohen-Tannoudji *et al* 1977, Kobe and Smirl 1978, Leubner and Zoller 1980, Kobe and Wen 1980, 1982, Leubner 1981, Kobe *et al* 1982, Kobe 1983, Lee and Albrecht 1983), together with the method of the gauge-invariant time-dependent perturbation theory (Yang 1982c). This formulation is based on the correspondence principle (Bohr 1928) and, as noted before, Poynting's theorem and the conservation of energy (e.g. Jackson 1975). It has been shown to remove all gauge ambiguity in the interpretation of transition probabilities (e.g. Leubner and Zoller 1980) and to satisfy the conservation of energy at all times (Yang 1982a, b, Kobe *et al* 1982). Furthermore, it is also consistent with the Foldy–Wouthuysen transformations (Foldy and Wouthuysen 1950), as shown by Kobe and Yang (1980) and Yang (1982a). This last property is especially important when spinning particles are concerned.

The arrangement of this paper is as follows. In § 2, we will briefly review the gauge-invariant formulation and the basic principles involved. In § 3, the concepts of the effective Hamiltonian and wavefunction will be introduced, and their perturbative solutions through the second order derived. Then, we will make a comparison with the Hamiltonian in the multipolar gauge (e.g. Power and Zienau 1959, Fiutak 1963, Woolley 1975). In § 4, the rotating-wave approximation will be made to derive the AC Poynting splitting which is then shown to reduce to the AC Stark splitting in

the dipole approximation of the fields. In § 5, we will consider the quantised electromagnetic fields and show that either quantising the vector potential or quantising the fields directly can be used in conjunction with our effective Hamiltonian with the same results. Finally we present a short discussion in § 6.

2. The gauge-invariant formulation

In this section, the basic theory and the underlying physical principles of the gauge-invariant formulation will be briefly reviewed. The all-important concept of manifest gauge invariance† can be found in Yang (1976, 1982a, b), Cohen-Tannoudji *et al* (1977), Kobe and Smirl (1978) and Kobe *et al* (1982). For an application of this formulation to resolve the ambiguity in the interpretation of transition probabilities, the works of Leubner and Zoller (1980) and Leubner (1981) are the clearest and simplest to comprehend. Kobe and Wen (1980, 1982) and Shirokov (1981) have compared the *exact* conventional and gauge-invariant probabilities for a charged simple-harmonic oscillator interacting with a radiation field in the dipole approximation. Recently, Lee and Albrecht (1983) have presented an excellent review on the applications of our formulation in molecular spectroscopies.

Consider a non-relativistic, spinless charged particle of mass m and charge e in the presence of a conservative, electrostatic field $\boldsymbol{E}_0(\boldsymbol{r}) = -\nabla V_0(\boldsymbol{r})$ and a time-varying radiation field $\boldsymbol{E}(\boldsymbol{r}, t)$ and $\boldsymbol{B}(\boldsymbol{r}, t)$. If we use the potentials $\boldsymbol{A}(\boldsymbol{r}, t)$ and $\Phi(\boldsymbol{r}, t)$ to represent the fields $\boldsymbol{E}$ and $\boldsymbol{B}$, then

$$\boldsymbol{E}(\boldsymbol{r}, t) = -\nabla\Phi(\boldsymbol{r}, t) - c^{-1}\partial\boldsymbol{A}(\boldsymbol{r}, t)/\partial t, \qquad \boldsymbol{B}(\boldsymbol{r}, t) = \nabla \times \boldsymbol{A}(\boldsymbol{r}, t). \tag{2.1}$$

The Schrödinger equation and the Hamiltonian in this gauge are then

$$\mathrm{i}\hbar\partial\Psi(\boldsymbol{r}, t)/\partial t = H(t)\Psi(\boldsymbol{r}, t), \tag{2.2}$$

$$H(t) = (\boldsymbol{p} - e\boldsymbol{A}/c)^2/2m + eV_0 + e\Phi, \tag{2.3}$$

with initial condition $\Psi(\boldsymbol{r}, t_0)$. Here, we note that the potentials and the fields are considered classical and external quantities.

The fundamental concept of the gauge-invariant formulation is to construct the energy operator H_B describing the particle's quantity that conserves with the radiation energy and its energy flux. This is done by using the classical Poynting theorem and conservation of energy (e.g. Jackson 1975, Yang 1976, 1982a, b, Kobe *et al* 1982) through the correspondence principle (Bohr 1928). If we neglect the self-interaction, then H_B is determined by

$$\partial H_B/\partial t + [H_B, H]/\mathrm{i}\hbar = \tfrac{1}{2}(\boldsymbol{J}\cdot\boldsymbol{E} + \boldsymbol{E}\cdot\boldsymbol{J}) \equiv P(t), \tag{2.4}$$

where $\boldsymbol{J} = e\boldsymbol{v} = e(\boldsymbol{p} - e\boldsymbol{A}/c)/m$ is the current operator associated with the Hamiltonian

† By 'manifest gauge invariance' we mean same forms and same values in all gauges (e.g. Cohen-Tannoudji *et al* 1977). This definition is analogous to the definition of Lorentz invariance in relativity (e.g. Jackson 1975, chap 11) (same forms and same values in all Lorentz frames, e.g. $\boldsymbol{r}^2 - c^2t^2 = \boldsymbol{r}'^2 - c^2t'^2$ where $(\boldsymbol{r}, t)$ and $(\boldsymbol{r}', t')$ are the space–time coordinates in two Lorentz frames). Thus, the expectation value of $\boldsymbol{\pi} = \boldsymbol{p} - e\boldsymbol{A}/c$ in wavefunction Ψ is gauge invariant since $\langle\Psi|\boldsymbol{\pi}|\Psi\rangle = \langle\Psi'|\boldsymbol{\pi}'|\Psi'\rangle$, where $\boldsymbol{\pi}' = \boldsymbol{p} - e\boldsymbol{A}'/c$, Ψ is the wavefunction in gauge $(\boldsymbol{A}, \Phi)$ and Ψ' is that in $(\boldsymbol{A}', \Phi')$, with both $(\boldsymbol{A}, \Phi)$ and $(\boldsymbol{A}', \Phi')$ describing the same fields.

in (2.3). One can easily show that

$$H_B = (\boldsymbol{p} - e\boldsymbol{A}/c)^2/2m + eV_0 = \tfrac{1}{2}m\boldsymbol{v}^2 + eV_0, \tag{2.5}$$

which is just the sum of the *Newtonian* kinetic energy (e.g. Cohen-Tannoudji *et al* 1977) and the potential energy.

If we use $\{E_j(t)\}$ and $\{\Psi_j(\boldsymbol{r}, t)\}$ to denote the eigenvalues and the orthonormal and complete (assumed) set of eigenfunctions of $H_B(t)$, then

$$H_B(t)\Psi_j(\boldsymbol{r}, t) = E_j(t)\Psi_j(\boldsymbol{r}, t), \qquad \langle\Psi_j(t)|\Psi_k(t)\rangle = \delta_{jk}. \tag{2.6}$$

The gauge-invariant procedure then defines the probability amplitudes $\{a_j(t)\}$ by

$$a_j(t) = \langle\Psi_j(t)|\Psi(t)\rangle, \tag{2.7}$$

and interprets $|a_j(t)|^2$ as the probability for finding the particle at time t with energy $E_j(t)$ (Yang 1976). This interpretation is consistent with the measurement theory in quantum mechanics (Cohen-Tannoudji *et al* 1977).

If we use (2.6) and (2.7) in conjunction with the Schrödinger equation, the differential equation governing the time evolution of the probability amplitudes is obtained:

$$\mathrm{i}\hbar\, \mathrm{d}a_j/\mathrm{d}t = E_j a_j + \sum_k a_k \langle\Psi_j|(e\Phi - \mathrm{i}\hbar\partial/\partial t)|\Psi_k\rangle. \tag{2.8}$$

The transition matrix elements in the above equation can be shown to relate to the matrix elements of the power or Poynting operator $P(t)$ in (2.4). If $E_j(t) \neq E_k(t)$, then

$$\langle\Psi_j|(e\Phi - \mathrm{i}\hbar\partial/\partial t)|\Psi_k\rangle = \mathrm{i}\hbar\langle\Psi_j|P(t)|\Psi_k\rangle/(E_j - E_k). \tag{2.9}$$

It should be noted that, according to (2.9), the transitions between any two particles' states of different energies are governed by the Poynting operator $P(t)$. The physical processes involved are therefore consistent with Poynting's theorem in the classical electromagnetic theory where energy exchanges between the fields and the particle can take place solely in the manner described by the power density. This concludes our review of the interaction of a quantised particle with classical electromagnetic fields.

3. The effective Hamiltonian and wavefunction

In this section, we shall define the effective Hamiltonian and wavefunction using what has been developed in § 2. After the concepts of the exact effective Hamiltonian and wavefunction are introduced, we will then solve the effective Hamiltonian using the perturbative method to derive its first- and second-order solutions. Then, we will compare our solutions with the Hamiltonian in the multipolar gauge. Finally, we stress here that the effective Hamiltonian is derived from the ordinary Hamiltonians through the Schrödinger equation.

3.1. The exact effective Hamiltonian

For convenience of arguments, we shall assume throughout this paper that the 'unperturbed' Hamiltonian

$$H_0 = \boldsymbol{p}^2/2m + eV_0(\boldsymbol{r}) \tag{3.1}$$

has a *non*-degenerate spectrum, with eigenvalues $\{\hbar\omega_j\}$ and the orthonormal and complete (assumed) set of eigenfunctions $\{\phi_j(\boldsymbol{r})\}$.

We begin by assuming that there exists a one-to-one correspondence between the spectrum $\{\hbar\omega_j\}$ of H_0 and $\{E_j(t)\}$ of $H_B(t)$. Then we define the effective wavefunction $\chi(\boldsymbol{r}, t)$ and Hamiltonian $\mathscr{H}(t)$ by

$$\chi(\boldsymbol{r}, t) = \sum_j a_j(t)\phi_j(\boldsymbol{r}), \tag{3.2}$$

$$\mathscr{H}(t) = \sum_{j,k} |\phi_j\rangle\mathscr{H}_{jk}(t)\langle\phi_k|, \tag{3.3}$$

where

$$\mathscr{H}_{jk}(t) = E_j(t)\delta_{jk} + \langle\Psi_j(t)|(e\Phi(\boldsymbol{r}, t) - i\hbar\partial/\partial t)|\Psi_k(t)\rangle. \tag{3.4}$$

Let us note here that both $\chi(\boldsymbol{r}, t)$ and $\mathscr{H}(t)$ are gauge invariant since $\{a_j(t)\}$, $\{E_j(t)\}$ and $\{\langle\Psi_j(t)|(e\Phi - i\hbar\partial/\partial t)|\Psi_k(t)\rangle\}$ are all gauge invariant and $\{\phi_j(\boldsymbol{r})\}$ are gauge *independent*. From (2.8), (3.2) and (3.3) it follows that we have the gauge-invariant effective Schrödinger equation

$$i\hbar\partial\chi(\boldsymbol{r}, t)/\partial t = \mathscr{H}(t)\chi(\boldsymbol{r}, t), \tag{3.5}$$

with gauge-invariant initial condition $\chi(\boldsymbol{r}, t_0)$.

One matter of importance in the effective wavefunction is in the specification of the *initial* wavefunction $\chi(\boldsymbol{r}, t_0)$. If the time-varying electromagnetic radiation fields $\boldsymbol{E}(\boldsymbol{r}, t)$ and $\boldsymbol{B}(\boldsymbol{r}, t)$ vanish identically everywhere at $t \leq t_0$ when the particle has energy $\hbar\omega_I$, then it can be shown (Yang 1976, Cohen-Tannoudji *et al* 1977, Kobe and Smirl 1978, Leubner and Zoller 1980) that

$$\chi(\boldsymbol{r}, t_0) = \exp(i\alpha)\phi_I(\boldsymbol{r}), \tag{3.6}$$

where α is a real number. We note here that (3.6) is the *conventional* way of specifying the initial condition for *all* gauges (e.g. Merzbacher 1960).

The second matter of importance, following the gauge invariance of the effective wavefunction, is the gauge-invariant effective time-evolution operator $\mathscr{U}(t, t_0)$ defined by

$$\chi(\boldsymbol{r}, t) = \mathscr{U}(t, t_0)\chi(\boldsymbol{r}, t_0). \tag{3.7}$$

This effective time-evolution operator also has the conventionally specified initial condition

$$\mathscr{U}(t_0, t_0) = 1. \tag{3.8}$$

Furthermore, it follows from (3.5)–(3.8) that

$$i\hbar\partial\mathscr{U}(t, t_0)/\partial t = \mathscr{H}(t)\mathscr{U}(t, t_0). \tag{3.9}$$

There are two different ways of solving equation (3.5) for the probability amplitudes. The first is to solve both the effective Hamiltonian and wavefunction perturbatively, resulting in the gauge-invariant time-dependent perturbation theory (Yang 1982c). The second method is to solve only the effective Hamiltonian perturbatively, and then use the result to solve for the probability amplitudes as accurately as possible. This second method is the one to be discussed in this paper. The first method can be applied only to *weak* radiation fields and, as this author has shown, produces *rates of net transitions* that agree completely with the conventional results. However, the

perturbative transition amplitudes and probabilities in general disagree with their conventional counterparts, consistent with the investigations of the exact transition probabilities by Leubner and Zoller (1980) and Leubner (1981).

However, when the atoms are in near resonance with an intense, coherent laser field where the back scattering is important, the first method can no longer give sufficiently detailed information concerning the behaviour of the atoms during the interaction, as is the case investigated by Knight and Milonni (1980). In this case, we must try to solve the truncated effective Schrödinger equation using a method to give as accurate solutions for the probability amplitudes as possible. The commonly used approximation is the rotating-wave approximation (e.g. Sargent *et al* 1977, Knight and Milonni 1980). Thus, we need to solve *only* for the effective Hamiltonian perturbatively. Another advantage of this method is that we can now make a meaningful comparison between the effective Hamiltonian and the ordinary Hamiltonians since the *initial conditions* for the wavefunctions are specified identically as in (3.6). In § 3.2, we shall briefly discuss the perturbative expression for the effective Hamiltonian.

3.2. Perturbative form of effective Hamiltonian

As is clear from the defining equation (3.4), one must first solve perturbatively for $E_j(t)$ and $\Psi_j(\boldsymbol{r}, t)$ in order to derive the perturbative expression for the effective Hamiltonian. For this purpose, we will use $E_j^{(n)}(t)$ for the nth-order eigenvalue correction and $\Psi_j^{(n)}(\boldsymbol{r}, t)$ for the nth-order eigenfunction correction of the state j of $H_B(t)$ as obtained from the usual Rayleigh–Schrödinger procedure (e.g. Messiah 1966) (see the appendix for more detailed information). Thus, we write

$$E_j(t) = \sum_{n=0}^{\infty} E_j^{(n)}(t) \qquad \text{and} \qquad \Psi_j(\boldsymbol{r}, t) = \sum_{n=0}^{\infty} \Psi_j^{(n)}(\boldsymbol{r}, t) \tag{3.10}$$

with $E_j^{(0)} = \hbar\omega_j$ and $\Psi_j^{(0)}(\boldsymbol{r}, t) = \phi_j(\boldsymbol{r})$. The normalisation requirements of $\{\Psi_j(\boldsymbol{r}, t)\}$ and $\{\phi_j(\boldsymbol{r})\}$ therefore require (Langhoff *et al* 1972) that

$$\sum_{m=1}^{n} \langle \Psi_j^{(n-m)} | \Psi_k^{(m)} \rangle = 0 \qquad \text{for all } j \text{ and } k, \text{ and all } n \geq 1. \tag{3.11}$$

If we now substitute (3.10) into (3.4), then

$$\mathscr{H}_{jk}(t) = \sum_{n=0}^{\infty} \mathscr{H}_{jk}^{(n)}(t), \tag{3.12}$$

where

$$\mathscr{H}_{jk}^{(0)}(t) = \hbar\omega_j \delta_{jk} = \langle \phi_j | H_0 | \phi_k \rangle, \tag{3.13}$$

$$\mathscr{H}_{jk}^{(n)}(t) = E_j^{(1)} \delta_{jk} + \sum_{m=1}^{n} \langle \Psi_j^{(n-m)} | \xi_k^{(m)} \rangle, \qquad n \geq 1, \tag{3.14}$$

$$\xi_k^{(m)}(t) = e\Phi\Psi_k^{(m-1)} - \mathrm{i}\hbar\partial\Psi_k^{(m)}/\partial t. \tag{3.15}$$

We now define the Nth-order effective Hamiltonian $\mathscr{H}^{[N]}$ by

$$\mathscr{H}^{[N]}(t) = \sum_{n=0}^{N} \sum_{j,k} |\phi_j\rangle \mathscr{H}_{jk}^{(n)} \langle \phi_k|. \tag{3.16}$$

Corresponding to this $\mathscr{H}^{[N]}$, we define the Nth-order effective wavefunction $\chi^{[N]}(\boldsymbol{r}, t)$

to be the solution of the Nth-order effective Schrödinger equation:

$$i\hbar\partial\chi^{[N]}/\partial t = \mathscr{H}^{[N]}\chi^{[N]}. \tag{3.17}$$

Because of the normalisation condition in (3.11), it can be shown that

$$\chi^{[N]}(\boldsymbol{r}, t_0) = \chi(\boldsymbol{r}, t_0) \qquad \text{for all } N \geq 0, \tag{3.18}$$

where the right-hand side is listed in (3.6). That (3.18) is valid for all $N \geq 0$ is important, since then there is no ambiguity in the specification of the initial wavefunction.

We now list the zeroth-, first- and second-order forms of the effective Hamiltonian. From (3.13) and (3.16) it is clear that

$$\mathscr{H}^{[0]} = \sum_{j,k} |\phi_j\rangle\langle\phi_j|H_0|\phi_k\rangle\langle\phi_k| = H_0. \tag{3.19}$$

We now consider $N = 1$. From (3.14)–(3.16), and (A5), (A12) and (A13),

$$\langle\phi_j|\mathscr{H}^{[1]}|\phi_j\rangle = \langle\phi_j|\{H_0 - e(\boldsymbol{A}\cdot p + \boldsymbol{p}\cdot\boldsymbol{A})/2mc + F[-e\boldsymbol{E}]\}|\phi_j\rangle, \tag{3.20}$$

$$\langle\phi_j|\mathscr{H}^{[1]}|\phi_k\rangle = (i/\omega_{jk})\langle\phi_j|P^{(1)}|\phi_k\rangle, \qquad j \neq k, \tag{3.21}$$

where $\omega_{jk} = \omega_j - \omega_k$, $P^{(1)}$ is the first-order Poynting (or power) operator

$$P^{(1)} = e(\boldsymbol{p}\cdot\boldsymbol{E} + \boldsymbol{E}\cdot\boldsymbol{p})/2m \tag{3.22}$$

and

$$F[-e\boldsymbol{E}] = -e\int_0^1 du\, \boldsymbol{r}\cdot\boldsymbol{E}(u\boldsymbol{r}, t). \tag{3.23}$$

Associated with the result (3.23) is the requirement that the scalar potential $\Phi(\boldsymbol{r}, t)$ satisfy the condition $\Phi(\boldsymbol{0}, t) = 0$. This requirement can be easily satisfied by the simple substitution $\Phi(\boldsymbol{r}, t) \to \Phi(\boldsymbol{r}, t) - \Phi(\boldsymbol{0}, t)$. As has been explained previously (Yang 1982c), such a requirement entails no consequence in either the transition matrix elements for states with different energies or the transition probabilities.

For the second-order effective Hamiltonian, we first define the second-order Poynting operator $P^{(2)}$ by

$$P^{(2)} = -e^2(\boldsymbol{A}\cdot\boldsymbol{E} + \boldsymbol{E}\cdot\boldsymbol{A})/2mc. \tag{3.24}$$

Note $P = P^{(1)} + P^{(2)}$, where P is defined in (2.4) and $P^{(1)}$ in (3.22). Furthermore, we define the operators $\{Q_j^{(0)}\}$ and the reduced resolvent operators (i.e. the reduced Green functions) $\{G_j^{(0)}\}$ by

$$G_j^{(0)} = Q_j^{(0)}/(\hbar\omega_j - H_0), \qquad Q_j^{(0)} = 1 - |\phi_j\rangle\langle\phi_j|. \tag{3.25}$$

With these operators, the functions $\{u_j^{(1)}\}$ and $\{\zeta_j^{(1)}\}$ defined in (A16) and (A18) can be expressed as

$$u_j^{(1)} = G_j^{(0)}V_1^B\phi_j, \qquad \zeta_j^{(1)} = i\hbar G_j^{(0)}P_B^{(1)}\phi_j, \tag{3.26}$$

where, using $V_1 = -e(\boldsymbol{A}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{A})/2mc$ defined in (A1),

$$V_1^B = V_1 + (ie/c\hbar)[H_0, F[\boldsymbol{A}]] = -(e/2mc)\{\boldsymbol{p}\cdot(\boldsymbol{A} - \boldsymbol{\nabla}F[\boldsymbol{A}]) + (\boldsymbol{A} - \boldsymbol{\nabla}F[\boldsymbol{A}])\cdot\boldsymbol{p}\}, \tag{3.27}$$

$$P_B^{(1)} = P^{(1)} + i\hbar^{-1}[H_0, F[-e\boldsymbol{E}]] = (e/2m)\{\boldsymbol{p}\cdot(\boldsymbol{E} - \boldsymbol{\nabla}F[\boldsymbol{E}]) + (\boldsymbol{E} - \boldsymbol{\nabla}F[\boldsymbol{E}])\cdot\boldsymbol{p}\}. \tag{3.28}$$

Note, $V_1^B = 0$ if $\boldsymbol{B} = 0$ and $P_B^{(1)} = 0$ if $\partial\boldsymbol{B}/\partial t = 0$.

We are now ready to give the explicit expression for the second-order effective Hamiltonian (where V_1 and V_2 are defined in (3.2)):

$$\begin{aligned}\langle\phi_j|\mathscr{H}^{[2]}|\phi_j\rangle = \langle\phi_j|\{&H_0 - e(\boldsymbol{p}\cdot\boldsymbol{A}+\boldsymbol{A}\cdot\boldsymbol{p})/2mc + F[-e\boldsymbol{E}] + (V_1 G_j^{(0)} V_1 + V_2)\\ &-\tfrac{1}{2}i\hbar(P_B^{(1)} G_j^{(0)} G_j^{(0)} V_1^B - V_1^B G_j^{(0)} G_j^{(0)} P_B^{(1)})\\ &+(F[-e\boldsymbol{E}] G_j^{(0)} V_1^B + V_1^B G_j^{(0)} F[-e\boldsymbol{E}])\\ &+(e^2/2i\hbar c^2)[F[\boldsymbol{A}], F[\dot{\boldsymbol{A}}]]\}|\phi_j\rangle,\end{aligned} \tag{3.29}$$

where the last term $[F[\boldsymbol{A}], F[\dot{\boldsymbol{A}}]]$ vanishes for the classical fields (they are shown here to illustrate the difference between classical and quantised fields). On the right-hand side of the above equation, the fourth term, $V_1 G_j^{(0)} V_1 + V_2$, comes from $E_j^{(2)}$ in (A6), and all the other second-order terms can be understood from (A17) and (3.26). The off-diagonal elements ($j \neq k$) of the second-order effective Hamiltonian are

$$\begin{aligned}\langle\phi_j|\mathscr{H}^{[2]}|\phi_k\rangle = (i/\omega_{jk})\langle\phi_j|\{&P^{(1)} + P^{(1)} G_j^{(0)} V_1^B + V_1^B G_j^{(0)} P^{(1)} + P^{(2)}\\ &+(ie/c\hbar)[P^{(1)}, F[\boldsymbol{A}]] - (\hbar\omega_{jk})^{-1}(V_1 \bar{Q}_j^{(0)} P^{(1)} - P^{(1)} \bar{Q}_k^{(0)} V_1)\}|\phi_k\rangle,\end{aligned} \tag{3.30}$$

where $\bar{Q}_k^{(0)} = 1 - Q_k^{(0)} = |\phi_k\rangle\langle\phi_k|$ is the projection operator† onto the 'unperturbed' state ϕ_k. In (3.30), all the second-order terms can be understood from (3.26) and (A15).

One particular characteristic of the effective Hamiltonian is that its elements extend beyond the second order, for example, one can easily show that the nth-order ($n > 2$) elements do not vanish if there is a magnetic field, i.e. $\nabla \times \boldsymbol{A} \neq 0$. If, however, some approximations are made such that the magnetic field is neglected, then all the elements higher than the first order can be shown to vanish identically. In contrast, the ordinary Hamiltonian can at most have only second-order terms as illustrated in (2.3).

3.3. Comparison with the multipolar-gauge Hamiltonian

It follows from the gauge invariance of the effective Hamiltonian that all its elements can, in principle, be expressible explicitly in terms of the fields. It is therefore tempting for us to make a brief comparison with the multipolar-gauge Hamiltonian (e.g. Power and Zienau 1959, Fiutak 1963, Woolley 1975). Here, we should perhaps emphasise that the comparison is made only with the *classical* multipolar-gauge Hamiltonian in which the *symbols* $\boldsymbol{E}$ and $\boldsymbol{B}$ refer to the electric and magnetic fields. This is in contrast with the *quantised* multipolar-gauge Hamiltonian where the displacement vector $\boldsymbol{D}$ and its magnetic counterpart $\boldsymbol{B}$, as opposed to $\boldsymbol{E}$ and $\boldsymbol{B}$, are used to denote the photon fields.

The multipolar-gauge classical Hamiltonian is

$$H_{\mathrm{mp}} = (\boldsymbol{p} - e\boldsymbol{A}_{\mathrm{mp}}/c)^2/2m + eV_0 + e\Phi_{\mathrm{mp}}, \tag{3.31}$$

where $\Phi_{\mathrm{mp}} = F[-\boldsymbol{E}]$ (see (3.23) and, e.g., Woolley (1975)) and

$$\boldsymbol{A}_{\mathrm{mp}}(\boldsymbol{r}, t) = -\int_0^1 \mathrm{d}u\, u\boldsymbol{r} \times \boldsymbol{B}(u\boldsymbol{r}, t). \tag{3.32}$$

† The conventional notation for the projection operator onto the state ϕ_k is denoted by P_k, rather than the $\bar{Q}_k^{(0)}$ used in this paper. Our reason for using $\bar{Q}_k^{(0)}$ is to avoid confusion since there are already too many P's for the Poynting (or power) operators.

For comparison, we shall write $H^{[0]}_{mp} = H_0$, $H^{[2]}_{mp} = H_{mp}$, and

$$H^{[1]}_{mp} = H_0 - e(\boldsymbol{p}\cdot\boldsymbol{A}_{mp} + \boldsymbol{A}_{mp}\cdot\boldsymbol{p})/2mc + e\Phi_{mp}. \tag{3.33}$$

It then follows from the above definitions that, for all j and k,

$$\langle\phi_j|H^{[1]}_{mp}|\phi_k\rangle = \langle\phi_j|\{H_0 - e(\boldsymbol{A}_{mp}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{A}_{mp})/2mc + e\Phi_{mp}\}|\phi_k\rangle. \tag{3.34}$$

The above matrix elements are to be compared with (3.20) and (3.21). Since $\langle\phi_j|(\boldsymbol{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{p})|\phi_j\rangle$ is gauge invariant (e.g. Yang 1977), it then follows that

$$\langle\phi_j|(\boldsymbol{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{p})|\phi_j\rangle = \langle\phi_j|(\boldsymbol{p}\cdot\boldsymbol{A}_{mp} + \boldsymbol{A}_{mp}\cdot\boldsymbol{p})|\phi_j\rangle, \tag{3.35}$$

which is a mathematical consequence of $\boldsymbol{A} = \boldsymbol{A}_{mp} + F[\boldsymbol{A}]$ where F is defined in (3.23). Thus, (3.20) is identical to (3.34) for $j = k$.

To make a comparison between (3.21) and (3.34) with $j \neq k$, we shall use

$$\boldsymbol{E}(\boldsymbol{r}, t) = -\nabla\Phi_{mp}(\boldsymbol{r}, t) - c^{-1}\partial\boldsymbol{A}_{mp}(\boldsymbol{r}, t)/\partial t. \tag{3.36}$$

Substituting this result into (3.21), we get, for $j \neq k$,

$$\langle\phi_j|\mathscr{H}^{[1]}|\phi_k\rangle = (i/\omega_{jk})(\partial/\partial t)\langle\phi_j| - e(\boldsymbol{p}\cdot\boldsymbol{A}_{mp} + \boldsymbol{A}_{mp}\cdot\boldsymbol{p})/2mc|\phi_k\rangle + \langle\phi_j|e\Phi_{mp}|\phi_k\rangle. \tag{3.37}$$

Thus we see that, for the first order, the effective Hamiltonian differs from the multipolar-gauge Hamiltonian in the *magnetic* interactions. This suggests that, when the interactions are dominated by the electric dipole, it is difficult to distinguish between the two. However, if an experiment can be designed in which the magnetic dipole interaction dominates, then one should be able to decide experimentally between the two even from the first-order results.

There is no need to make an explicit comparison between the effective Hamiltonian and the multipolar-gauge Hamiltonian for the second-order results. It is obvious that these two are very different simply by inspecting (3.29)–(3.31). Note, in (3.29), one can replace $\boldsymbol{A}$ in $(V_1 G^{(0)}_j V_1 + V_2)$ by $\boldsymbol{A}_{mp}$. This is due to the gauge invariance of $E^{(2)}_j$ in (A6). The difference in the second-order elements also suggests that one can distinguish between them by investigating the second-order physical predictions (one must include the magnetic field, though).

4. The AC Poynting splitting

In this section, we shall solve the first-order effective Schrödinger equation when the external radiation field is a single-frequency field with angular frequency ω tuned to near-resonance with two energies $\hbar\omega_1$ and $\hbar\omega_2$ of the 'unperturbed' Hamiltonian. We shall use the two-state and rotating-wave approximations to derive the AC Poynting splitting for the *exact* fields. Then we will show that it reduces to the more familiar AC Stark splitting when the dipole approximation on the fields is made. We will also show that, for those first-order interactions in which the magnetic dipole dominates (i.e. the electric dipole transitions are forbidden), it reduces to the AC Zeeman splitting under the long wavelength approximation.

Assume that the radiation fields have the form

$$\boldsymbol{E}(\boldsymbol{r}, t) = \boldsymbol{E}_+(\boldsymbol{r})\,e^{i\omega t} + \boldsymbol{E}_-(\boldsymbol{r})\,e^{-i\omega t}, \qquad (\boldsymbol{E}_+)^* = \boldsymbol{E}_-, \tag{4.1}$$

and similarly for $\boldsymbol{B}(\boldsymbol{r}, t)$, where * denotes the complex conjugate. Since the first-order effective Hamiltonian as indicated in (3.20) and (3.21) is manifestly gauge invariant,

we may choose whatever potentials we please as long as they generate the correct fields. For example, one may choose them to be such that $\Phi(\boldsymbol{r}, t) = 0$ and

$$\boldsymbol{A}(\boldsymbol{r}, t) = \boldsymbol{A}_+(\boldsymbol{r})\, \mathrm{e}^{\mathrm{i}\omega t} + \boldsymbol{A}_-(\boldsymbol{r})\, \mathrm{e}^{-\mathrm{i}\omega t}. \tag{4.2}$$

If we use $\omega_0 = \omega_2 - \omega_1 \approx \omega$, then according to (3.2), (3.17), (3.20) and (3.21), we have

$$\mathrm{i}\, \mathrm{d}a_2/\mathrm{d}t = (\omega_2 + \Delta_2)a_2 + Va_1, \tag{4.3}$$

$$\mathrm{i}\, \mathrm{d}a_1/\mathrm{d}t = (\omega_1 + \Delta_1)a_1 + V^* a_2, \tag{4.4}$$

where

$$\Delta_j = \langle \phi_j | \{ -e(\boldsymbol{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{p})/2mc + F[-e\boldsymbol{E}] \} | \phi_j \rangle, \tag{4.5}$$

$$V(t) = (\mathrm{i}/\hbar\omega_0)\langle \phi_2 | e(\boldsymbol{p}\cdot\boldsymbol{E} + \boldsymbol{E}\cdot\boldsymbol{p})/2m | \phi_1 \rangle \equiv V_+\, \mathrm{e}^{\mathrm{i}\omega t} + V_-\, \mathrm{e}^{-\mathrm{i}\omega t}. \tag{4.6}$$

The effects of Δ_1 and Δ_2 on the solutions of a_1 and a_2 can be seen to be of second order in the fields. If we define (Keldysh 1965)

$$b_j = a_j \exp(\mathrm{i}\omega_j t + \mathrm{i}\tilde{\Delta}_j), \qquad \tilde{\Delta}_j(t) = \int_0^t \mathrm{d}t'\, \Delta_j(t'), \tag{4.7}$$

then, using $\tilde{\Delta}_0 = \tilde{\Delta}_2 - \tilde{\Delta}_1$,

$$\mathrm{i}\, \mathrm{d}b_2/\mathrm{d}t = Vb_1 \exp(\mathrm{i}\omega_0 t + \mathrm{i}\tilde{\Delta}_0) = Vb_1 \exp(\mathrm{i}\omega_0 t)(1 + \mathrm{i}\tilde{\Delta}_0 + \ldots), \tag{4.8}$$

and similarly for $\mathrm{d}b_1/\mathrm{d}t$. Thus for all practical purposes in the first-order investigation, Δ_1 and Δ_2 can be neglected from (4.3) and (4.4).

If we solve (4.3) and (4.4) using the rotating-wave approximation with the initial conditions that $a_1(0) = 1$ and $a_2(0) = 0$, then (e.g. Knight and Milonni 1980)

$$a_2(t) = [K_+ \exp(\mathrm{i}\mu_+ t) + K_- \exp(\mathrm{i}\mu_- t)] \exp(-\mathrm{i}\omega_2 t), \tag{4.9}$$

where

$$\mu_\pm = \tfrac{1}{2}\{(\omega_0 - \omega) \pm [(\omega_0 - \omega)^2 + 4|V_-|^2]^{1/2}\}, \tag{4.10}$$

$$K_\pm = \mp V_-[(\omega_0 - \omega)^2 + 4|V_-|^2]^{-1/2}. \tag{4.11}$$

From (4.6) and (4.10), it is seen that the Rabi flopping frequency,

$$\mu = \mu_+ - \mu_- = [(\omega_0 - \omega)^2 + 4|V_-|^2]^{1/2}, \tag{4.12}$$

is caused intrinsically by the first-order Poynting (power) operator $P^{(1)} = e(\boldsymbol{p}\cdot\boldsymbol{E} + \boldsymbol{E}\cdot\boldsymbol{p})/2m$ as defined in (3.22). Hence, the frequency splitting is the AC Poynting splitting.

If the states ϕ_1 and ϕ_2 are of opposite parities, and if the long wavelength approximation applies, then the AC Poynting splitting reduces to the more familiar AC Stark splitting (e.g. Knight and Milonni 1980) since

$$(\mathrm{i}/\omega_0)\langle \phi_2 | e\boldsymbol{p}\cdot\boldsymbol{E}(\boldsymbol{0}, t)/m | \phi_1 \rangle = \langle \phi_2 | -e\boldsymbol{r}\cdot\boldsymbol{E}(\boldsymbol{0}, t) | \phi_1 \rangle. \tag{4.13}$$

If these two states are of the same parity, the long wavelength applies and the transition is dominated by the magnetic dipole, then the AC Poynting splitting reduces to the AC Zeeman splitting since (Yang 1976, § IV)

$$\boldsymbol{E}(\boldsymbol{r}, t) \approx -\boldsymbol{\nabla}[\boldsymbol{M}_E^{(1)} + \boldsymbol{M}_E^{(2)}] - (1/2c)[\partial \boldsymbol{B}(\boldsymbol{0}, t)/\partial t] \times \boldsymbol{r}, \tag{4.14}$$

where $M_E^{(1)} = -\boldsymbol{r}\cdot\boldsymbol{E}(\boldsymbol{0}, t)$ and

$$M_E^{(2)} = -(\tfrac{1}{6})\sum_{j,k}(3x_jx_k - r^2\delta_{jk})[\partial E_j(\boldsymbol{r}'t)/\partial x'_k]_{\boldsymbol{r}'=\boldsymbol{0}}, \tag{4.15}$$

with $\boldsymbol{r} = (x_1, x_2, x_3)$ and similarly for $\boldsymbol{r}'$. If we substitute (4.14) into (4.6) and use the fact that the magnetic dipole interaction dominates, then

$$V_- \approx \hbar^{-1}(\omega/\omega_0)\langle\phi_2| - (e/2mc)\boldsymbol{r}\times\boldsymbol{p}\cdot\boldsymbol{B}_-(\boldsymbol{0})|\phi_1\rangle. \tag{4.16}$$

One should note that the magnetic dipole *transition* operator, as can be seen from (4.6) and (4.14), involves the *time derivative* of the magnetic field. This is in contrast with the magnetic dipole operator in the multipolar-gauge Hamiltonian which is $-(e/2mc)\boldsymbol{r}\times\boldsymbol{p}\cdot\boldsymbol{B}$. Because of this difference, we have the extra factor (ω/ω_0) appearing in (4.16). Such a difference, as noted in § 3.3, should have some experimental consequences in the measurement of the Rabi flopping frequencies.

5. Treatment of quantised fields

In § 3, we have shown that the introduction of the effective Hamiltonian and wavefunction does eliminate the gauge ambiguity in the quantum mechanical formulation of a quantised particle interacting with classical fields. This thus raises hopes that maybe it is able to do so also for the quantised fields. That is, it does not matter whether the fields are quantised directly (without any reference to how to quantise the potentials) or the potentials are quantised first (as is usually done). (For a discussion concerning this point, see Scully and Lamb (1967).) In this section we shall show that if certain rules are observed†, one can use either scheme of quantisation in conjunction with the effective Hamiltonian and end up with the same results. As an illustration, we shall use the field Hamiltonian and the first-order particle's effective Hamiltonian to derive the gauge-invariant Jaynes–Cummings doublets (Jaynes and Cummings 1963, see also Knight and Milonni 1980) by using the usual quantised transverse *vector potential.*

5.1. *The Scully–Lamb quantisation procedure*

The Scully–Lamb (1967) quantisation procedure, designed to sidestep the $\boldsymbol{A}\cdot\boldsymbol{p}$ against $\boldsymbol{r}\cdot\boldsymbol{E}$ ambiguity as noted in the introduction, is to quantise the (transverse) electric and magnetic fields $\boldsymbol{E}$ and $\boldsymbol{B}$ (*not* $\boldsymbol{D}$ and $\boldsymbol{B}$) directly, starting from Maxwell's equations in the *absence* of all charge and current densities. We will not repeat the procedure here but merely quote their results. If we have a finite volume V with linear dimension L, and consider only the x component of the electric field propagating in the z direction

† For the purposes of this paper, these rules consist of some mathematical identities and the correspondence between the quantised field equations and the classical Maxwell equations (§ 5.2). In a later paper, we shall derive all the results in §§ 3.2, 5.2 and 5.3 starting from the total (fields plus particles) Hamiltonian within the framework of the fully quantised scheme in the radiation gauge (e.g. Fermi 1932), together with two added physical assumptions. These two assumptions are: (i) that a photon detector measures only the radiation energy flux reaching the detector (i.e. it cannot measure the physical states of the particles), and (ii) that the self-interaction of a charged particle *cannot* be turned off during such a measurement (i.e. such a measurement is done in the presence of the self-interactions of the particles).

(their details will be followed as much as possible), then

$$\hat{\boldsymbol{E}}(\boldsymbol{r}, t) = \boldsymbol{e}_x \sum_s C_s(b_s + b_s^\dagger) \sin(K_s z), \tag{5.1}$$

$$\hat{\boldsymbol{B}}(\boldsymbol{r}, t) = -\mathrm{i}\boldsymbol{e}_y \sum_s C_s(b_s - b_s^\dagger) \cos(K_s z), \tag{5.2}$$

where $K_s = s\pi/L$ and s is a positive integer. The vectors $\boldsymbol{e}_x$ and $\boldsymbol{e}_y$ are the unit vectors in the x and y directions, $C_s = (2\pi\hbar\Omega_s/V)^{1/2}$ and $\Omega_s = cK_s$. Throughout this section, a caret will be used to indicate that the fields involved are quantised. The operator b_s ($b_s^\dagger$) is a photon annihilation (creation) operator and satisfies the commutation relation $[b_s, b_{s'}^\dagger] = \delta_{ss'}$.

The free-field Hamiltonian is

$$H_{\mathrm{FF}} = \sum_s \hbar\Omega_s(b_s^\dagger b_s + \tfrac{1}{2}). \tag{5.3}$$

The eigenstates of H_{FF} will be denoted by the usual notation. In particular, $|n_s\rangle$ will represent the normalised state with n photons having wavevector $\boldsymbol{K}_s$.

Let us note one important consequence of this particular quantisation procedure. It is that the operation represented by $\hat{\boldsymbol{A}}(\boldsymbol{r}, t)|n_s\rangle$, for example, is not mathematically defined for $\boldsymbol{A}$ in any arbitrary gauge; it is defined only for those vector potentials that can be *explicitly* expressed in terms of $\boldsymbol{E}$ and $\boldsymbol{B}$.

We now discuss how the effective Hamiltonian method can be used with this quantisation procedure. If we use only the particle's first-order effective Hamiltonian, then the total effective Hamiltonian is

$$\mathscr{H}_{\mathrm{T}}^{[1]} = \hat{\mathscr{H}}^{[1]} + H_{\mathrm{FF}}, \tag{5.4}$$

where $\hat{\mathscr{H}}^{[1]}$ is defined by (3.20) and (3.21), with quantised $\hat{\boldsymbol{A}}$ and $\hat{\boldsymbol{E}}$. First, we use the fact that $\{\langle\phi_j|(\boldsymbol{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\boldsymbol{p})|\phi_j\rangle\}$ are gauge invariant (for both classical and quantised vector potentials) to write

$$\langle\phi_j|\hat{\mathscr{H}}^{[1]}|\phi_j\rangle = \langle\phi_j|\{H_0 - e(\boldsymbol{p}\cdot\hat{\boldsymbol{A}}_{\mathrm{mp}} + \hat{\boldsymbol{A}}_{\mathrm{mp}}\cdot\boldsymbol{p})/2mc + F[-e\hat{\boldsymbol{E}}]\}|\phi_j\rangle, \tag{5.5}$$

where, by (5.2) and (3.32),

$$\hat{\boldsymbol{A}}_{\mathrm{mp}}(\boldsymbol{r}, t) = \mathrm{i}\sum_s C_s(b_s - b_s^\dagger) \times \int_0^1 \mathrm{d}u\,(u\boldsymbol{r}\times\boldsymbol{e}_y)\cos(K_s u z), \tag{5.6}$$

and the operator $F[-e\hat{\boldsymbol{E}}]$ can be similarly expressed using (5.1) and (3.23). The off-diagonal elements $\langle\phi_j|\hat{\mathscr{H}}^{[1]}|\phi_k\rangle$ can be obtained by replacing $\boldsymbol{E}$ in (3.21) by $\hat{\boldsymbol{E}}$ in (5.1).

Since, after the procedure in (5.4)–(5.6), the total effective Hamiltonian $\mathscr{H}_{\mathrm{T}}^{[1]}$ is completely expressed in terms of the operators $\{b_s\}$, all of its elements are operationally defined with respect to how they operate on the photon states. Hence, there is no ambiguity as to how one can use the total effective Hamiltonian in (5.4) to derive the probability amplitudes for finding the particle and the photons in any states to compare with experiment.

5.2. Some mathematical identities

In this subsection, we shall derive a few important results from (5.1)–(5.6) that will be necessary for showing that the Scully–Lamb procedure is equivalent to the usual

procedure of quantising the transverse vector potential (e.g. Heitler 1960, Sakurai 1967), *provided* that the effective Hamiltonian is used to obtain physically meaningful quantities. Let us point out here that all results in this subsection are derived using the Scully–Lamb quantisation procedure, i.e. all photon operators are expressed in the $\{b_s\}$ operators and the vector potential is an auxiliary, rather than a fundamental, quantity.

Let us first define a vector potential $\hat{\boldsymbol{A}}_t(\boldsymbol{r}, t)$ by

$$\hat{\boldsymbol{A}}_t(\boldsymbol{r}, t) = -\mathrm{i}\boldsymbol{e}_x \sum_s (c/\Omega_s) C_s (b_s - b_s^\dagger) \sin(K_s z). \tag{5.7}$$

Then it can be shown that the following relation is true:

$$\langle \phi_j | (\boldsymbol{p} \cdot \hat{\boldsymbol{A}}_t + \hat{\boldsymbol{A}}_t \cdot \boldsymbol{p}) | \phi_j \rangle = \langle \phi_j | (\boldsymbol{p} \cdot \boldsymbol{A}_{\mathrm{mp}} + \boldsymbol{A}_{\mathrm{mp}} \cdot \boldsymbol{p}) | \phi_j \rangle, \tag{5.8}$$

where $\hat{\boldsymbol{A}}_{\mathrm{mp}}$ is listed in (5.6). The proof of (5.8) follows by observing the complete equality between each s component of $\boldsymbol{B}$ in (5.2) and that of $\nabla \times \hat{\boldsymbol{A}}_t$ and by using the usual techniques associated with the multipolar gauge (see especially Woolley (1975)).

Next, we observe that the following relations are also true:

$$\hat{\boldsymbol{E}}(\boldsymbol{r}, t) = -c^{-1}\{[\hat{\boldsymbol{A}}_t(\boldsymbol{r}, t), H_{\mathrm{FF}}]/\mathrm{i}\hbar\}, \tag{5.9}$$

$$\hat{\boldsymbol{B}}(\boldsymbol{r}, t) = \nabla \times \hat{\boldsymbol{A}}_t(\boldsymbol{r}, t), \tag{5.10}$$

$$\nabla \times \hat{\boldsymbol{E}}(\boldsymbol{r}, t) = -c^{-1}\{[\hat{\boldsymbol{B}}(\boldsymbol{r}, t), H_{\mathrm{FF}}]/\mathrm{i}\hbar\}, \tag{5.11}$$

where $\hat{\boldsymbol{E}}$, $\hat{\boldsymbol{B}}$, H_{FF} and $\hat{\boldsymbol{A}}_t$ are listed respectively in (5.1), (5.2), (5.3) and (5.7). The result (5.11) follows from (5.9) and (5.10). The above three field equations will serve as our quantised equivalent of the following three *classical* Maxwell equations which do not *explicitly* involve the charge and current densities (using only the transverse component $\boldsymbol{E}$ of the total electric fields):

$$\boldsymbol{E}(\boldsymbol{r}, t) = -c^{-1}\partial \boldsymbol{A}_t(\boldsymbol{r}, t)/\partial t, \tag{5.12}$$

$$\boldsymbol{B}(\boldsymbol{r}, t) = \nabla \times \boldsymbol{A}_t(\boldsymbol{r}, t), \tag{5.13}$$

$$\nabla \times \boldsymbol{E}(\boldsymbol{r}, t) = -c^{-1}\partial \boldsymbol{B}(\boldsymbol{r}, t)/\partial t. \tag{5.14}$$

That (5.9) and (5.11) involve only the free-field Hamiltonian H_{FF} can be understood from the correspondence principle and the classical equations (5.12) and (5.14). According to the classical Maxwell equations, (5.12) and (5.14) are valid whether or not there are charge and current densities present (there is no need to assume that there are no sources or that the sources are at infinity). Since (5.12) and (5.14) do not explicitly involve the sources, the classical operations denoted by $\partial/\partial t$ in these two equations should produce the net effects that their corresponding quantised equivalents do not explicitly involve the particle's Hamiltonian (H in (2.3), for example). Such a statement can be justified rigorously from the fully quantised ordinary Hamiltonian, which is outside the scope of the present paper (see the footnote at the beginning of § 5). For the purposes of this paper, we simply assume that (5.9) is equivalent to (5.12), and proceed to treat (5.9) as one equation defining the relationship between the transverse electric field $\hat{\boldsymbol{E}}$ and the transverse vector potential $\hat{\boldsymbol{A}}_t$.

5.3. Quantisation of the vector potential

The assumption that equations (5.9)–(5.11) are the quantised equivalents of the three Maxwell equations (5.12)–(5.14) has enabled us to realise one important and favourable result. It is that the Scully–Lamb procedure and the usual procedure of quantising the transverse vector potential (e.g. Heitler 1960, Sakurai 1967) will give the same results *provided* the effective total Hamiltonian in (5.4) is used. This is because we have been able to construct A_t and prove (5.8) completely in terms of the Scully–Lamb photon operators. For this reason, we now make no distinction between these two quantisation procedures and proceed to write $\mathscr{H}_T^{[1]}$ in (5.4) in the usual notation.

Let us use $a_\lambda^\dagger$ (a_λ) to denote a photon creation (annihilation) operator in the scheme of quantising the transverse vector potential $\hat{\boldsymbol{A}}_t$, where $\lambda = (\boldsymbol{k}, \alpha)$ and $\boldsymbol{k}$ is the wavevector and α is the polarisation index. Then (in gaussian units)

$$\hat{\boldsymbol{A}}_t(\boldsymbol{r}, t) = \sum_\lambda (cC_\lambda/\omega_\lambda)\boldsymbol{e}_\lambda(a_\lambda\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + a_\lambda^\dagger\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}), \tag{5.15}$$

where $\boldsymbol{e}_\lambda$ is a real polarisation vector satisfying $\boldsymbol{k}\cdot\boldsymbol{e}_\lambda = 0$, $\omega_\lambda = c|\boldsymbol{k}|$ and $C_\lambda = (2\pi\hbar\omega_\lambda/V)^{1/2}$ where V is the normalisation volume. In this notation, H_{FF} is

$$H_{FF} = \sum_\lambda \hbar\omega_\lambda(a_\lambda^\dagger a_\lambda + \tfrac{1}{2}), \tag{5.16}$$

and $\hat{\boldsymbol{E}}(\boldsymbol{r}, t)$ and $\hat{\boldsymbol{B}}(\boldsymbol{r}, t)$ are obtained by (5.9) and (5.10):

$$\hat{\boldsymbol{E}}(\boldsymbol{r}, t) = i\sum_\lambda C_\lambda \boldsymbol{e}_\lambda(a_\lambda\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} - a_\lambda^\dagger\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}), \tag{5.17}$$

$$\hat{\boldsymbol{B}}(\boldsymbol{r}, t) = i\sum_\lambda (C_\lambda/|\boldsymbol{k}|)\boldsymbol{k}\times\boldsymbol{e}_\lambda(a_\lambda\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} - a_\lambda^\dagger\, e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}). \tag{5.18}$$

The diagonal and off-diagonal matrix elements of $\mathscr{H}^{[1]}$ are obtained by using $\tilde{\boldsymbol{A}}_t$ and $\hat{\boldsymbol{E}}$ in (5.15) and (5.17) to replace the $\boldsymbol{A}$ and $\boldsymbol{E}$ in (3.20) and (3.21). In § 5.4, we shall use this first-order total effective Hamiltonian to derive the AC Poynting splitting.

5.4. The gauge-invariant Jaynes–Cummings doublets

The original Jaynes–Cummings (1963) doublets were derived in the quantisation procedure of (5.15) using the ordinary total first-order Hamiltonian

$$H_T^{[1]} = \boldsymbol{p}^2/2m + eV_0 - e(\boldsymbol{p}\cdot\hat{\boldsymbol{A}}_t + \hat{\boldsymbol{A}}_t\cdot\boldsymbol{p})/2mc + H_{FF}. \tag{5.19}$$

If the photon state $|n_s\rangle$ is such that $\omega_s \approx \omega_2 - \omega_1$, where ω_2 and ω_1 are two eigenvalues (divided by $\hbar$) of the unperturbed Hamiltonian H_0, then the states $|1, n_s\rangle$ and $|2, (n-1)_s\rangle$ are almost degenerate in energy. The energies of $H_T^{[1]}$ are then the eigenvalues of the 2×2 matrix with elements $\langle 2, (n-1)_s|H_T^{[1]}|2, (n-1)_s\rangle$, $\langle 2, (n-1)_s|V_t^{(1)}|1, n_s\rangle$, $\langle 1, n_s|V_t^{(1)}|2, (n-1)_s\rangle$ and $\langle 1, n_s|H_T^{[1]}|1, n_s\rangle$ in the rotating-wave approximation, where $V_t^{(1)} = -e(\boldsymbol{p}\cdot\hat{\boldsymbol{A}}_t + \hat{\boldsymbol{A}}_t\cdot\boldsymbol{p})/2mc$. It then follows that, for the exact field,

$$\langle 2, (n-1)_s|V_t^{(1)}|1, n_s\rangle = -(e/m\omega_s)(n_s)^{1/2}C_s\langle\phi_2|e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\boldsymbol{e}_s\cdot\boldsymbol{p}|\phi_1\rangle. \tag{5.20}$$

On the other hand, if we apply the same procedure and approximation to our effective first-order total Hamiltonian $\mathscr{H}_T^{[1]}$, then

$$\langle 2, (n-1)_s|\mathscr{H}_T^{[1]}|1, n_s\rangle = -(e/m\omega_{21})(n_s)^{1/2}C_s\langle\phi_2|e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\boldsymbol{e}_s\cdot\boldsymbol{p}|\phi_1\rangle, \tag{5.21}$$

which differ from (5.20) if $\omega_s \neq \omega_2 - \omega_1 = \omega_{21}$. The two diagonal matrix elements of $\mathscr{H}_T^{[1]}$ are equal to those of $H_T^{[1]}$. Hence the eigenenergies obtained from our effective total Hamiltonian are slightly different from those of the ordinary total Hamiltonian. As can be seen from § 4, our result in (5.21) is exactly the AC Poynting splitting, which reduces to the AC Stark splitting in the dipole approximation. Thus, we have shown that our effective Hamiltonian can still produce gauge-invariant results even in the quantisation scheme in which the transverse vector potential is quantised first.

6. Conclusions

The approach of the effective Hamiltonian and wavefunction used in this paper has its origin in a manifestly gauge-invariant formulation of a quantised particle interacting with classical electromagnetic fields (see § 2 for references) and in the formulation of the gauge-invariant time-dependent perturbation theory (Yang 1981, 1982c). However, in order to consider the interaction with quantised electromagnetic fields, the introduction of the particle's effective Hamiltonian is a necessary step for each manipulation of the mathematics involved, for specifying the initial conditions of the particle's state (see § 3.1), and for easy recognition of all quantities of interest. It is also necessary to construct the effective *total* Hamiltonian since it is precisely in this form that the effective total Hamiltonian (e.g. see (5.4)) can be constructed very simply by applying Sakurai's correspondence rule (Sakurai 1967, equation (2.102)). We have demonstrated that the effective Hamiltonian approach can resolve the gauge problem for the classical fields and makes the procedures of quantisation of vector potentials and of fields completely equivalent.

Throughout this paper and other works of this author (see § 2 for references), we emphasise only one physical point: conservation of energy in the form of Poynting's theorem (e.g. Jackson 1975) through the correspondence principle in the equations of motion. By carrying this point into the form of mathematical formulation, we have shown that the physical principles can indeed produce results that are gauge invariant and agree with experimental observations. The AC Poynting splitting, which reduces to the familiar AC Stark splitting in the electric dipole approximation, is just one consequence of the conservation of energy. The gauge-invariant Jaynes–Cummings doublets as derived in § 5 also illustrate that the same physical principles can be applied to quantised fields.

As a final note, let us emphasise here that the *effective* Hamiltonian is derived from the ordinary Hamiltonians by considering only how to derive the gauge-invariant (and correct) transition amplitudes and probabilities. Its applications are therefore limited only to these and other related quantities, for example, the resonant frequencies. One should *not* use the effective Hamiltonian to derive the equations of motion of operators. The correct equations of motion of operators, on the other hand, must *always* be derived from the *ordinary* Hamiltonians. To illustrate this point more clearly, let us consider the equations of motion of the position operator $\boldsymbol{r}$ as determined by the ordinary Hamiltonian in (2.3) and the effective Hamiltonian in § 3.1. From (2.3), we get†

$$(\mathrm{d}\boldsymbol{r}/\mathrm{d}t)_H = [\boldsymbol{r}, H]/\mathrm{i}\hbar = m^{-1}(\boldsymbol{p} - e\boldsymbol{A}/c),$$

† If $f = f(\boldsymbol{r}, \boldsymbol{p}, t)$, then $(\mathrm{d}f/\mathrm{d}t)_H$ is defined to be $(\mathrm{d}f/\mathrm{d}t)_H \equiv \partial f/\partial t + [f, H]/\mathrm{i}\hbar$. The notation $(\mathrm{d}f/\mathrm{d}t)_{\mathscr{H}}$ is then defined to be such that the H in the above definition is replaced by the effective Hamiltonian $\mathscr{H}$.

which is obviously not equal to $(\mathrm{d}\boldsymbol{r}/\mathrm{d}t)_{\mathscr{H}}$ since $\mathscr{H}$ explicitly involves the electric field $\boldsymbol{E}$ whereas H does not. The only exception occurs when $\boldsymbol{B}=0$, in which case $(\mathrm{d}\boldsymbol{r}/\mathrm{d}t)_{\mathscr{H}}$ gives the equation of motion in the multipolar gauge. This example clearly demonstrates our caution concerning when and when not to apply the effective Hamiltonian approach proposed here.

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Appendix. Perturbative solutions of eigenfunctions

The main purpose is to briefly outline the procedure for solving the eigenvalues and eigenfunctions of the energy operator $H_B(t)$ in (2.6) and to provide enough information leading to the perturbative solutions of the effective Hamiltonian discussed in § 3.2. Most of the material here has been presented in a previous paper for the time-dependent perturbation formulation (Yang 1982c). If one is interested in more detailed information concerning this appendix, one should refer to that paper.

Our objective is to solve for the eigenvalues $\{E_j(t)\}$ and the eigenfunctions $\{\Psi_j(\boldsymbol{r},t)\}$ perturbatively using the Rayleigh–Schrödinger procedure (e.g. Messiah 1966). Let us therefore first decompose H_B as

$$H_B(t)=H_0+V_1(t)+V_2(t), \tag{A1}$$

where $H_0=\boldsymbol{p}^2/2m+eV_0$ is the 'unperturbed' Hamiltonian and

$$V_1(t)=-e(\boldsymbol{A}\cdot\boldsymbol{p}+\boldsymbol{p}\cdot\boldsymbol{A})/2mc, \qquad V_2(t)=(e\boldsymbol{A})^2/2mc^2. \tag{A2}$$

If we substitute (3.10) and (A1) into (2.6) treating time t as a parameter, then we get $H_0\phi_j(\boldsymbol{r})=\hbar\omega_j\phi_j(\boldsymbol{r})$ and

$$(H_0-\hbar\omega_j)\Psi_j^{(1)}(\boldsymbol{r},t)+(V_1-E_j^{(1)}(t))\phi_j(\boldsymbol{r})=0, \tag{A3}$$

$$(H_0-\hbar\omega_j)\Psi_j^{(2)}+(V_1-E_j^{(1)})\Psi_j^{(1)}+(V_2-E_j^{(2)})\phi_j=0, \tag{A4}$$

and so on. These perturbative eigenfunctions are required to satisfy the normalisation condition (3.11) so that the effective Hamiltonian is normalised to any order. These eigenvalue corrections can be obtained by the standard procedure; they are

$$E_j^{(1)}=\langle\phi_j|V_1|\phi_j\rangle, \tag{A5}$$

$$E_j^{(2)}=\langle\phi_j|V_1|\Psi_j^{(1)}\rangle+\langle\phi_j|V_2|\phi_j\rangle-E_j^{(1)}\delta_j^{(1)}, \tag{A6}$$

and so on. Here, $\delta_j^{(n)}$ are defined by

$$\delta_j^{(n)}=\langle\phi_j|\Psi_j^{(n)}\rangle, \qquad n\geqslant 1, \tag{A7}$$

and their values are chosen by the normalisation requirement in (3.11) and by the proper behaviour under gauge transformations. Our choices are:

$$\delta_j^{(1)} = (ie/c\hbar)\langle\phi_j|F[\boldsymbol{A}]|\phi_j\rangle, \tag{18}$$

$$\delta_j^{(2)} = -\tfrac{1}{2}\langle\Psi_j^{(1)}|\Psi_j^{(1)}\rangle + (ie/2c\hbar)\{\langle\phi_j|F[\boldsymbol{A}]|\Psi_j^{(1)}\rangle + \langle\Psi_j^{(1)}|F[\boldsymbol{A}]|\phi_j\rangle\}, \tag{A9}$$

where

$$F[\boldsymbol{A}] = \int_0^1 \mathrm{d}u\, \boldsymbol{r}\cdot\boldsymbol{A}(u\boldsymbol{r}, t). \tag{A10}$$

All higher δ's can be derived by following the procedure outlined in Yang (1982c, appendix). Finally, we note that the eigenvalue corrections $\{E_j^{(n)}\}$ are gauge invariant and independent of the values of $\{\delta_j^{(n)}\}$ (e.g. Yang 1977).

Because of our needs in § 3.2, we now evaluate $\langle\Psi_j^{(n-m)}|\xi_k^{(m)}\rangle$ where $\xi_k^{(m)}$ is defined in (3.15). If we use $H_0\phi_j = \hbar\omega_j\phi_j$, (A3) and the first-order Poynting's operator $P^{(1)}$ in (3.22), then it can be shown that

$$(H_0 - \hbar\omega_j)\xi_j^{(1)} = \mathrm{i}\hbar(P^{(1)} - \dot{E}_j^{(1)})\phi_j, \tag{A11}$$

where $\dot{E}_j^{(1)} = \mathrm{d}E_j^{(1)}/\mathrm{d}t$. It then follows from (A8) and (A11) that

$$\langle\phi_j|\xi_j^{(1)}\rangle = \langle\phi_j|F[-e\boldsymbol{E}]|\phi_j\rangle, \tag{A12}$$

$$\langle\phi_j|\xi_k^{(1)}\rangle = (\mathrm{i}/\omega_{jk})\langle\phi_j|P^{(1)}|\phi_k\rangle, \qquad j \neq k. \tag{A13}$$

These results will show up in the matrix elements of the first-order effective Hamiltonian in (3.20) and (3.21).

In order to derive the second-order elements in the effective Hamiltonian, we get from (A3) and (A4) the following equation:

$$(H_0 - \hbar\omega_j)\xi_j^{(2)} + (V_1 - E_j^{(1)})\xi_j^{(1)} = \mathrm{i}\hbar(P^{(1)} - \dot{E}_j^{(1)})\Psi_j^{(1)} + \mathrm{i}\hbar(P^{(2)} - \dot{E}_j^{(2)})\phi_j, \tag{A14}$$

where $\dot{E}_j^{(2)} = \mathrm{d}E_j^{(2)}/\mathrm{d}t$ and $P^{(2)}$ is the second-order Poynting operator in (3.24). From this equation one can show after a lengthy but straightforward procedure that, for $j \neq k$,

$$\begin{aligned}\langle\Psi_j^{(1)}|\xi_k^{(1)}\rangle + \langle\phi_j|\xi_k^{(2)}\rangle &= (\mathrm{i}/\omega_{jk})\{\langle\phi_j|P^{(1)}|u_k^{(2)}\rangle + \langle u_j^{(1)}|P^{(1)}|\phi_k\rangle \\ &\quad + \langle\phi_j|(P^{(2)} + (ie/c\hbar)[P^{(1)}, F[\boldsymbol{A}]])|\phi_k\rangle\} \\ &\quad -(\mathrm{i}/\hbar\omega_{jk}^2)\{E_j^{(1)}\langle\phi_j|P^{(1)}|\phi_k\rangle - \langle\phi_j|P^{(1)}|\phi_k\rangle E_k^{(1)}\},\end{aligned} \tag{A15}$$

where

$$u_j^{(1)} = \Psi_j^{(1)} - (ie/c\hbar)F[\boldsymbol{A}]\phi_j. \tag{A16}$$

For $j = k$, we use (A9) and $\xi_j^{(n)}$ defined in (3.24). If the ordering of the operators involving $\boldsymbol{A}$ and $\boldsymbol{E}$ is preserved (for later purposes), then

$$\begin{aligned}\langle\Psi_j^{(1)}|\xi_j^{(1)}\rangle + \langle\phi_j|\xi_j^{(2)}\rangle &= \tfrac{1}{2}\{\langle\zeta_j^{(1)}|u_j^{(1)}\rangle + \langle u_j^{(1)}|\zeta_j^{(1)}\rangle\} + \{\langle\phi_j|F[-e\boldsymbol{E}]|u_j^{(1)}\rangle + \langle u_j^{(1)}|F[-e\boldsymbol{E}]|\phi_j\rangle\} \\ &\quad + (e^2/2\mathrm{i}\hbar c^2)\langle\phi_j|[F[\boldsymbol{A}], F[\dot{\boldsymbol{A}}]]|\phi_j\rangle,\end{aligned} \tag{A17}$$

where $\dot{\boldsymbol{A}} = \partial\boldsymbol{A}(\boldsymbol{r}, t)/\partial t$ and, in parallel with (A16),

$$\zeta_j^{(1)} = \xi_j^{(1)} - F[-e\boldsymbol{E}]\phi_j. \tag{A18}$$

The main advantage of defining the $u_j^{(1)}$ in (A16) and $\zeta_j^{(1)}$ in (A18) is that they vanish identically whenever $\boldsymbol{B}(\boldsymbol{r}, t)$ vanishes, regardless of the forms of the vector and the scalar potentials. A minor convenience is that they are both orthogonal to ϕ_j, i.e. $\langle\phi_j|u_j^{(1)}\rangle = \langle\phi_j|\zeta_j^{(1)}\rangle = 0$.

We now discuss one special case of particular interest restricting to *classical* potentials and fields. If $\boldsymbol{B} = \nabla\times\boldsymbol{A} = 0$, then it can be shown (e.g. Yang 1977, 1982c) that (i) all $E_j^{(n)}$, $n \geq 1$, vanish identically, (ii) $u_j^{(1)} = 0$, and (iii) $P^{(2)} + (ie/c\hbar)([P^{(1)}, F(\mathbf{A}]] = 0$. Thus, *all* the second-order elements of the effective Hamiltonian vanish identically. (This conclusion is valid for all other higher orders by carrying out the details of the mathematical procedure, and is consistent with previous results obtained by this author (Yang 1976).) This conclusion is derived, as shown in (A16)–(A18), using the potentials in any *arbitrary* gauge.

The consequence of the gauge invariance of all $E_j^{(n)}$, $n \geq 1$, is that they depend only on the magnetic field, $\boldsymbol{B} = \nabla\times\boldsymbol{A}$, represented by the vector potentials. In other words, the $E_j^{(n)}$ derived in the Coulomb gauge will be identical to those derived in the Lorentz or the multipolar gauge, and therefore there is no need to choose any particular gauge to work with simply because this gauge has some 'special' properties.

Because of the manifest gauge invariance (i.e. same forms and same values in *all* gauges), we may therefore extend all our previous perturbative results in this appendix to the quantised potentials and fields. This will, however, make all our quantities operators in the photon space. The main item now is to see whether the $E_j^{(n)}$ will be gauge invariant for the quantised potentials. For this purpose, let us consider a quantised vector potential of the usual transverse form (omitting the normalisation factor):

$$\hat{\boldsymbol{A}}_t(\boldsymbol{r}, t) = \boldsymbol{e}_\lambda(a_\lambda\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + a_\lambda^\dagger\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}), \tag{A19}$$

where $\boldsymbol{e}_\lambda$ (real) is a polarisation vector, $\boldsymbol{k}$ is the propagation vector with $\boldsymbol{k}\cdot\boldsymbol{e}_\lambda = 0$, and a_λ ($a_\lambda^\dagger$) is a photon annihilation (creation) operator. Then it can be shown that

$$\langle\phi_j|\hat{\boldsymbol{A}}_t(\boldsymbol{0}, t)\cdot\boldsymbol{p}|\phi_j\rangle = 0 \qquad \text{for all } j, \tag{A20}$$

which agrees with our classical results and implies that the $E_j^{(1)}$, now an operator in the photon space, still depends on the magnetic field. All other higher-order eigenvalue corrections can probably be shown in a similar manner.

The differences between the classical potentials and the quantised ones in (A17) and (A18) can be read immediately from the commutators involved by noting that $u_j^{(1)}$ still vanishes for the quantised potentials. Once again, these commutators are gauge invariant whether or not the scalar potential is used to quantise the fields (since the scalar potential commutes with the vector potentials). This concludes this appendix.

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