

Theory of spontaneous light emission

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Understanding the discrete spectrum of light emitting atoms had been the primary motivation for developing a theory beyond classical mechanics and electrodynamics. It was far from being likely that Planck's constant h which he introduced to explain the continuous spectrum of light emitting incandescent "black bodies" could have anything to do with those discrete spectra. For this reason it came much as a surprise when Niels Bohr [1] could explain the well studied spectrum of the hydrogen atom by requiring the associated electron to orbit around the nucleus on concentric circles where its angular momentum L equals integer multiples of Planck's constant h : $L = n h$ and $n = 1, 2, \dots$. In each of the orbitals the electron was considered to be in a stable state, but it was allowed to jump spontaneously to another orbital of lower energy and convert the energy difference into light. Those "quantum jumps" still belong to the vocabulary of present-day quantum mechanics (see e. g. [2]) although their existence lacks any foundation as we shall demonstrate. In Bohr's theory the electron always possesses a non-vanishing angular momentum so that the centrifugal force keeps it well separated from the nucleus and thereby ensures a well defined size of the hydrogen atom for $n = 1$, its state of lowest energy. In reality, i. e. according to our approach, the particle under study, the electron, is driven by the combined action of the static classical Coulomb force exercised by the nucleus and by the stochastic forces of the vacuum. As a consequence, its probability amplitude obeys the Schrödinger equation, the time-independent solutions of which, $\hat{\psi}_{nlm}(\mathbf{r})$, are characterized by integer quantum numbers n, l, m where \mathbf{r} is referenced to the position of the nucleus. The latter is considered to be a clamped point charge for simplicity. The state $\hat{\psi}_{100}(\mathbf{r})$ refers to the groundstate where $\langle \mathbf{L} \rangle = 0$, distinctly different from Bohr's theory. Only excited states ($n > 1$) for which l equals $|m|$ display a toroidal probability density and resemble diffuse circular Bohr orbitals.

The energies that are associated with the eigensolutions $\hat{\psi}_{nlm}(\mathbf{r})$ are given by

$$E_{nlm} = -\frac{R}{n^2} \quad \text{where } n > l + |m| \quad l = 0, 1, 2, \dots, \quad m = -l, \dots, 0, \dots, +l \quad (1)$$

and

$$R = \frac{1}{2} \alpha^2 m_0 c^2 = \text{Rydberg constant}; \quad R = 13.6059 \text{ eV}.$$

Here m_0 denotes the electron's rest mass, c the velocity of light in vacuo and α the fine structure constant:

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} = \frac{1}{137.036}; \quad \hbar = \frac{h}{2\pi}.$$

The quantity ϵ_0 represents the permittivity of the vacuum and e is the elementary charge.

It is one of the fundamental credos of conventional quantum mechanics that eigenvalues of the energy as in (1) constitute results of appropriate measurements, more precisely, as Mermin [7] states in a widely recognized article:

“...quantum mechanics requires that the result of measuring an observable be an eigenvalue of the corresponding Hermitian operator.....”

Although this statement belongs to the seemingly incredible rituals in teaching quantum mechanics, it is not even wrong but rather void of meaning. Of course, there has always been the discrete hydrogen spectrum in the back of the minds of the founding fathers, and that spectrum seemed to be clearly some map of the eigenvalues (1). But in actual fact one commonly measures the wave length of the emitted light by a spectrometer about 10^{10} atomic diameters away from the emitter. When the packet of the light wave enters the “measurement process”, i.e. the spectrometer, the atom has long left its original state. The phraseology “measuring eigenvalues” invites the impression as if one were dealing with something like measuring somebody’s collar size. Moreover, as we shall show, in the emission process the energy of the atom attains all values between the eigenvalues that are involved in the transition, but the frequency and the measured associated wavelength of the emitted light remain constant.

Before I go into the details of my approach to spontaneous light emission, I want to emphasize that its basic idea is almost identical with what has been popularized by E. T. Jaynes already in 1963 [3] and the following years [4], [5] under the name “neoclassical theory (NCT)”. This name is incorrect and therefore completely misleading. In my theory (and in Jaynes’ theory as well) the electromagnetic field is generated by an oscillating electronic current density which sets up a vector potential and this, in turn, appears in the kinetic energy operator of the electronic Hamiltonian. What - in the world - should be considered “neoclassical” in using this interrelation?

The present theory of spontaneous light emission is developed within the framework that we have elaborated in our article on “Stochastic Foundation of Quantum Mechanics and the Origin of Particle Spin” [6].

Our point of departure from the standard approach consists in questioning the assumption that eigenstates “can be prepared”. A thoughtless assumption! How should such a “preparation” be achieved? By definition, an eigenstate is associated with zero variance of its energy. Hence, because of

$$\Delta E \Delta t \approx \hbar \quad \text{where} \quad \Delta E = \sqrt{(E - E_{nlm})^2} \quad (2)$$

the preparation time Δt is infinite for an eigenstate.¹ That is, in reality, an excited state can only be a solution to the **time-dependent** Schrödinger equation and hence may be cast as

$$\psi(\mathbf{r}, t) = \sum_{n,l,m} c_{nlm} \hat{\psi}_{nlm}(\mathbf{r}) e^{-i \frac{E_{nlm}}{\hbar} t} \quad (3)$$

where

$$\int \hat{\psi}_{n'l'm'}^*(\mathbf{r}) \hat{\psi}_{nlm}(\mathbf{r}) d^3r = \delta_{n'n} \delta_{l'l} \delta_{m'm} \quad (4)$$

¹A similar situation occurs if one wants to excite a superconducting cavity in one of its modes. If the cavity can lose energy to the outside at a small rate it behaves as if it were slightly attenuated. The time it takes to arrive at a stationary state grows longer and longer the weaker the energy loss becomes. The excitation time tends to infinity as the loss rate tends to zero.

and because of

$$\int |\psi(\mathbf{r}, t)|^2 d^3r = 1 \quad \text{one has} \quad \sum_{n,l,m} |c_{nlm}|^2 = 1. \quad (5)$$

Each term under the sum in Eq.(3) satisfies individually the time-dependent Schrödinger equation of the hydrogen electron since by definition

$$\hat{H}\hat{\psi}_{nlm}(\mathbf{r}) = E_{nlm}\hat{\psi}_{nlm}(\mathbf{r}) \quad \text{where} \quad \hat{H} = \frac{\hat{\mathbf{p}}^2}{2m_0} - \frac{e^2}{4\pi\epsilon_0 r} \quad \text{and} \quad \hat{\mathbf{p}} = -i\hbar\nabla. \quad (6)$$

A realistic “eigenstate” is characterized by the property that the square modulus of one the coefficients c_{nlm} in Eq.(3) is close to unity, that of the others correspondingly small.

In the following we consider the situation in which the hydrogen atom has been excited from the ground state 1s to the state 2p where $m = 0$. The excitation may have been caused by absorbing linearly polarized light. As stated above, it is, as a matter of fact, impossible that the atom in the excitation process really ends up in the eigenstate 2p. Its state will rather have the form

$$\psi(\mathbf{r}, t) = c_0 \hat{\psi}_{1s}(\mathbf{r}) e^{-i\frac{E_{1s}}{\hbar}t} + c_1 \hat{\psi}_{2p}(\mathbf{r}) e^{-i\frac{E_{2p}}{\hbar}t} \quad \text{where} \quad 0 < |c_0| \ll |c_1| < 1. \quad (7)$$

Using Eq.(7) we obtain

$$\int \psi^*(\mathbf{r}, t) \hat{H} \psi(\mathbf{r}, t) d^3r = \underbrace{|c_1|^2}_{=1-|c_0|^2} E_{2p} + |c_0|^2 E_{1s} \quad \text{that is} \quad E = E_{2p} - \tilde{E} |c_0|^2 \quad (8)$$

where

$$\tilde{E} = E_{2p} - E_{1s}. \quad (9)$$

The expression $\tilde{E} |c_0|^2$ represents obviously the uncertainty ΔE with which the 2p-state has been “prepared”.

From Eq.(7) we may form the electronic charge density $\rho(\mathbf{r}, t) = e |\psi(\mathbf{r}, t)|^2$ which we cast as

$$\rho(\mathbf{r}, t) = \rho_0(\mathbf{r}) + \tilde{\rho}(\mathbf{r}, t) \quad (10)$$

where

$$\rho_0(\mathbf{r}) = e \left[|c_0|^2 \hat{\psi}_{1s}^2(\mathbf{r}) + |c_1|^2 \hat{\psi}_{2p}^2(\mathbf{r}) \right] \quad (11)$$

and

$$\tilde{\rho}(\mathbf{r}, t) = |c_0^* c_1| e \hat{\psi}_{1s}(\mathbf{r}) \hat{\psi}_{2p}(\mathbf{r}) \left[e^{i\left[\frac{E_{2p}-E_{1s}}{\hbar}t + \varphi\right]} + e^{-i\left[\frac{E_{2p}-E_{1s}}{\hbar}t + \varphi\right]} \right]. \quad (12)$$

where φ is defined through

$$c_0^* c_1 = |c_0^* c_1| e^{i\varphi}. \quad (13)$$

Here we have exploited the fact that $\hat{\psi}_{1s}(\mathbf{r})$ and $\hat{\psi}_{2p}(\mathbf{r})$ are real-valued functions. Eq.(10) may hence be rewritten

$$\rho(\mathbf{r}, t) = \rho_0(\mathbf{r}) + 2 |c_0^* c_1| \tilde{\rho}_0(\mathbf{r}) \cos(\omega t + \varphi) \quad (14)$$

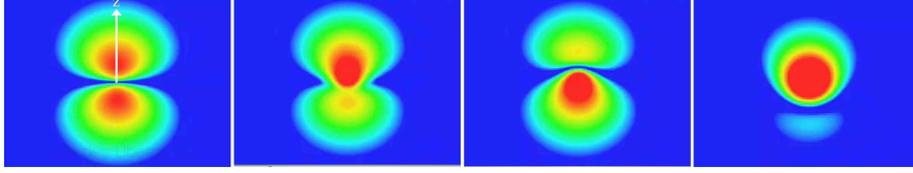


Figure 1: Four snapshots of the color coded density of a H-atom in the transition $2p \rightarrow 1s$

where

$$\tilde{\rho}_0(\mathbf{r}) = e \hat{\psi}_{1s}(\mathbf{r}) \hat{\psi}_{2p}(\mathbf{r}) \quad \text{and} \quad \omega = \frac{E_{2p} - E_{1s}}{\hbar} \quad \text{i. e.} \quad \hbar \omega = E_{2p} - E_{1s} \quad (15)$$

The figure above shows four snapshots of the time evolution of $\rho(\mathbf{r}, t)$. As one can see from Eq.(8):

$$E = |c_0|^2 E_{1s} + |c_1|^2 E_{2p} \quad \text{and} \quad 0 \leq |c_0|; 0 \leq |c_1| \quad |c_0|^2 + |c_1|^2 = 1$$

the energy of the electron can have any value between E_{2p} and E_{1s} . **Irrespective of the value of E** its charge density oscillates sharply at ω ! In the following calculation we shall derive a transition time which the electron takes to change its state from (7) with $0 < |c_0| \ll |c_1| < 1$ to a form of $\psi(\mathbf{r}, t)$ where $|c_0| \approx 1$ and $|c_1| \approx 0$. This transition time turns out to be of the order of $10^{-9} s$, that is, **there are no quantum jumps!**

The function $\psi(\mathbf{r}, t)$ defined by Eq.(7) is a solution to the time-dependent Schrödinger equation

$$\hat{H}\psi(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) \quad (16)$$

only as long as the coefficients c_0, c_1 are constant. However, even when c_0 is very small compared to unity, $\rho(\mathbf{r}, t)$ oscillates at the frequency ω and thus gives rise to the emission of an electromagnetic wave. The latter is polarized in the direction of the quantization axis of $\hat{\psi}_{2p}(\mathbf{r})$ which also defines the symmetry axis of $\hat{\psi}_{1s}(\mathbf{r}) \hat{\psi}_{2p}(\mathbf{r})$ in Eq.(15). As the atom loses energy in building up the electromagnetic wave, E in Eq.(8) decreases, and hence c_0 must now increase as a function of time. This is a consequence of the fact that the radiation field acts back on the atom, and therefore the Hamiltonian in Eq.(16) is now modified:

$$\hat{H}'\psi(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) \quad \text{where} \quad \hat{H}' = \frac{(\hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r}, t))^2}{2m_0} - \frac{e^2}{4\pi\epsilon_0 r} \quad (17)$$

with $\mathbf{A}(\mathbf{r}, t)$ denoting the vector potential of the radiation field. We mention here only in passing that a quantization of the radiation field does not change the line of argument we shall pursue in the following. This will be outlined at the end of this section.

To obtain $\mathbf{A}(\mathbf{r}, t)$ we first determine the current density

$$\mathbf{j}(\mathbf{r}, t) = \frac{e\hbar}{2im_0} [\psi^*(\mathbf{r}, t)\nabla\psi(\mathbf{r}, t) - \psi(\mathbf{r}, t)\nabla\psi^*(\mathbf{r}, t)]. \quad (18)$$

On inserting $\psi(\mathbf{r}, t)$ from Eq.(7) the current density takes the form

$$\mathbf{j}(\mathbf{r}, t) = \frac{e\hbar}{m_0} |c_0^* c_1| [\hat{\psi}_{1s}(\mathbf{r})\nabla\hat{\psi}_{2p}(\mathbf{r}) - \hat{\psi}_{2p}(\mathbf{r})\nabla\hat{\psi}_{1s}(\mathbf{r})] \sin(\omega t + \varphi). \quad (19)$$

The vector potential $\mathbf{A}(\mathbf{r}, t)$ and $\mathbf{j}(\mathbf{r}, t)$ are interconnected by

$$\mathbf{A}(\mathbf{r}, t) = \frac{\mu_0}{4\pi} \int \frac{\mathbf{j}(\mathbf{r}', t - \frac{|\mathbf{r}' - \mathbf{r}|}{c})}{|\mathbf{r}' - \mathbf{r}|} d^3r' \quad \text{where} \quad \mu_0 = \frac{1}{\epsilon_0 c^2}. \quad (20)$$

Because of Eq.(18) $\mathbf{A}(\mathbf{r}, t)$ is a functional of $\psi(\mathbf{r}, t)$. It follows then from inspection of Eq.(17) that the modified Schrödinger equation (17) constitutes now a **non-linear** partial differential equation since the Hamiltonian \hat{H}' depends on $\psi(\mathbf{r}, t)$. Below we shall derive a detailed solution to this equation. If one is not interested in the details of the time dependence one can take a short-cut:

First we give the expressions

$$\hat{\psi}_{1s}(\mathbf{r})\nabla\hat{\psi}_{2p}(\mathbf{r}) \quad \text{and} \quad \hat{\psi}_{2p}(\mathbf{r})\nabla\hat{\psi}_{1s}(\mathbf{r})$$

a different form by using the identity (which is just an application of the chain rule):

$$[\hat{H}\mathbf{r} - \mathbf{r}\hat{H}]\hat{\psi}(\mathbf{r}) = -i\frac{\hbar}{m_0}\hat{\mathbf{p}}\hat{\psi}(\mathbf{r}) = -\frac{\hbar^2}{m_0}\nabla\hat{\psi}(\mathbf{r}). \quad (21)$$

This yields

$$\hat{\psi}_{1s}(\mathbf{r})\nabla\hat{\psi}_{2p}(\mathbf{r}) = \frac{m_0}{\hbar^2}[\hat{\psi}_{1s}(\mathbf{r})\mathbf{r}\hat{H}\hat{\psi}_{2p}(\mathbf{r}) - \hat{\psi}_{1s}(\mathbf{r})\hat{H}\mathbf{r}\hat{\psi}_{2p}(\mathbf{r})]$$

and

$$\hat{\psi}_{2p}(\mathbf{r})\nabla\hat{\psi}_{1s}(\mathbf{r}) = \frac{m_0}{\hbar^2}[\hat{\psi}_{2p}(\mathbf{r})\mathbf{r}\hat{H}\hat{\psi}_{1s}(\mathbf{r}) - \hat{\psi}_{2p}(\mathbf{r})\hat{H}\mathbf{r}\hat{\psi}_{1s}(\mathbf{r})].$$

Forming the integral of Eq.(19), exploiting the hermiticity of \hat{H} , using Eq.(6) and $\hbar\omega = E_{2p} - E_{1s}$ we thus obtain

$$I(t)\mathbf{e}_z = 2|c_0^*c_1|e\omega \int \hat{\psi}_{1s}(\mathbf{r})\mathbf{r}\hat{\psi}_{2p}(\mathbf{r})d^3r \sin(\omega t + \varphi) \quad \text{where} \quad \mathbf{e}_z || z - \text{axis}. \quad (22)$$

The quantity $I(t)$ denotes the alternating current that is set up in the atom as a result of c_0 not being zero. The quantization axis of $\hat{\psi}_{2p}(\mathbf{r})$ is taken along the z -axis. We may rewrite the above integral

$$\int \hat{\psi}_{1s}(\mathbf{r})\mathbf{r}\hat{\psi}_{2p}(\mathbf{r})d^3r = \int \rho_{dipole}(\mathbf{r})\mathbf{r}d^3r = \bar{\mathbf{r}}$$

where we have expressed the fact that $\hat{\psi}_{1s}(\mathbf{r})\hat{\psi}_{2p}(\mathbf{r})$ represents a dipole-type probability density. Hence, Eq.(22) can be cast as

$$I(t)\mathbf{e}_z = -\frac{d}{dt}\mathbf{p}(t) \quad \text{where} \quad \mathbf{p}(t) = g(t)|e|\bar{\mathbf{r}}\cos\omega t \quad \text{and} \quad g(t) = 2|c_0^*(t)c_1(t)|.$$

As the emission of the electromagnetic wave proceeds, the coefficient c_0 becomes larger and will finally attain its largest value 1 at the end of the transition. According to Eq.(3) it will be equal to $\frac{1}{\sqrt{2}}$ in the middle of the transition. The coefficient c_1 changes in reverse since the sum of the square of the coefficients must be unity at any time. Hence, in the middle of the transition the function $g(t)$ defined above attains its maximum value 1 and drops asymptotically to zero on either side. To serve the purpose of the present short-cut, we approximate the actually bell-shape

time-dependence of $g(t)$ by a rectangle of width $\hat{\tau}$ and height unity.

We now invoke Hertz's result on the density $\mathbf{S}(\mathbf{r}, t)$ of the energy flow from an oscillating dipole:

$$\mathbf{S}(r, \theta, t) = \frac{1}{16\pi^2 \varepsilon_0 c^3} \frac{\sin^2 \theta}{r^2} \left[\frac{d^2}{dt^2} \mathbf{p}(t) \right]^2$$

where θ is the angle that \mathbf{r} encloses with the dipole axis.

Forming a surface integral with $\mathbf{S}(r, \theta, t)$ over a concentric sphere of radius r and averaging over one oscillation period one arrives at

$$S(t) = [g(t)]^2 \frac{e^2 \omega^4}{6\pi \varepsilon_0 c^3} |\mathbf{p}_{n'n}|^2 \quad \text{where} \quad n' = 1s; n = 2p$$

and

$$\mathbf{p}_{n'n} = \int \hat{\psi}_{n'}(\mathbf{r}) \mathbf{r} \hat{\psi}_n(\mathbf{r}) d^3r; \quad [g(t)]^2 = \begin{cases} 1 & \text{for } |t| \leq \hat{\tau}/2 \\ 0 & \text{for } |t| > \hat{\tau}/2 \end{cases} \quad (23)$$

Integration of $S(t)$ over the transition time $\hat{\tau}$ must yield $E_{2p} - E_{1s} = \hbar \omega$:

$$\int_{-\hat{\tau}/2}^{+\hat{\tau}/2} S(t) dt = \hbar \omega = \frac{e^2 \omega^4}{6\pi \varepsilon_0 c^3} |\mathbf{p}_{n'n}|^2 \hat{\tau}.$$

From this we obtain an expression for the inverse of the transition time

$$\frac{1}{\hat{\tau}} = \frac{e^2 \omega^3}{6\pi \varepsilon_0 c^3 \hbar} |\mathbf{p}_{n'n}|^2 \quad \text{or} \quad \frac{1}{\hat{\tau}} = \alpha \frac{2\omega^3}{3c^2} |\mathbf{p}_{n'n}|^2 \quad \text{where} \quad \alpha = \frac{e^2}{4\pi \varepsilon_0 \hbar} \quad (24)$$

in agreement with the result of the standard calculation (s. e. g. [9]) which is based on a remarkably different concept. It should be observed, however, that this calculation yields an expression for the transition rate $\frac{1}{\hat{\tau}}$ which is identified with $\frac{d}{dt} |c_0|^2(t)|_{t=0} = \frac{2}{\hat{\tau}}$. Hence

$$\frac{1}{\hat{\tau}'} = \frac{e^2 \omega^3}{3\pi \varepsilon_0 c^3 \hbar} |\mathbf{p}_{n'n}|^2.$$

It is worth noting that the problem of spontaneous light emission has for the first time been treated by Fermi [8] in 1927. He chose an approach very similar to ours, but used the classical expression for the radiation back action $\propto \frac{d^3}{dt^3} p$ which led to a frequency shift of the emitted light depending on the transition time. However, this is at variance with the observation.

We now turn back to the problem of calculating the detailed time-dependence of $|c_0(t)|^2, |c_1(t)|^2$. To this end we first observe that

$$\hat{H}' = \hat{H} + \hat{H}_{int} = \frac{(\hat{\mathbf{p}} - e\mathbf{A}(\mathbf{r}, t))^2}{2m_0} - \frac{e^2}{4\pi \varepsilon_0 r} = \hat{H} - \frac{e}{m_0} \mathbf{A}(\mathbf{r}, t) \cdot \hat{\mathbf{p}} + \dots \quad (25)$$

where the dots stand for $\frac{(e\mathbf{A}(\mathbf{r}, t))^2}{2m_0}$ which will be neglected for the term linear in $\mathbf{A}(\mathbf{r}, t)$. Inserting (25) and $\psi(\mathbf{r}, t)$ from (7) into the time-dependent Schrödinger equation Eq.(17), multiplying this equation by $\hat{\psi}_{2p}(\mathbf{r}) e^{i\frac{E_{2p}}{\hbar} t}$ or alternatively by $\hat{\psi}_{1s}(\mathbf{r}) e^{i\frac{E_{1s}}{\hbar} t}$ and performing a real-space integration one arrives at

$$i\hbar \dot{c}_1 = c_0 M_{10} e^{i\omega t} + c_1 M_{11} \quad (26)$$

where $M_{10} = \int \hat{\psi}_{2p}(\mathbf{r}) \hat{H}_{int} \hat{\psi}_{1s}(\mathbf{r}) d^3r$ and $M_{11} = \int \hat{\psi}_{2p}(\mathbf{r}) \hat{H}_{int} \hat{\psi}_{2p}(\mathbf{r}) d^3r$

and

$$\hat{H}_{int} = i \frac{e\hbar}{m_0} \mathbf{A}(\mathbf{r}, t) \cdot \nabla. \quad (27)$$

Analogously we have, in obvious notation

$$i\hbar \dot{c}_0 = c_1 M_{01} e^{-i\omega t} + c_0 M_{00}. \quad (28)$$

According to Eqs.(19) and (20) one has

$$\begin{aligned} \mathbf{A}(\mathbf{r}, t) = & \quad (29) \\ |c_0^* c_1| \frac{e\hbar}{4\pi\epsilon_0 m_0 c^2} \int \frac{[\hat{\psi}_{1s}(\mathbf{r}') \nabla' \hat{\psi}_{2p}(\mathbf{r}') - \hat{\psi}_{2p}(\mathbf{r}') \nabla' \hat{\psi}_{1s}(\mathbf{r}')] \sin[\omega(t - \frac{|\mathbf{r}-\mathbf{r}'|}{c}) + \varphi]}{|\mathbf{r} - \mathbf{r}'|} d^3 r'. \end{aligned}$$

For light frequencies $\nu = \frac{\omega}{2\pi} \approx 10^{15} s^{-1}$ and $|\mathbf{r} - \mathbf{r}'| \lesssim 4 \cdot 10^{-8} cm$ for points within the atomic volume we have $\frac{\omega}{c} |\mathbf{r} - \mathbf{r}'| \lesssim 10^{-2}$, and hence we may approximate:

$$\sin[\omega(t - \frac{|\mathbf{r}-\mathbf{r}'|}{c}) + \varphi] \approx \sin(\omega t + \varphi) - \omega \frac{|\mathbf{r}-\mathbf{r}'|}{c} \cos(\omega t + \varphi)$$

Inserting this into Eq.(29) one obtains

$$\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_1(\mathbf{r}, t) + \mathbf{A}_2(\mathbf{r}, t) = \hat{\mathbf{A}}_1(\mathbf{r}) \sin(\omega t + \varphi) + \hat{\mathbf{A}}_2(\mathbf{r}) \cos(\omega t + \varphi) \quad (30)$$

where

$$\hat{\mathbf{A}}_1(\mathbf{r}) = |c_0^* c_1| \frac{e\hbar}{4\pi\epsilon_0 m_0 c^2} \int \frac{[\hat{\psi}_{1s}(\mathbf{r}') \nabla' \hat{\psi}_{2p}(\mathbf{r}') - \hat{\psi}_{2p}(\mathbf{r}') \nabla' \hat{\psi}_{1s}(\mathbf{r}')] d^3 r'}{|\mathbf{r} - \mathbf{r}'|} \quad (31)$$

and

$$\hat{\mathbf{A}}_2(\mathbf{r}) = -|c_0^* c_1| \frac{e\hbar\omega}{4\pi\epsilon_0 m_0 c^3} \int [\hat{\psi}_{1s}(\mathbf{r}') \nabla' \hat{\psi}_{2p}(\mathbf{r}') - \hat{\psi}_{2p}(\mathbf{r}') \nabla' \hat{\psi}_{1s}(\mathbf{r}')] d^3 r' \quad (32)$$

The integral in Eq.(32) can be rewritten by using the identity (21):

$$\begin{aligned} \mathbf{A}_2(\mathbf{r}, t) = \mathbf{A}_2 \cos(\omega t + \varphi) = \\ -2|c_0^* c_1| \frac{e\omega^2}{4\pi\epsilon_0 c^3} \underbrace{\int \hat{\psi}_{1s}(\mathbf{r}') \mathbf{r}' \hat{\psi}_{2p}(\mathbf{r}') d^3 r'}_{=\mathbf{p}_{n'n}} \cos(\omega t + \varphi). \end{aligned} \quad (33)$$

We now form the matrix element of $\hat{H}_{int} = i \frac{e\hbar}{m_0} \mathbf{A}(\mathbf{r}, t) \cdot \nabla$ according to Eq.(26) using again the identity (21).

$$M_{10} = \frac{i\hbar}{m_0} 2|c_0^* c_1| \frac{e^2 \omega^2}{4\pi \epsilon_0 c^2} \mathbf{p}_{n'n} \cdot \underbrace{\int \hat{\psi}_{2p} \nabla \hat{\psi}_{1s} d^3 r}_{=-\omega \frac{m_0}{\hbar} \mathbf{p}_{n'n}} \cos(\omega t + \varphi) \quad (34)$$

$$+ \frac{i\hbar}{m_0} \int \hat{\psi}_{2p}(\mathbf{r}) \frac{e}{m_0} \hat{\mathbf{A}}_1(\mathbf{r}) \cdot \nabla \hat{\psi}_{1s}(\mathbf{r}) d^3 r \sin(\omega t + \varphi)$$

We multiply Eq.(26) by c_1^* and form the sum with its complex conjugate. The result may be written:

$$\begin{aligned} \frac{\partial}{\partial t}|c_1(t)|^2 &= -4\gamma |c_0^*(t)c_1(t)|^2 \cos^2(\omega t + \varphi) \\ &+ 2|c_0^*(t)c_1(t)| \int \hat{\psi}_{2p}(\mathbf{r}) \frac{e}{m_0} \hat{\mathbf{A}}_1(\mathbf{r}) \cdot \nabla \hat{\psi}_{1s}(\mathbf{r}) d^3r \cos(\omega t + \varphi) \sin(\omega t + \varphi) \\ &+ 2|c_1(t)|^2 \int \hat{\psi}_{2p}(\mathbf{r}) \frac{e}{m_0} \hat{\mathbf{A}}_1(\mathbf{r}) \cdot \nabla \hat{\psi}_{2p}(\mathbf{r}) d^3r \sin(\omega t + \varphi) \\ &+ 2|c_1(t)|^2 \int \hat{\psi}_{2p}(\mathbf{r}) \frac{e}{m_0} \hat{\mathbf{A}}_2(\mathbf{r}) \cdot \nabla \hat{\psi}_{2p}(\mathbf{r}) d^3r \cos(\omega t + \varphi). \end{aligned} \quad (35)$$

The quantity γ in the first line of this equation stands for

$$\gamma = \frac{e^2 \omega^3}{4\pi \varepsilon_0 c^3 \hbar} |\mathbf{p}_{n'n}|^2. \quad (36)$$

We now perform a time average on the right-hand side of Eq.(35) over successive oscillation periods $T = \frac{2\pi}{\omega}$ of the emitted light. Since the emission time $\hat{\tau}$ is many orders of magnitude larger than T , one may approximate $|c_{0/1}(t)|$ by $|c_{0/1}(\bar{t}_\nu)|$ where $\nu = 1, 2, \dots$ counts successive oscillation intervals and \bar{t}_ν denotes an appropriately chosen time in the respective interval. On performing the time average all terms on the right-hand side of Eq.(35) now drop out except for the first one. Hence we arrive at

$$\frac{\partial}{\partial t}|c_1(t)|^2 = -2\gamma |c_0(t)|^2 |c_1(t)|^2 \quad (37)$$

where we have used $\overline{\cos^2(\omega t + \varphi)} = \frac{1}{2}$ with the bar denoting time averaging. We have, furthermore, replaced the histogram-type functions of time $|c_{0/1}(\bar{t}_\nu)|^2$ on the right-hand side by their smooth least mean-square fits.

In complete analogy we obtain

$$\frac{\partial}{\partial t}|c_0(t)|^2 = 2\gamma |c_0(t)|^2 |c_1(t)|^2. \quad (38)$$

Since $|c_0(t)|^2 + |c_1(t)|^2 = 1$, the time derivative of this sum must vanish. This is obviously ensured by the above two coupled equations (37) and (38). It can readily be verified that their two solutions are

$$|c_0(t)|^2 = \frac{1}{2} (1 + \tanh \frac{2t}{\tau}) \quad \text{and} \quad |c_1(t)|^2 = \frac{1}{2} (1 - \tanh \frac{2t}{\tau}). \quad (39)$$

On multiplying these two functions one gets

$$|c_0(t)|^2 |c_1(t)|^2 = \frac{1}{4} \frac{1}{\cosh^2 \frac{2t}{\tau}}.$$

From Eq.(37) we have

$$\frac{\partial}{\partial t}|c_1(t)|^2 = -2\gamma |c_0(t)|^2 |c_1(t)|^2 = -\frac{1}{2} \gamma \frac{1}{\cosh^2 \frac{2t}{\tau}}.$$

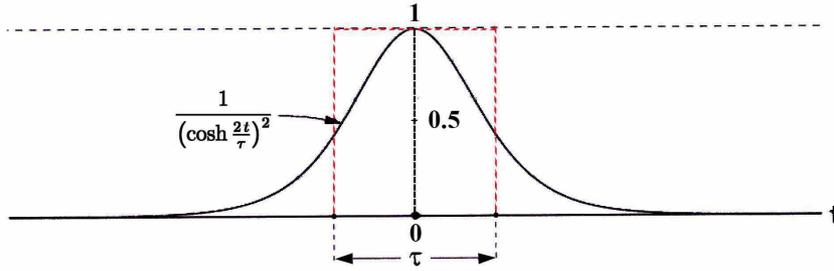


Figure 2: Optical transition: time-dependence of the “driving force” $\propto \mathbf{A}_2^2$

On the other hand it follows from Eq.(39) on differentiating $|c_1(t)|^2$

$$\frac{\partial}{\partial t}|c_1(t)|^2 = -\frac{1}{\tau} \frac{1}{\cosh^2 \frac{2t}{\tau}}.$$

That means, the functions $|c_1(t)|^2$ and $|c_0(t)|^2$ fulfill Eqs.(37) and (38) if

$$\frac{1}{\tau} = \frac{1}{2} \gamma = \frac{e^2 \omega^3}{8\pi \varepsilon_0 c^3 \hbar} |\mathbf{p}_{n'n}|^2.$$

Comparing this result with our “short-cut calculation” (24) we see that it is 25% smaller than the latter:

$$\frac{1}{\tau} = 0.75 \frac{1}{\hat{\tau}}.$$

This difference originates in the simplification of the time dependence of $|c_1(t)|^2$ and $|c_0(t)|^2$ in taking the short-cut.

The following figure illustrates the time dependences according to Eq.(39).

We have marked two points A and B on the left-hand side of the curve for $|c_1(t)|^2$. As explained in connection with Eq.(8), the quantity $[E_{2p} - E_{1s}] |c_0|^2$ represents the energy uncertainty with which the state $\hat{\psi}_{2p}(\mathbf{r})$ has been “prepared” as a result of the finite preparation time Δt . With the aid of Eq.(2) and $|c_1(t)|^2 = 1 - |c_0(t)|^2$ this can be recast

$$1 - |c_1(t)|^2 = \frac{\hbar}{[E_{2p} - E_{1s}] \Delta t}.$$

The shorter the excitation time, the more $|c_1(t)|^2$ departs from unity. Hence, point A refers to a longer excitation time than point B. Correspondingly, if the system has landed in A after the excitation process, it takes a longer time to reach the transition interval (marked by two vertical dashed lines) than it would take if it would start at B. One may refer to these residence times prior to emission as “dead times”. It should be noticed, however, that the “emission time”, limited by the two vertical dashed lines, remains largely unaffected by the different lengths of the dead times. That is to say, largely independent of the form of the excitation one observes a spectral line of a natural width that is only determined by the two states of the atom under study.

The result obtained above contrasts remarkably with that of Weisskopf and Wigner [9]. Their article is still considered groundlaying for the theory of spontaneous

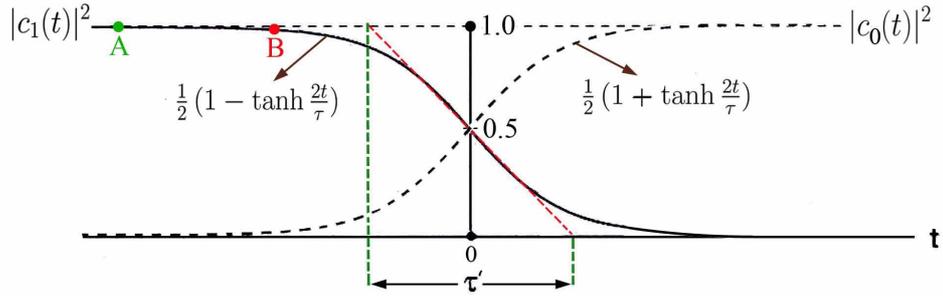


Figure 3: Optical transition between two states: Time dependence of the modulus square of the two-state related coefficients

light emission. However, these authors arrive at $|c_1(t)|^2 = e^{-\frac{t}{\tau}}$ which appears to be plausible, but is inconsistent with a solution to the time-dependent Schrödinger equation as follows from our derivation.

Another point of misunderstanding concerns “the measurement” of that exponential decay law $e^{-\frac{t}{\tau}}$. Clearly, neither $|c_1(t)|^2$ nor any related quantity, for example $E = |c_0(t)|^2 E_{1s} + |c_1(t)|^2 E_{2p}$, is experimentally accessible in any ways since one can only detect the light when it has been fully emitted. What is actually done in the experiments is measuring the time-dependence of the photon-capture rate at which a photon detector fires after a large number of identical atoms has been excited by a flash. In the ensuing process the atoms reemit the light spontaneously. The moment at which the flash is released serves as a reference point with respect to which the detector records the flow of the incoming photons, and this flow is exponentially decaying in time. But each atom contributes only one single photon. Obviously, the photons are emitted at different times from different atoms. What has the time-dependence of their flow to do with Weisskopf-Wigner’s decay law which refers to the time evolution of a single atom?

To simplify the following considerations we assume that the spectrum of the flash is rectangular around the frequency ω_0 for which the atom under study would be completely transferred from its ground state $1s$ to the excited state $2p$ if the atom would be exposed to the associated electromagnetic wave for an infinitely long time. Hence

$$\hbar \omega_0 = E_{2p} - E_{1s} = \Delta E \quad \text{and} \quad |c_1(t)|^2 = 1.$$

If the atom absorbs a photon of lower frequency from the flash ($\omega < \omega_0$) it ends up in a state where $|c_1(t)|^2$ is now smaller than unity and we have because of Eq.(8)

$$\hbar \Delta\omega = \Delta E [1 - |c_1(t)|^2] \quad \text{which can be recast} \quad \hbar \Delta\omega = \Delta E |c_0(t)|^2 \quad (40)$$

with $\Delta\omega$ denoting $\omega_0 - \omega$. We temporarily abbreviate $\frac{2t}{\tau}$ into x and observe

$$\tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}} \approx -1 + e^{2x} \quad \text{if} \quad x \ll -1 \quad \text{and hence} \quad \frac{1}{2}(1 + \tanh x) \approx \frac{1}{2} e^{2x}.$$

Eq.(40) may therefore be rewritten

$$\hbar \Delta\omega = \frac{\Delta E}{2} e^{\frac{4t}{\tau}}. \quad (41)$$

Here $t \ll -\tau$ is referenced to the middle of the transition interval. If one wants to find the position of some point like A or B in the above figure for some atom that has absorbed a photon of energy $\hbar(\omega_0 - \Delta\omega)$, one has to insert the particular $\Delta\omega$ in Eq.(41) and one obtains the associated t that gives the distance of that point from the middle of the transition interval. If the spectrum of the flash is rectangular the probability that an atom absorbs such a photon is equal for all frequencies of the spectrum. That means that the length of the dead times t associated with the various values of $\Delta\omega$ are ordered in an exponential fashion. As follows from Eq.(41) the decay constant in that exponential function is given by the transition time τ . Deviations from that exponential form are connected with a departure from the rectangular form of the flash spectrum.

As for the validity of the above assumption $x \ll -1$, that is $-t \gg \tau$, one has to keep in mind that there are experimental limitations which allow monitoring the incoming photons only many transition times after the flash.

In concluding this section we pick up on a statement made in the beginning that the above considerations are not affected by a quantization of the emitted electromagnetic wave.

We recall from classical electrodynamics that the energy \mathcal{E} of an electromagnetic field in empty space is given by

$$\mathcal{E} = \frac{1}{2} \int_{\mathcal{V}} [\varepsilon_0 \mathbf{E}^2(\mathbf{r}, t) + \mu_0 \mathbf{H}^2(\mathbf{r}, t)] d^3r \quad (42)$$

where \mathcal{V} stands for the volume under study and \mathbf{E} and \mathbf{H} denote the electric and magnetic field, respectively. Using

$$\mathbf{E}(\mathbf{r}, t) = -\dot{\mathbf{A}}(\mathbf{r}, t) \quad (43)$$

and

$$\mathbf{B}(\mathbf{r}, t) = \mu_0 \mathbf{H}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t)$$

one may express

$$\mathbf{E}(\mathbf{r}, t) = i \sum_{\mathbf{k}, \sigma} \omega_{\mathbf{k}} \vec{\epsilon}_{\mathbf{k}, \sigma} [A_{\mathbf{k}, \sigma} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} - A_{\mathbf{k}, \sigma}^* e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)}]$$

and

$$\mathbf{B}(\mathbf{r}, t) = i \sum_{\mathbf{k}, \sigma} \mathbf{k} \times \vec{\epsilon}_{\mathbf{k}, \sigma} [A_{\mathbf{k}, \sigma} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} - A_{\mathbf{k}, \sigma}^* e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)}]$$

where we have used an expansion of $\mathbf{A}(\mathbf{r}, t)$ in terms of plane waves that satisfy the wave equation for the empty space under study

$$\Delta \mathbf{A}(\mathbf{r}, t) - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{A}(\mathbf{r}, t) = 0,$$

and hence

$$\mathbf{A}(\mathbf{r}, t) = \sum_{\mathbf{k}, \sigma} \vec{\epsilon}_{\mathbf{k}, \sigma} [A_{\mathbf{k}, \sigma} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} + A_{\mathbf{k}, \sigma}^* e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)}] \quad \text{where } \omega_{\mathbf{k}} = c|\mathbf{k}|. \quad (44)$$

Here σ can attain two values $\sigma = \pm 1$ and correspondingly $\vec{\epsilon}_{\mathbf{k}, \sigma}$ denotes two orthogonal unit vectors defining the polarization of the associated plane waves. On

inserting $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ into Eq.(42) and performing the real-space integral one may cast the result as

$$\mathcal{E} = \mathcal{V} \sum_{\mathbf{k}, \sigma} 2\varepsilon_0 \omega_{\mathbf{k}}^2 A_{\mathbf{k}, \sigma} A_{\mathbf{k}, \sigma}^*. \quad (45)$$

The following consideration is aimed at clarifying whether the formalism of “quantization” really explains the occurrence of photons or merely describes the experimental findings.

There are three striking experimental facts that make the existence of photons as particles of the electromagnetic field undeniable

- Planck’s radiation law for a black body
- the observable recoil that a free atom experiences on emitting radiation of a certain frequency
- the observation that the energy emitted from an atom (or nucleus) is quantitatively transferred to an absorber atom (or nucleus) irrespective of the distance between emitter and absorber

The photoelectric effect cannot be taken as another example of proving the existence of photons though it is usually quoted to the contrary. The photoelectric effect merely proves that a charged massive particle exposed to light of a frequency ω obeys quantum mechanics:

Under the influence of the light acting as a time-dependent perturbation the particle can only make a transition from its quantum mechanical ground state of energy E_0 to an excited state of energy $E_1 = E_0 + \hbar\omega$. The transition rate according to Fermi’s Golden Rule is

$$P_{10} = \frac{2\pi}{\hbar} |M_{10}|^2 \delta(E_1 - E_0 - \hbar\omega)$$

where M_{10} is the Matrixelement of the perturbation. Any perturbation of classical origin which oscillates at a frequency ω would lead to the same result. Hence, the energy reservoir from which the perturbation is fed, may contain a continuous amount of energy, but it can lose energy to the electron only in portions $\hbar\omega$.

Planck considered a box that consisted of ideally reflecting walls and was filled with standing electromagnetic waves which are in heat contact with a small grain of carbon inside the box. That grain serves as a heat bath, which means it possesses a certain temperature. It is assumed to absorb and reemit electromagnetic waves such that its own temperature doesn’t change and the system of electromagnetic waves attains this temperature when equilibrium is established, that is when there is no net flux of energy between the two systems any more.

The basic idea on which Planck’s law of black body radiation rests is that the observed frequency dependence of the intensity of the emitted light, its striking departure from the classical law of Rayleigh and Jeans at high frequencies, can only be explained if one makes a single, but very fundamental assumption: the energy of each of the electromagnetic waves consists of an integer number of photons whose energy is $\hbar\omega$ if the frequency of the associated wave is ω .

The energy contribution to \mathcal{E} in Eq.(45) of a wave

$$A_{\mathbf{k}, \sigma} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} + A_{\mathbf{k}, \sigma}^* e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} \quad (46)$$

is therefore at its $n_{\mathbf{k},\sigma}^{th}$ “excitation step” (i. e. when the wave consists of $n_{\mathbf{k},\sigma}$ photons)

$$\mathcal{E}_{\mathbf{k},\sigma} = n_{\mathbf{k},\sigma} \hbar\omega_{\mathbf{k}} = 2\varepsilon_0 \mathcal{V} \omega_{\mathbf{k}}^2 A_{\mathbf{k},\sigma} A_{\mathbf{k},\sigma}^* \quad \text{where} \quad n_{\mathbf{k},\sigma} = 0, 1, 2, \dots \quad (47)$$

In contact with a heat bath (=carbon grain of temperature T) one obtains for the thermal average energy $\bar{\mathcal{E}}_{\mathbf{k},\sigma}$

$$\bar{\mathcal{E}}_{\mathbf{k},\sigma} = \frac{1}{\sigma_{\mathbf{k},\sigma}} \sum_{\mathcal{E}_{\mathbf{k},\sigma}} \mathcal{E}_{\mathbf{k},\sigma} e^{-\beta \mathcal{E}_{\mathbf{k},\sigma}}$$

where

$$\sigma_{\mathbf{k},\sigma} = \sum_{\mathcal{E}_{\mathbf{k},\sigma}} e^{-\beta \mathcal{E}_{\mathbf{k},\sigma}} \quad \text{denotes the partition sum and} \quad \beta \stackrel{def}{=} \frac{1}{k_B T}.$$

Using Eq.(47) one can rewrite the right-hand side

$$\bar{\mathcal{E}}_{\mathbf{k},\sigma} = \frac{\hbar\omega_{\mathbf{k}}}{\sigma_{\mathbf{k},\sigma}} \sum_{n_{\mathbf{k},\sigma}} n_{\mathbf{k},\sigma} [e^{-\beta \hbar\omega_{\mathbf{k}}}]^{n_{\mathbf{k},\sigma}}. \quad (48)$$

The sum on the right-hand side has the form

$$\sum_{n=1}^{\infty} n Q^n = \frac{d}{dQ} \sum_{n=0}^{\infty} Q^n = \frac{d}{dQ} \frac{1}{1-Q} = \frac{Q}{(1-Q)^2} \quad \text{where} \quad Q = e^{-\beta \hbar\omega_{\mathbf{k}}}.$$

Correspondingly we have

$$\sigma_{\mathbf{k}} = \sum_{n_{\mathbf{k}}} [e^{-\beta \hbar\omega_{\mathbf{k}}}]^{n_{\mathbf{k}}} = \frac{1}{1-Q}. \quad \text{Hence} \quad \bar{\mathcal{E}}_{\mathbf{k},\sigma} = \hbar\omega_{\mathbf{k}} \frac{Q}{(1-Q)},$$

One can therefore cast the average energy $\bar{\mathcal{E}}_{\mathbf{k},\sigma}$ as

$$\bar{\mathcal{E}}_{\mathbf{k},\sigma} \equiv \bar{\mathcal{E}}_{\mathbf{k}} = \hbar\omega_{\mathbf{k}} \bar{n}_{\mathbf{k}}, \quad (49)$$

where

$$\bar{n}_{\mathbf{k}} = \frac{1}{e^{\frac{\hbar\omega_{\mathbf{k}}}{k_B T}} - 1}. \quad (50)$$

The total radiation energy in a hollow rectangular box with linear dimensions L_1, L_2, L_3 and volume $\mathcal{V} = L_1 L_2 L_3$ is therefore

$$\mathcal{E} = \sum_{\mathbf{k},\sigma} \bar{\mathcal{E}}_{\mathbf{k}} = 2 \sum_{\mathbf{k}} \bar{\mathcal{E}}_{\mathbf{k}} \quad (51)$$

Each plane wave (46) is subject to boundary conditions at the interior plane surfaces of the box. As a result, the components $\mathbf{k}_j = k_j \mathbf{e}_j ; j = 1, 2, 3$ of the wave vector \mathbf{k} are quantized

$$k_j = \begin{cases} (2n_j - 1) \frac{\pi}{L_j}; & n_j = 1, 2, 3, \dots \\ n_j \frac{2\pi}{L_j}; & n_j = 1, 2, 3, \dots \end{cases}$$

In any case one has

$$k_{j,n_{j+1}} - k_{j,n_j} \stackrel{def}{=} \Delta k_j = \frac{2\pi}{L_j}$$

and hence

$$\Delta^3 k \stackrel{def}{=} \Delta k_1 \Delta k_2 \Delta k_3 = \frac{2\pi}{L_1} \frac{2\pi}{L_2} \frac{2\pi}{L_3} = \frac{(2\pi)^3}{\mathcal{V}}, \quad \text{that is} \quad \frac{\mathcal{V}}{(2\pi)^3} \Delta^3 k = 1.$$

Eq.(51) may therefore be rewritten

$$\mathcal{E} = 2 \frac{\mathcal{V}}{(2\pi)^3} \sum_{\mathbf{k}} \bar{\mathcal{E}}_{\mathbf{k}} \Delta^3 k \approx 2 \frac{\mathcal{V}}{(2\pi)^3} \int \bar{\mathcal{E}}_{\mathbf{k}} d^3 k = \frac{\mathcal{V}}{\pi^2} \int_0^\infty \bar{\mathcal{E}}_k k^2 dk$$

where it has been exploited that $\omega_{\mathbf{k}}$ depends only on $k = |\mathbf{k}|$.

Substituting k with $\frac{\omega}{c}$ and inserting $\bar{\mathcal{E}}_k$ from Eq.(49) one arrives at

$$\frac{\mathcal{E}}{\mathcal{V}} \stackrel{def}{=} u = \int_0^\infty \underbrace{\frac{\hbar}{\pi^2 c^3} \omega^3 \frac{1}{e^{\frac{\hbar\omega_{\mathbf{k}}}{k_B T}} - 1}}_{\stackrel{def}{=} \hat{u}_\omega} d\omega.$$

The quantity u denotes the energy density, and \hat{u}_ω stands for the spectral energy density. The latter expression represents Planck's radiation law.

We now return to Eq.(47) which may be recast

$$|A_{\mathbf{k},\sigma}|^2 = \frac{n_{\mathbf{k},\sigma} \hbar}{2 \varepsilon_0 \mathcal{V} \omega_{\mathbf{k}}}. \quad (52)$$

This serves as a crucial input in going through the formal procedure of “quantization”. In so doing one should keep in mind that the decisive step of quantization has already been taken by introducing $n_{\mathbf{k},\sigma} \hbar \omega_{\mathbf{k}}$ in Eq.(47). The ensuing formalization does not bring about any more substance. It should be observed that $n_{\mathbf{k},\sigma} \hbar \omega_{\mathbf{k}}$ has been **introduced** to fit the experiments and not been **derived** from some theory.

Inserting $|A_{\mathbf{k},\sigma}|^2$ from above Eq.(44) one obtains

$$\mathbf{A}(\mathbf{r}, t) = \sum_{\mathbf{k},\sigma} \vec{\epsilon}_{\mathbf{k},\sigma} \underbrace{\sqrt{\frac{\hbar}{2 \varepsilon_0 \mathcal{V} \omega_{\mathbf{k}}}} [a_{\mathbf{k},\sigma} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t)} + a_{\mathbf{k},\sigma}^* e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t)}]}_{\stackrel{def}{=} \tilde{\mathbf{A}}_{\mathbf{k},\sigma}(\mathbf{r}, t)}. \quad (53)$$

where

$$a_{\mathbf{k},\sigma}^* a_{\mathbf{k},\sigma} = n_{\mathbf{k},\sigma}. \quad (54)$$

The step into “quantum electrodynamics” consists in the following assumption: One introduces the notion of a “state” $|0, 0, \dots, n_{\mathbf{k},\sigma}, 0, \dots\rangle$ which describes a situation where $n_{\mathbf{k},\sigma}$ photons of energy $\hbar \omega_{\mathbf{k}} = \hbar c |\mathbf{k}|$ are present. The zeros stand for photons of different \mathbf{k} and/or different σ which are absent in the situation under study. We abbreviate the notation of this state into $|n_{\mathbf{k},\sigma}\rangle$ and imagine to span a Hilbert space with these states by requiring them to be orthonormal:

$$\langle n'_{\mathbf{k}',\sigma'} | n_{\mathbf{k},\sigma} \rangle = \delta_{n'_{\mathbf{k}',\sigma'}, n_{\mathbf{k},\sigma}}. \quad (55)$$

One now replaces the ‘‘occupation number amplitudes’’ $a_{\mathbf{k},\sigma}^*$, $a_{\mathbf{k},\sigma}$ in Eq.(53) by creation- and annihilation operators:

$$a_{\mathbf{k},\sigma}^* \rightarrow \hat{a}_{\mathbf{k},\sigma}^\dagger; \quad a_{\mathbf{k},\sigma} \rightarrow \hat{a}_{\mathbf{k},\sigma} \quad (56)$$

with the following properties:

$$\begin{aligned} \hat{a}_{\mathbf{k},\sigma}^\dagger |n_{\mathbf{k},\sigma}\rangle &= \sqrt{n_{\mathbf{k},\sigma} + 1} |n_{\mathbf{k},\sigma} + 1\rangle \\ \hat{a}_{\mathbf{k},\sigma} |n_{\mathbf{k},\sigma}\rangle &= \sqrt{n_{\mathbf{k},\sigma}} |n_{\mathbf{k},\sigma} - 1\rangle. \end{aligned} \quad (57)$$

The two operators hence obey the commutation relation (‘‘minus commutation’’)

$$\hat{a}_{\mathbf{k},\sigma} \hat{a}_{\mathbf{k},\sigma}^\dagger - \hat{a}_{\mathbf{k},\sigma}^\dagger \hat{a}_{\mathbf{k},\sigma} \stackrel{def}{=} [\hat{a}_{\mathbf{k},\sigma}, \hat{a}_{\mathbf{k},\sigma}^\dagger] = 1. \quad (58)$$

As a consequence of the substitution (56) and because of Eq.(53) $\mathbf{A}(\mathbf{r}, t)$ becomes a field operator:

$$\hat{\mathbf{A}}(\mathbf{r}, t) = \sum_{\mathbf{k},\sigma} \vec{\epsilon}_{\mathbf{k},\sigma} \sqrt{\frac{\hbar}{2\varepsilon_0 \mathcal{V} \omega_{\mathbf{k}}}} \left[\hat{a}_{\mathbf{k},\sigma} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t)} - \hat{a}_{\mathbf{k},\sigma}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t)} \right] \quad (59)$$

and analogously

$$\hat{\mathbf{E}}(\mathbf{r}, t) = i \sum_{\mathbf{k},\sigma} \vec{\epsilon}_{\mathbf{k},\sigma} \sqrt{\frac{\hbar \omega_{\mathbf{k}}}{2\varepsilon_0 \mathcal{V}}} \left[\hat{a}_{\mathbf{k},\sigma} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t)} - \hat{a}_{\mathbf{k},\sigma}^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t)} \right]. \quad (60)$$

From Eq.(57) we have

$$\hat{a}_{\mathbf{k},\sigma}^\dagger \hat{a}_{\mathbf{k},\sigma} |n_{\mathbf{k},\sigma}\rangle = n_{\mathbf{k},\sigma} |n_{\mathbf{k},\sigma}\rangle$$

which means

$$\langle n_{\mathbf{k},\sigma} | \hat{a}_{\mathbf{k},\sigma}^\dagger \hat{a}_{\mathbf{k},\sigma} |n_{\mathbf{k},\sigma}\rangle = n_{\mathbf{k},\sigma}.$$

This is equivalent to Eq.(54).

The quantization procedure defined through Eqs.(56) to (59) is standard but not entirely consistent: An implausible consequence of this procedure is that it does not exactly reproduce Eq.(47) which contains the input information

$$\mathcal{E}_{\mathbf{k},\sigma} = n_{\mathbf{k},\sigma} \hbar \omega_{\mathbf{k}} \quad \leftrightarrow \quad \mathcal{E} = \sum_{\mathbf{k},\sigma} \mathcal{E}_{\mathbf{k},\sigma} = \sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma} \hbar \omega_{\mathbf{k}}. \quad (61)$$

The functions

$$e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t)}$$

are orthogonal for different wave vectors \mathbf{k} within the normalization volume \mathcal{V} . As the two contributions to \mathcal{E} in Eq.(42) are equal, \mathcal{E} can be calculated by taking twice the contribution of the electric field. From Eqs.(42), (55), (57) and (60) we obtain then

$$\begin{aligned} \mathcal{E} &= \sum_{\mathbf{k},\sigma} \int_{\mathcal{V}} \langle n_{\mathbf{k},\sigma} | \varepsilon_0 \hat{\mathbf{E}}^\dagger \cdot \hat{\mathbf{E}} |n_{\mathbf{k},\sigma}\rangle d^3 r = \\ &= \sum_{\mathbf{k},\sigma} \langle n_{\mathbf{k},\sigma} | \sum_{\mathbf{k}',\sigma'} \frac{\hbar \omega_{\mathbf{k}'}}{2} \underbrace{(a_{\mathbf{k}',\sigma'}^\dagger a_{\mathbf{k}',\sigma'} + a_{\mathbf{k}',\sigma'} a_{\mathbf{k}',\sigma'}^\dagger)}_{=\delta_{\mathbf{n}',\sigma',\mathbf{n},\sigma} (2n_{\mathbf{k},\sigma} + 1)} |n_{\mathbf{k},\sigma}\rangle = \sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma} \hbar \omega_{\mathbf{k}} + \underbrace{\frac{1}{2} \sum_{\mathbf{k},\sigma} \hbar \omega_{\mathbf{k}}}_{\text{‘‘zero-point energy’’}} \end{aligned} \quad (62)$$

This is identical with the input information (61) except for the extra term “zero-point energy” whose appearance is all the more puzzling as it is infinite since there is no physical reason for a cut-off frequency in the summation over contributions $\hbar\omega_{\mathbf{k}}$.

Despite the vexing occurrence of this infinite term, there is an overwhelming majority of theorists who regard it as an indisputable piece of quantum electrodynamics and even take the phenomenon of Casimir forces as proving the existence of zero point energy. There is a widely held belief that the Casimir forces with which two metal plates attract each other within a submicron distance is caused by a lowering of the zero point energy in the space between the plates. By contrast, we advance the opinion that the above extra term does actually not exist and that the Casimir forces can be explained without drawing on the existence of zero point energy.

The formal occurrence of this term is caused by introducing $\hat{a}_{\mathbf{k},\sigma}^\dagger, \hat{a}_{\mathbf{k},\sigma}$ one step too soon. At the pre-quantization step the electric field has still the form

$$\mathbf{E}(\mathbf{r}, t) = i \sum_{\mathbf{k},\sigma} \vec{\epsilon}_{\mathbf{k},\sigma} \sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2\varepsilon_0\mathcal{V}}} [a_{\mathbf{k},\sigma} e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} - a_{\mathbf{k},\sigma}^* e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)}].$$

If this expression is used in determining the total energy, one obtains

$$\mathcal{E} = \int_{\mathcal{V}} \varepsilon_0 \mathbf{E}^*(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t) d^3r = \sum_{\mathbf{k},\sigma} \hbar\omega_{\mathbf{k}} a_{\mathbf{k},\sigma}^* a_{\mathbf{k},\sigma}$$

Substituting $a_{\mathbf{k},\sigma}^*, a_{\mathbf{k},\sigma}$ according to Eq.(56)

$$a_{\mathbf{k},\sigma}^* \rightarrow \hat{a}_{\mathbf{k},\sigma}^\dagger; \quad a_{\mathbf{k},\sigma} \rightarrow \hat{a}_{\mathbf{k},\sigma}$$

one arrives at

$$\hat{\mathcal{E}} = \sum_{\mathbf{k},\sigma} \hbar\omega_{\mathbf{k}} \hat{a}_{\mathbf{k},\sigma}^\dagger \hat{a}_{\mathbf{k},\sigma} \text{ and hence } \mathcal{E} = \sum_{\mathbf{k},\sigma} \hbar\omega_{\mathbf{k}} \langle n_{\mathbf{k},\sigma} | \hat{a}_{\mathbf{k},\sigma}^\dagger \hat{a}_{\mathbf{k},\sigma} | n_{\mathbf{k},\sigma} \rangle = \sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma} \hbar\omega_{\mathbf{k}} \quad (63)$$

without an additional zero point energy.

We now turn to the question: what is the meaning of $\mathbf{A}(\mathbf{r}, t)$ in the perturbed Hamiltonian (25)?

On forming the expectation value of $\hat{\mathbf{E}}(\mathbf{r}, t)$, that is

$$\begin{aligned} \langle n_{\mathbf{k},\sigma} | \hat{\mathbf{E}}(\mathbf{r}, t) | n_{\mathbf{k},\sigma} \rangle = \\ i \sum_{\mathbf{k}',\sigma'} \vec{\epsilon}_{\mathbf{k}',\sigma'} \sqrt{\frac{\hbar\omega_{\mathbf{k}'}}{2\varepsilon_0\mathcal{V}}} \langle n_{\mathbf{k},\sigma} | \left[\hat{a}_{\mathbf{k}',\sigma'} e^{i(\mathbf{k}'\cdot\mathbf{r}-\omega_{\mathbf{k}'}t)} - \hat{a}_{\mathbf{k}',\sigma'}^\dagger e^{-i(\mathbf{k}'\cdot\mathbf{r}-\omega_{\mathbf{k}'}t)} \right] | n_{\mathbf{k},\sigma} \rangle \end{aligned} \quad (64)$$

one recognizes that $\langle n_{\mathbf{k},\sigma} | \hat{\mathbf{E}}(\mathbf{r}, t) | n_{\mathbf{k},\sigma} \rangle \equiv 0$ because the states $\hat{a}_{\mathbf{k}',\sigma'}^\dagger | n_{\mathbf{k},\sigma} \rangle$ and $\hat{a}_{\mathbf{k}',\sigma'} | n_{\mathbf{k},\sigma} \rangle$ are all orthogonal to $| n_{\mathbf{k},\sigma} \rangle$. However, this result does not have any physical relevance since it cannot be checked experimentally. If one wants to detect the existence of an electric field at a point \mathbf{r} , any measurement of a force $\mathbf{F} = e \mathbf{E}$ involves somehow a displacement of a charge e , and hence leads to the absorption of energy from the electromagnetic wave. For example, if one would place a charged, point-like harmonic oscillator with frequency $\omega_{\mathbf{k}}$ in the electric field, one could verify that it is driven by the electric field only when it is damped.

Otherwise it would - in general - also oscillate without any driving force. To correlate $\hat{\mathbf{E}}(\mathbf{r}, t)$ with a measurable quantity, one must therefore consider a photon state

$$|\phi(t)\rangle = c_1(t) |n_{\mathbf{k},\sigma}\rangle + c_0(t) |n_{\mathbf{k},\sigma} - 1\rangle. \quad (65)$$

The state $|n_{\mathbf{k},\sigma}\rangle$ refers to an electromagnetic wave of wave vector \mathbf{k} and polarization σ which contains n photons. Correspondingly, the state $|n_{\mathbf{k},\sigma} - 1\rangle$ represents the same electromagnetic wave with one photon less. If $|c_0(t)|^2$ and $|c_1(t)|^2$ are functions of time similar to those shown in Fig.3, then (65) describes a transition in which the electromagnetic wave loses a photon to some charged quantum mechanical object. For this transition state $|\phi(t)\rangle$ the expectation value of $\hat{\mathbf{E}}(\mathbf{r}, t)$ yields two non-vanishing portions

$$\begin{aligned} \langle \phi(t) | \hat{\mathbf{E}}(\mathbf{r}, t) | \phi(t) \rangle &= -i \vec{\epsilon}_{\mathbf{k},\sigma} \sqrt{\frac{\hbar \omega_{\mathbf{k}}}{2 \varepsilon_0 \mathcal{V}}} e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} c_1(t) c_0(t) \underbrace{\langle n_{\mathbf{k},\sigma} | \hat{a}_{\mathbf{k},\sigma}^\dagger | n_{\mathbf{k},\sigma} - 1 \rangle}_{=n_{\mathbf{k},\sigma} |n_{\mathbf{k},\sigma}\rangle} + \\ & i \vec{\epsilon}_{\mathbf{k},\sigma} \sqrt{\frac{\hbar \omega_{\mathbf{k}}}{2 \varepsilon_0 \mathcal{V}}} e^{i(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t)} c_0(t) c_1(t) \langle n_{\mathbf{k},\sigma} - 1 | \underbrace{\hat{a}_{\mathbf{k},\sigma} | n_{\mathbf{k},\sigma} \rangle}_{=n_{\mathbf{k},\sigma} |n_{\mathbf{k},\sigma} - 1\rangle}. \quad (66) \end{aligned}$$

This may be cast

$$\tilde{\mathbf{E}}_{\mathbf{k},\sigma}(\mathbf{r}, t) \stackrel{def}{=} \langle \hat{\mathbf{E}}(\mathbf{r}, t) \rangle = -2 \vec{\epsilon}_{\mathbf{k},\sigma} |c_0(t) c_1(t)| \sqrt{\frac{n_{\mathbf{k},\sigma} \hbar \omega_{\mathbf{k}}}{2 \varepsilon_0 \mathcal{V}}} \sin(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t + \varphi). \quad (67)$$

Here φ is defined as in Eq.(13). Analogously one obtains

$$\tilde{\mathbf{A}}_{\mathbf{k},\sigma}(\mathbf{r}, t) = 2 \vec{\epsilon}_{\mathbf{k},\sigma} |c_0(t) c_1(t)| \sqrt{\frac{n_{\mathbf{k},\sigma} \hbar}{2 \varepsilon_0 \mathcal{V} \omega_{\mathbf{k}}}} \cos(\mathbf{k} \cdot \mathbf{r} - \omega_{\mathbf{k}} t + \varphi). \quad (68)$$

One is hence led to conclude that $\mathbf{A}(\mathbf{r}, t)$ in the perturbed Hamiltonian (25) is just the expectation value of $\hat{\mathbf{A}}(\mathbf{r}, t)$ in the course of energy exchange between the charged quantum mechanical object and the electromagnetic field. Within this time interval, which is the only one of physical significance, the expectation values $\tilde{\mathbf{A}}_{\mathbf{k},\sigma}(\mathbf{r}, t)$ and $\tilde{\mathbf{E}}_{\mathbf{k},\sigma}(\mathbf{r}, t)$ display a completely classical behavior, and the product $|c_1(t) c_0(t)|$ can roughly be approximated by a constant as indicated in Fig.2 by the red dashed line.

So far it seems to be clear that “quantum electrodynamics”, that is the formal apparatus of “quantization” only describes Planck’s hypothesis, which means, the energy quantization of free electromagnetic waves. The latter explains in detail the experimental findings and, in particular, the high-frequency behavior of black body radiation. Beyond that, does quantum electrodynamics also explain the occurrence of a momentum carrying particle associated with each individual plane wave? We believe, it does not. Its existence is simply implied. And it neither explains the photon’s point-like character which one is forced to assume. Otherwise it could hardly be understood that an atom which absorbs the photon receives the full energy amount of the photon irrespective of the distance between the emitter and the absorber. Moreover, it does not explain the recoil that the emitter experiences in the reverse direction of the photon’s propagation towards the absorber. The occurrence of a photon’s momentum $\hbar \mathbf{k}$ associated with a plane wave of wave vector \mathbf{k} derives from the classical expression for the light pressure. But the photon

that is emitted from a hydrogen atom in a $2p \rightarrow 1s$ -transition is associated with a Hertzian-type wave field. Outside the atom the latter can be expanded in terms of plane waves, but the energy of the photon relates to the entire field and not to one of its plane wave components. Still, it carries the momentum $\frac{\hbar\omega}{c} \mathbf{e}_\gamma$ as if it were in a plane wave state with $\mathbf{k} = \frac{\omega}{c} \mathbf{e}_\gamma$ where \mathbf{e}_γ denotes the direction of its propagation. This is evidenced by the experiment, but remains unexplained within our approach and in quantum electrodynamics as well.

Besides, our treatment invites an interesting experiment: One could use the experimental setup by Dehmelt and associates [2] in which a single Ba^+ -ion is kept in a Paul-trap. The ion contains one outer electron which behaves very similar to a hydrogen electron considered so far. One can transfer this electron from its $6s$ -groundstate to a $6p$ -state by the absorption of linearly polarized light of the appropriate energy. According to our theory the ion will spontaneously emit light then which is polarized in the same plane as the light that was previously absorbed. A detector monitors the emitted photon at some fixed distance d . It can be moved on a sphere of radius d . If the excitation has been repeated sufficiently often, the lateral distribution of detection events should display the characteristic feature of the Hertzian dipole radiation.

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