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THEORY OF NATURAL LINE SHAPE

Luis Davidovich*
Institut für Theoretische Physik, ETH
CH-8093 Zürich, Switzerland
and
H.M. Nussenzveig+
Instituto de Física, Universidade de São Paulo
São Paulo, Brazil

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1. INTRODUCTION

The quantum-electrodynamical treatment of the emission of light by an atom has been strongly influenced by Weisskopf and Wigner's early contribution[1] to this subjet. While their work was highly successful in accounting for the observed line shape, several disturbing theoretical questions concerning the underlying assumptions remained unsettled:

(i) An initial state for the system corresponding to an excited atomic eigenstate with no photons present was assumed, which seems quite unphysical. The state preparation and the dependence of the decay on the excitation should be discussed.

(ii) It is well known that the exponential decay "Ansatz" cannot be valid for all times, although deviations from it are expected to be extremely small for long-lived decaying states such as the atomic ones. However, the range of validity of the exponential decay law should be determined.

(iii) The state space was restricted to a two-level atom and to the vacuum and one-photon sectors, without any indication of how to proceed in order to improve the approximation. For such a basic problem as this one, one should start from a clearcut formulation, and a systematic procedure for deriving corrections to the Weisskopf-Wigner approximation should be given.

Measurements of the Lamb shift in hydrogen provided a sensitive experimental test of the predicted line shape. It was remarked by Lamb[2] that the Weisskopf-Wigner line shape disagrees with experiment in this case if the usual

minimal-coupling interaction Hamiltonian is employed, and that one must use instead the interaction $-e\underset{\sim}{r}.\underset{\sim}{E}^{\perp}$, where $\underset{\sim}{E}^{\perp}$ is the transverse electric field. As will be seen below, the discrepancy is orders of magnitude larger than the present accuracy in the measurement. Since the minimal-coupling Hamiltonian is widely employed in quantum electrodynamics, this discrepancy should be resolved.

An extensive study of the line shape problem was made around 1950 by Heitler, Arnous and collaborators[3,4,5]. They applied a dressing transformation in order to go over from "bare" states of the system to physical states. They began[3] by imposing unphysical constraints on the dressing transformation; later[4,5], these constraints were removed, but they employed a cumbersome formalism, and their attention was focussed on the evaluation of radiative corrections to the resonant term in a transition between two atomic states. The effect of nonresonant terms was not considered, and there was no discussion of the time development of the system. Similar remarks apply to Low's[6] covariant $\underline{S}$-matrix treatment.

The relationship between time evolution and the analytic properties of the $\underline{S}$-matrix as a function of energy has been clarified in nonrelativistic potential scattering, where decaying states can be described in terms of propagators associated with complex poles on unphysical sheets[7]. This has also been verified in some models of unstable particles in quantum field theory.

The present paper is a survey of results that were recently obtained[8] in a new treatment of the line shape problem. We deal with a nonrelativistic hydrogen atom

interacting with the quantized radiation field. This is the simplest and best-known atomic system; the corresponding exact transition matrix elements including retardation have been recently determined[9] and they lead to an extremely simple analytic structure of the transition probabilities (Sect.2).

We employ Van Hove's[10] resolvent operator approach. An outline of its main features is given in Sect.3. In Sect. 4, we discuss the physical consequences of some of the approximations employed in previous treatments[11], where various terms in the Hamiltonian are omitted or simplified. We proceed by successive approximations.

We begin with a simplified multi-level model in which "counter-rotating" terms are omitted. This eliminates persistent perturbation effects in the sense of Van Hove (incuding self-energy and dressing effects), and leads to a decomposition of Hilbert space into sectors, such that the model becomes exactly soluble in the sector of interest. Unlike previously solved models, transitions from the resonant level to other excited states are taken into account.

Employing the exact transition probabilities of Sect.2, the resolvent is explicitly obtained and its analytic behavior is found (Sect.5). This allows one to describe the time evolution of the system. In particular, we discuss the decay of a Weisskopf-Wigner initial state and the dependence on the excitation in the scattering of a wave packet, determining the range of validity of the exponential decay law within this model (Sect.6).

The effect of adding back the "counter-rotating" terms is considered next. In order to remove the associated persistent effects, we apply a generalized version of a

dressing transformation proposed by Faddeev[12], which is defined order-by-order in perturbation theory (Sect.7). The previously described resolvent operator method can then be applied to the transformed Hamiltonian, which generates the dynamics of "dressed" states.

The results obtained by applying this procedure to second order in the coupling constant, in dipole approximation, are described in Sect. 8. The dressing transformation yields the nonrelativistic Lamb-shift correction to the ground-state energy. The corresponding Lamb-shift corrections to excited-state energies appear, as they should, in the poles of the resolvent on unphysical sheets.

Finally, in Sect.9, we discuss the relation between the minimal coupling and $-e\underset{\sim}{r}.\underset{\sim}{E}^{\perp}$ interaction Hamiltonians, as well as the results they yield for the line shape. While these results are equivalent when both the resonant and all nonresonant terms are included, this is not so when, as is usually done, only the resonant term is taken into account. The background contribution due to transitions to all nonresonant levels can be explicitly computed with the help of the Coulomb Green's function. For the Lamb-shift transition, the background correction to the minimal-coupling resonant term is important, and it resolves the discrepancy observed by Lamb. For the Lyman-α line, although the correction is much smaller, it is the minimal-coupling resonant term that yields better results. The evaluation of corrections to the line shape should become of increasing importance as the accuracy of Lamb-shift measurements increases.

2. The Model

We consider a nonrelativistic hydrogen atom (recoil is neglected) interacting with the quantized radiation field. The Hamiltonian of the system is (we take $\hbar=c=1$ throughout

$$H = H_A + H_F + H_{I,1} + H_{I,2} \quad , \tag{2.1}$$

with

$$H_A = \underset{\sim}{p}^2/2m - e^2/r, \tag{2.2}$$

$$H_F = \frac{1}{8\pi} \int d^3r \left[(\underset{\sim}{E}^{\perp})^2 + (\underset{\sim}{\nabla} \times \underset{\sim}{A})^2 \right], \tag{2.3}$$

where $\underset{\sim}{A}$ is the vector potential in the Coulomb gauge, and $\underset{\sim}{E}^{\perp}$ is the transverse electric field; the linear and quadratic parts of the interaction Hamiltonian are respectively given by

$$H_{I,1} = -\frac{e}{m} \underset{\sim}{p}.\underset{\sim}{A}(\underset{\sim}{r}) \quad , \tag{2.4}$$

$$H_{I,2} = \frac{e^2}{2m} \underset{\sim}{A}^2(\underset{\sim}{r}). \tag{2.5}$$

We rewrite the atomic Hamiltonian in terms of the hydrogen-atom stationary states $|n\rangle$ (where n stands for a complete set of quantum numbers) and the corresponding energies E_{On} , as

$$H_A = \sum_n E_{On} |n\rangle\langle n| \quad , \tag{2.6}$$

where the summation is to be understood as integration for eigenstates in the continuum. We will be concerned, however, mainly with the discrete spectrum.

We employ the multipole expansion[13]

$$\underset{\sim}{A}(\underset{\sim}{r}) = 2 \sum_{\tau=0}^{1} \sum_{J=1}^{\infty} \sum_{M=-J}^{J} \int_0^\infty dk \sqrt{k}\ a_{JM\tau}(k)\ \underset{\sim}{A}_{JM\tau}(k,\underset{\sim}{r}) + h.\ c., \quad (2.7)$$

in terms of the usual basis[13], where $\underset{\sim}{A}_{JM\tau}$ represents an electric ($\tau = 0$) or magnetic ($\tau = 1$) multipole field of order 2^J. The operator $a_{JM\tau}(k)$ annihilates photons of frequency k with the set of quantum numbers

$$\beta = (JM\tau), \quad (2.8)$$

so that

$$[a_\beta(k),\ a_{\beta'}{}^{+}(k')] = \delta_{\beta\beta'}\ \delta(k - k'). \quad (2.9)$$

The field Hamiltonian becomes (after zero-point energy subtraction)

$$H_F = \sum_\beta \int_0^\infty dk\ k\ a_\beta{}^{+}(k)\ a_\beta(k)\ . \quad (2.10)$$

The exact matrix elements $\langle n|\ \underset{\sim}{p}.\underset{\sim}{A}_\beta|m\rangle$ for the nonrelativistic hydrogen atom have been evaluated by Moses[9]. To express $H_{I,1}$ in terms of them, it is convenient to adopt "atomic units" for the frequency k, measuring it in units of the inverse Bohr radius a_B^{-1}, i. e., setting

$$a_B^{-1} \equiv \alpha\, m = 1, \quad (2.11)$$

where α is the fine-structure constant. We then have

$$H_{I,1} = \sqrt{\lambda} \sum_{nm\beta} \int_0^\infty dk \sqrt{k}\ f_{nm\beta}(k)\ a_\beta(k)\,|n\rangle\langle m| + h.\ c., \quad (2.12)$$

where we have defined a coupling constant (in the units (2.11))

$$\lambda = (e/m)^2 = \alpha^3 \qquad (\approx 4 \times 10^{-7})\ . \quad (2.13)$$

Let $n = (N_n, j_n, M_n)$, where N_n, j_n and M_n are the principal quantum number, angular momentum and magnetic quantum number of the state n, respectively. The matrix elements $f_{nm\beta}$ vanish unless they fulfil the following exact selection rules, which follow from angular momentum and parity conservation:

$$|j_n - j_m| \leq J \leq j_n + j_m \; ; \quad M = M_n - M_m \; ;$$

$$J + j_n + j_m \equiv \tau \pmod 2 . \qquad (2.14)$$

Under these conditions, it can be shown[8] that $|f_{nm\beta}(k)|^2$ (derived from the results of Ref.9) is a rational function of k^2, of the following remarkably simple form:

$$|f_{nm\beta}(k)|^2 = P_{nm\beta}(k) \, (k^2 + K_{nm}^{\,2})^{-P_{nm}} , \qquad (2.15)$$

where $P_{nm\beta}(k)$ is a polynomial (in k^2) with real coefficients, that are $\mathcal{O}(1)$ in the units (2.11), P_{nm} is an integer ≥ 4, such that

$$| f_{nm\beta}(k) |^2 = \mathcal{O}(k^{-8}) \qquad \text{as} \quad k \to \infty , \qquad (2.16)$$

and $K_{nm}^{-1} = \mathcal{O}(1)$ is an atomic transition radius of the order of the Bohr radius. For example, for the Lyman-α and Lyman-β lines (electric dipole transitions), $|f_{nm\beta}(k)|^2$ is proportional to, respectively,

$$\left[k^2 + (3/2)^2 \right]^{-4} , \quad \left[(4/3)^2 + 2k^2 \right]^2 \left[k^2 + (4/3)^2 \right]^{-6} .$$

The functions $|f_{nm\beta}(k)|^2$ play the role of exact atomic form factors, introducing a natural cutoff at distances

of the order of the Bohr radius. The Yukawa-like denominators in (2.15) reflect the exponential fall-off of the bound-state wave functions. The extremely simple analytic properties of (2.15) play an important role in the soluble model discussed below.

3. The Resolvent Operator

Our treatment is based on the resolvent operator method, as developed by Van Hove[10]. We briefly recall its main features.

The resolvent operator $\mathcal{G}(z)$ associated with the Hamiltonian $H = H_0 + H_I$ is an operator-valued function of the complex variable z defined, for $\mathrm{Im}\, z \neq 0$, by

$$\mathcal{G}(z) = (z - H)^{-1}. \tag{3.1}$$

It is expected to be holomorphic for $\mathrm{Im}\, z \neq 0$. The time evolution operator may be expressed in terms of $\mathcal{G}(z)$ as

$$\exp(-iHt) = -\frac{1}{2\pi i}\int_C \exp(-izt)\,\mathcal{G}(z)\,dz \quad (t>0), \tag{3.2}$$

where C is a straight line taken above the real axis, from $-\infty + i\varepsilon$ to $\infty + i\varepsilon$ $(\varepsilon > 0)$.

The operator $\mathcal{G}(z)$ can be split into a diagonal part with respect to H_0, $\mathcal{D}(z)$, and a nondiagonal part with respect to H_0, $\mathcal{N}(z)$:

$$\mathcal{G}(z) = \mathcal{D}(z) + \mathcal{N}(z), \tag{3.3}$$

where, for every eigenstate $|\alpha\rangle$ of H_0,

$$H_0|\alpha\rangle = E_{0\alpha}|\alpha\rangle, \tag{3.4}$$

we have

$$\mathcal{D}(z)|\alpha\rangle = \mathcal{D}_\alpha(z)|\alpha\rangle. \tag{3.5}$$

The eigenvalue $\mathcal{D}_\alpha(z)$ determines the persistence amplitude of the state $|\alpha\rangle$, i. e., if we start out from the initial state $|\alpha\rangle$ at $t = 0$, the probability amplitude to find the system in the state $|\alpha\rangle$ at time t is given by

$$\langle\alpha|\exp(-iHt)|\alpha\rangle = -\frac{1}{2\pi i}\int_C \exp(-izt)\ \mathcal{D}_\alpha(z)\ dz. \quad (3.6)$$

This amplitude therefore depends crucially on the analytic properties of $\mathcal{D}_\alpha(z)$.

The unperturbed resolvent operator $\mathcal{G}_0(z)$ is defined by

$$\mathcal{G}_0(z) = (z - H_0)^{-1}. \quad (3.7)$$

The analogue $\Sigma(z)$ of Dyson's mass operator[14] satisfies

$$\mathcal{D}(z) = \mathcal{G}_0(z) + \mathcal{D}(z)\ \Sigma(z)\ \mathcal{G}_0(z) \quad (3.8)$$

and it can be pictured diagrammatically by

$$\Sigma(z) = \left[H_I + H_I\,\mathcal{D}(z)\,H_I + \ldots\right]_{\text{i.d.}}, \quad (3.9)$$

where the index "i.d." stands for a summation over all irreducible diagonal[10] diagrams.

As z approaches a point E on the real axis, we have[10]

$$\lim_{z \to E \pm i0} \Sigma(z) = \Delta(E) \mp \frac{i}{2}\,\Gamma(E), \quad (3.10)$$

where $\Gamma(E)$ is a positive semidefinite operator, $\Gamma(E) \geqslant 0$. Thus, denoting by an index α the eigenvalues of diagonal operators in the state $|\alpha\rangle$,

$$\lim_{z \to E \pm i0} \mathcal{D}_\alpha(z) = \left[E - E_{0\alpha} - \Delta_\alpha(E) \mp \frac{i}{2}\,\Gamma_\alpha(E)\right]^{-1}. \quad (3.11)$$

If $\Gamma_\alpha(E) \neq 0$, we see that E lies on a cut of $\mathcal{D}_\alpha(z)$, which is holomorphic for Im $z \neq 0$ (physical sheet).

The Weisskopf-Wigner approximation would correspond to

$$\mathcal{D}_\alpha(z) = \left[z - E_\alpha - \frac{i}{2}\Gamma_\alpha \right]^{-1} , \qquad (3.12)$$

which would violate the analyticity on the physical sheet. By comparison with (3.11), we see that $\Delta(E)$ and $\Gamma(E)$ in (3.10) play the roles of level shift and level width operators, respectively.

The nondiagonal part $\mathcal{N}(z)$ in (3.3) may be written as

$$\mathcal{N}(z) = \mathcal{D}(z)\ \mathcal{U}(z)\ \mathcal{D}(z) , \qquad (3.13)$$

where the transition operator $\mathcal{U}(z)$ is diagrammatically represented by

$$\mathcal{U}(z) = \left[H_I + H_I\, \mathcal{D}(z)\ H_I + \ldots . \right]_{i.n.d.} , \qquad (3.14)$$

summed over all irreducible nondiagonal diagrams (i.n. d.)[10]. As will be seen below, $\mathcal{U}(z)$ determines the transition amplitude in scattering processes.

Let $|\alpha\rangle$ stand, as in (3.4), for an eigenstate of H_0 with unperturbed energy $E_{0\alpha}$, and let us assume that the equation (cf. (3.11))

$$E - E_{0\alpha} - \Delta_\alpha(E) = 0 \qquad (3.15)$$

has one and only real root $E = E_\alpha$. Then, there are only three possibilities:

$$\text{(i)} \quad \Gamma_\alpha(E_\alpha) \neq 0 ; \qquad (3.16)$$

In this case, by (3.11), $E = E_\alpha$ lies on a cut of $\mathcal{D}_\alpha(z)$. Van Hove[10] calls this a <u>dissipative state</u> ; typically, it decays in the presence of the interaction, and $\Delta_\alpha(E_\alpha)$ and $\Gamma_\alpha(E_\alpha)$ represent the energy shift and

linewidth due to the interaction. This situation is well illustrated by a Weisskopf-Wigner initial state,

$$|\alpha\rangle = |r;0\rangle = |r\rangle|0) \ , \qquad (3.17)$$

where $|r\rangle$ is an excited state of H_A and $|0)$ denotes the photon vacuum (we employ round brackets for photon state vectors). It will be discussed below in Sect. 6(a).

(ii) $$\Gamma_\alpha(E) = 0 \quad \text{for all real } E. \qquad (3.18)$$

In this case, $\mathcal{D}_\alpha(z)$ has a simple pole at $E = E_\alpha$ and no cut. The state $|\alpha\rangle$ is classified by Van Hove as asymptotically stationary[10] , because its asymptotic evolution is not affected by the interaction. The interaction produces only transient effects, as in ordinary scattering from a short-range potential. An example will be provided by the scattering of a one-photon wave packet from the ground state for the exactly soluble model discussed in Sect. 6(b).

(iii) $$\Gamma_\alpha(E_\alpha) = 0 \ , \text{ but } \ \Gamma_\alpha(E) \neq 0 \text{ for some real } E. \qquad (3.19)$$

In this case, the state $|\alpha\rangle$ is not asymptotically stationary. The interaction produces persistent perturbation effects; besides self-energy effects, they include, typically, "dressing" ("cloud") effects. Thus (cf. Sect. 8), the state $|\alpha\rangle = |1;0\rangle = |1\rangle|0)$, where $|1\rangle$ is the ground state of H_A, is not asymptotically stationary; the interacting ground state of the system is "dressed".

If $|\alpha\rangle$ and $|\alpha'\rangle$ are asymptotically stationary, the S - matrix element $\langle\alpha|S|\alpha'\rangle$ between these states can be shown to exist (with no need to adopt the unphysical procedure of adiabatic switching of the interaction). It is then given

by

$$\langle\alpha|S|\alpha'\rangle = \delta(\alpha-\alpha') - 2i\pi\,\delta(E_\alpha - E_{\alpha'})\mathcal{U}_{\alpha\alpha'}(E_\alpha), \quad (3.20)$$

where

$$\mathcal{U}_{\alpha\alpha'} = \langle\alpha|\mathcal{U}|\alpha'\rangle, \quad (3.21)$$

with $\mathcal{U}$ given by (3.13)-(3.14), is the transition amplitude matrix. The corresponding differential cross-section, for one-photon incidence, is given by

$$\sigma_{\alpha\alpha'} = (2\pi)^4 |\mathcal{U}_{\alpha\alpha'}(E_\alpha)|^2 \rho_\alpha(E_\alpha), \quad (3.22)$$

where ρ_α is the density of final states.

4. Possible Approximations

Our approach is based on the idea of sucessive approximations, retaining first only a part of the Hamiltonian, such that the problem becomes exactly soluble, and then adding back the omitted pieces of the Hamiltonian and investigating how they affect the solution. A somewhat related approach for Weisskopf-Wigner type theories has been advocated by Grimm and Ernst[15]. We start with a physical discussion of some of the main approximations that have previously been employed[11], as well as an extended version to be employed in Sect.5.

(I) Finite number of atomic states: This amounts to cutting off the spectrum of H_A beyond some discrete level N, so that, in (2.6) and (2.12),

$$(n,m) \leq N . \quad (4.1)$$

In particular, if only two states are kept, this is the two level atom. The accumulation point at the ionization

threshold as well as transitions to the continuum are eliminated by this approximation.

(II) Generalized RWA ("Rotating-Wave Approximation"): We consider a specific excited state $|r\rangle$, to be kept fixed, where "r" stands for "resonant", because this state is supposed to be selectively singled out by resonant processes, as will be seen below. Keeping only those terms in (2.12) where one of the levels involved in the transition is r, the generalized RWA corresponds to the following choice of interaction Hamiltonian:

$$H_I = \sqrt{\lambda} \sum_{n\beta} \int_0^\infty dk \sqrt{k}\ f_{rn\beta}(k)\ a_\beta(k)\ |r><n| + h.c., \quad (4.2)$$

where the "counter-rotating terms", which differ from those in (4.2) by the interchange of r and n within the summation, are neglected.

This is an extended version of the usual RWA, to which it reduces for a two-level atom. It corresponds to coupling the absorption of a photon only with transitions that end in r, and emission of a photon only with those that start from r, whether the transitions are to levels above or below r.

If we call "resonant atomic excitation" the occupation of level r (so that the atom is not "resonantly excited" whenever it occupies a level $n \neq r$), the generalized RWA leads to an additional conservation law, corresponding to the conservation of the number of photons plus the resonant atomic excitation. This is represented by the operator

$$\mathcal{E} = \frac{1}{2} |r\rangle\langle r| - \frac{1}{2} \sum_{n \neq r} |n\rangle\langle n| + \sum_{\beta} \int_0^{\infty} dk \; a_\beta^{+}(k) \; a_\beta(k) , \quad (4.3)$$

which commutes with

$$H = H_0 + H_I = H_A + H_F + H_I , \quad (4.4)$$

i.e.,

$$[\mathcal{E} , H] = 0 \quad . \quad (4.5)$$

This leads to a splitting of Hilbert space into sectors, allowing an exact solution in the sector of interest, as will be seen below.

Furthermore, (4.2) allows a transition from the ground state (n = 1) to level r only in the presence of a photon, so that the unperturbed ground state of the system

$$|1 ; 0\rangle = |1\rangle |0) \quad (4.6)$$

is also the interacting ground state, an eigenstate of H in the sector $\mathcal{E} = -1/2$ (so long as (5.6) below is satisfied). Thus, the generalized RWA exludes persistent perturbation effects.

(III) Dipole Approximation: This amounts to substituting, in (2.4) and (2.5),

$$\underset{\sim}{A}(\underset{\sim}{r}) = \underset{\sim}{A}(0) . \quad (4.7)$$

As a consequence of this, only electric dipole waves remain coupled to the atom, i.e., the photon index ranges only over the values

$$J = 1 ; \quad M = 0, \pm 1 ; \tau = 0 . \quad (4.8)$$

At the same time, this corresponds to neglecting retardation over atomic dimensions, so that the electric dipole form factors in (2.15) go over into their $k \rightarrow 0$ limit, which is

just a constant. This would lead to divergent integrals, so that this approximation is often coupled with

(IV) Sharp Cutoff : To avoid divergences in the dipole approximation, one replaces the effect of the atomic form factors by a sharp cutoff,

$$\rho(k) = \theta(K - k), \tag{4.9}$$

where θ is the Heaviside step function, and the cutoff parameter K is of the order of the inverse Bohr radius, $K \sim a_B^{-1}$.

The combination of approximations (III) and (IV), although it has often been employed in conjunction with two-level atomic models, leads to spurious effects. It introduces a spurious pole of the resolvent on the real axis, which gives rise to a non-decaying, non-ergodic contribution to the time evolution[8], for the state (3.17). This does not happen for a smooth form factor, such as (2.15).

We do not employ either (III) or (IV) in the soluble model that will now be discussed.

5. Exactly Soluble Multilevel Moldel

This model is defined by the Hamiltonian (4.4),

$$H = \sum_n E_{on} |n><n| + \sum_\beta \int_0^\infty dk\, k\, a_\beta^+(k) a_\beta(k) + \sqrt{\lambda} \sum_{n\beta} \int_0^\infty dk \sqrt{k} \left[f_{nn\beta}(k) a_\beta(k) |n><n| + h.c. \right], \tag{5.1}$$

where $n \leq N$, and β also ranges only over a finite set of values, due to the selection rules (2.14). The coefficients $f_{rn\beta}(k)$ are taken to be the exact hydrogen-atom matrix ele

ments. This corresponds to making approximations (I) and (II) of Sect. 4 and neglecting the quadratic interaction Hamiltonian (2.5).

The transitions allowed by the interaction Hamiltonian in (5.1) are schematically represented in Fig.1. In contrast with the multilevel model treated by Davies[16], the present model allows for transitions (within the generalized RWA) between the resonant level and other excited levels, but it does not take into account the decay of the other levels.

We restrict our discussion to the Hilbert Space sector associated with the eigenvalue $\xi = 1/2$ of the operator (4.3). Any state vector in this sector is of the form

$$|\psi\rangle = u\,|r;0\rangle + |\phi\rangle\,, \tag{5.2}$$

where

$$|\phi\rangle = \sum_{n\neq r,\beta} \int_0^\infty dk\ \varphi_{n\beta}(k)\,|n;1\beta,k\rangle\,, \tag{5.3}$$

$$|r;0\rangle = |r\rangle|0\rangle\,,\quad |n;1\beta,k\rangle = a^+_\beta(k)\,|n\rangle|0\rangle\,, \tag{5.4}$$

$$\langle\psi|\psi\rangle = |u|^2 + \sum_{n\neq r,\beta} \int_0^\infty |\varphi_{n\beta}(k)|^2\,dk = 1\,. \tag{5.5}$$

The state vector $|\psi\rangle$ evolves in the 0 photon + 1 photon subspace. Thus, cascade and multiphoton processes are excluded, but the effects of transitions to other levels on the excitation and decay of the resonant level are partially taken into account.

The condition

$$\frac{\lambda}{E_{or}} \sum_{n\neq r,\beta} \int_0^\infty \frac{|f_{rn\beta}(k)|^2}{k + E_{on}}\,k\,dk < 1\,, \tag{5.6}$$

which follows for this model from the smallness of the coupling constant (2.13), ensures that H has only a continuous spectrum[17], ranging from the unperturbed ground-state energy E_{01} to infinity. We take the unperturbed ground-state energy as the zero level of energy,

$$E_{01} = 0 . \tag{5.7}$$

The resolvent then has a cut along the real axis ranging from 0 to ∞ .

The matrix elements of the resolvent in the sector under consideration follow from the identity

$$\mathcal{G}(z) = \mathcal{G}_0(z) + \mathcal{G}(z)\, H_I\, \mathcal{G}_0(z). \tag{5.8}$$

They are explicitly given by[8]

$$\langle \pi;0|\mathcal{G}(z)|\pi;0\rangle = \langle \pi;0|\mathcal{D}(z)|\pi;0\rangle = \mathcal{D}_{\pi;0}(z) = \frac{1}{D(z)}, \tag{5.9}$$

$$\langle \pi;0|\mathcal{G}(z)|\Phi\rangle = \frac{\sqrt{\lambda}}{D(z)} \sum_{n\neq\pi,\beta} \int_0^\infty \frac{\sqrt{k}\, f^*_{\pi n\beta}(k)\, \varphi_{n\beta}(k)}{z-k-E_{on}}\, dk, \tag{5.10}$$

$$\langle \Phi|\mathcal{G}(z)|\Phi'\rangle = \sum_{n\neq\pi,\beta} \int_0^\infty \frac{\varphi^*_{n\beta}(k)\,\varphi'_{n\beta}(k)}{z-k-E_{on}}\, dk + \frac{\lambda}{D(z)} \sum_{n\neq\pi,\beta} \int_0^\infty \frac{\sqrt{k}\,\varphi^*_{n\beta}(k)\, f_{\pi n\beta}(k)}{z-k-E_{on}}\, dk \sum_{m\neq\pi,\beta} \int_0^\infty \frac{\sqrt{k}\, f^*_{\pi m\beta}(k)\,\varphi'_{m\beta}(k)}{z-k-E_{om}}\, dk, \tag{5.11}$$

where

$$D(z) = z - E_{on} - \frac{1}{2\pi} \sum_{n\neq\pi,\beta} \int_0^\infty \frac{\Gamma_{\pi n\beta}(k)}{z-k-E_{on}}\, dk, \tag{5.12}$$

$$\Gamma_{\pi n\beta}(k) = 2\pi\lambda k\, |f_{\pi n\beta}(k)|^2 . \tag{5.13}$$

The analytic properties of $\mathcal{D}_{r;0}(z)$ and of the other matrix elements of the resolvent are therefore determined by those of the denominator function D (z). This

function can be explicitly computed[8] from (2.15). It is given by

$$D(z) = z - E_{Or} - \frac{1}{2\pi}\sum_{n\neq r,\beta} \Gamma_{rn\beta}(z-E_{On})\ \ln\left[(E_{On}-z)/K_{rn}\right] + \lambda \sum_{n\neq r,\beta} \frac{Q_{rn\beta}(z-E_{On})}{\left[(z-E_{On})^2+K_{rn}^2\right]^{p_{rn}}} \quad , \qquad (5.14)$$

where, on the physical sheet,

$$\ln\left[(E_{On} - E \mp i0)/K_{rn}\right] = \ln\left|(E_{On}-E)/K_{rn}\right| \mp i\pi\,\theta(E-E_{On}) \quad , \qquad (5.15)$$

θ being the Heaviside step function, and $Q_{rn\beta}(z)$ is a polynomial with real coefficients, that are $\mathcal{O}(1)$ in the units (2.11), with degree $Q_{rn\beta} \leq 2p_{rn} - 1$. Thus,

$$D(z) = \mathcal{O}(z) \quad (\ |z| \to \infty\ ) \quad . \qquad (5.16)$$

The function D(z) is holomorphic and zero-free on the physical sheet. The coefficients of the polynomial $Q_{rn\beta}(z)$ follow from (2.15), (5.13), (5.14) and the condition that D(z) has no singularities at $z = E_{On} \pm i K_{rn}$ on the physical sheet.

According to (5.14), D(z) has a logarithmic branch point at each unperturbed bound-state energy E_{On}, except the resonant one, n=r. The logarithmic terms, while reminiscent of the "Bethe-log" contributions to the Lamb shift (cf.Sect. 8), are exact within this model.

6. Applications to Decay and Resonance Scattering

We now apply the exactly soluble model of Sect.5 to

investigate the decay of a Weisskopf-Wigner initial state and the resonance scattering of a wave packet.

(a) Decay of a Weisskopf-Wigner initial state:

The initial state $|r;0\rangle$ defined by (5.4) is a dissipative state in the sense of Van Hove (cf. (3.16) and (5.15)). According to (3.6) and (5.9),

$$\langle r;0 \mid \exp(-iHt) \mid r;0\rangle = -\frac{1}{2\pi i}\int_C \frac{\exp(-izt)}{D(z)}\,dz. \qquad (6.1)$$

Let us now deform the path C in the manner indicated in Fig. 2, into a series of paths $C_1, C_2, \ldots, C_N$ directed parallel to the bisector of the fourth quadrant, such that the path C_j winds around the branch point E_{0j}. Thus, the left-hand side of C_j and the right-hand side of C_j are on different Riemann sheets, but the left-hand side of each path is on the same sheet as the right-hand side of the preceding one. These deformations are allowed by (5.16), with no contribution from portions of the "circle at infinity".

Each time the path winds around a branch point E_{0j} in the indicated manner, a new term

$$+ i \sum_{\beta} \Gamma_{rj\beta}(z-E_{0j})$$

is added to the determination of $D(z)$ in the corresponding Riemman sheet (cf. (5.14) - (5.15)). On each sheet, the integrand has a finite number of poles, the positions of which can be determined[8] from (5.14). With the above choice of contour it may be shown[8] that only one pole z_r (indicated in Fig. 2) will be crossed, with

$$z_r = E_r - \frac{i}{2}\Gamma_r = E_{0r} + \frac{1}{2\pi}\sum_{n\neq n,\beta} P\int_0^{\infty} \frac{\Gamma_{rn\beta}(k)}{E_{0r} - k - E_{0n}}\,dk$$

$$- \frac{i}{2} \sum_{\beta, n=1}^{r-1} \Gamma_{rn\beta} (E_{Or} - E_{On}) + \mathcal{O}(\lambda) , \qquad (6.2)$$

where only those thresholds crossed up to E_{Or} contribute to the imaginary part, and P denotes Cauchy's principal value.

For times much longer than the optical period ($E_{Or} t \gg 1$), the asymptotic behavior of (6.1) is given by[8]

$$\langle r;0 \mid \exp(-iHt) \mid r;0 \rangle \approx [1 + \mathcal{O}(\lambda^2)] \exp(-iE_r t - \tfrac{1}{2} \Gamma_r t)$$
$$+ \sum_{n \neq r, \beta} A_{rn\beta} \, t^{-2\gamma_{rn\beta}} \exp(-iE_{On} t) , \qquad (6.3)$$

where $A_{rn\beta}$ are constants and

$$\gamma_{rn\beta} = J_{rn\beta} + \tau_{rn\beta} , \qquad (6.4)$$

where $J_{rn\beta}$ and $\tau_{rn\beta}$ are associated with the multipolarity of the transition (cf. (2.8)); for electric dipole transitions, $\gamma_{rn\beta} = 1$.

The first term in (6.3) corresponds to the Wigner-Weisskopf exponential "Ansatz", with the level shift $E_r - E_{Or}$ given by the principal-value integral in (6.2) (which already contains, as we have seen, pieces of "Bethe-log"-like contributions). The half-width Γ_r, according to (6.2), is the sum of the partial widths for transitions to all lower levels, as it should be. Both the level shift and half-width include contributions that were not taken into account in previous exactly solved models (in particular, those involving two-level atoms).

The terms in the second line of (6.3) represent corrections to exponential decay, arising from the integrals around the cuts C_j in Fig. 2. A rigorous estimate[8] shows that, for electric dipole transitions, such corrections are negligible up to times t_0 such that

$$t_0^2 \quad \exp\left(-\frac{1}{2}\Gamma_r t_0\right) \sim \frac{2e^2}{3\pi} \langle r \mid \underset{\sim}{r}^2 \mid r \rangle . \qquad (6.5)$$

For the Lyman-α line, this yields a value of t_0 of the order of 96 lifetimes, so that corrections to the Weisskopf-Wigner "Ansatz" in this case are extremely small. It is interesting to note that such corrections behave as t^{-2} for $t \to \infty$, just like a free-photon wave packet when account is taken of causal propagation[18]. Analogous features have been found for decay involving massive particles[7], suggesting that limitations in the validity of the exponential decay law are to be traced to the limitations in the validity of of the particle concept itself when applied to unstable particles. In order to discuss the observability of such deviations, however, one would need a theoretical analysis of the measurement process.

(b) Resonance scattering of a wave packet:

The dependence of the decay on the excitation in the present model can be investigated by discussing the scattering of a photon wave packet by the atom. In order for the model to remain reasonably realistic, we must assume that the mean energy $\bar{E}$ of the incident wave packet is close to resonance (cf. (6.7) below), so that we are discussing resonance fluorescence.

As a consequence of the generalized RWA employed in our model, the state $|1;\ 1\beta, k\rangle$ defined by (5.4) (atom in the ground state + 1 photon) is asymptotically stationary in the sense of Van Hove, so that the incident wave takes the form

$$|\Phi\rangle = \int_0^\infty dk \ \varphi(k) \ | \ 1;1\beta \ , \ k\rangle , \qquad (6.6)$$

where $\varphi(k)$ is associated with a mean energy $\bar{E}$ and a half-width γ such that

$$|\bar{E} - E_{0r}| \ll |E_{0,r} - E_{0,r\pm1}|, \gamma \ll |E_{0,r} - E_{0,r\pm1}|. \qquad (6.7)$$

The excitation amplitude of the atom is given by (cf. (5.10))

$$\langle r;0 \,|\, \exp(-iHt) \,|\, \Phi \rangle = -\frac{1}{2\pi i} \int_C \exp(-izt) \langle r;0 \,|\, \mathcal{G}(z) \,|\, \phi \rangle dz. \qquad (6.8)$$

By suitable choice of $\varphi(k)$ (e. g., a Lorentzian wave packet), this can be treated[8] similarly to (6.1). Typically, the excitation probability is characterized by a rise time T_{rise} and by a decay time T_{decay} such that[5,7]

$$T_{rise} \sim \min(\gamma^{-1}, \Gamma_r^{-1}) \; ; \; T_{decay} \sim \max(\gamma^{-1}, \Gamma_r^{-1}). \qquad (6.9)$$

For excitation by a broad line ($\gamma \gg \Gamma_r$), the excitation and the decay may be regarded as to some extent independent processes; for a Lorentzian wave packet, the Weisskopf-Wigner state is excited with a probability $\sim(\Gamma_r/\gamma)^2$ and it decays with the natural line shape.

The scattered wave packet, as well as the emitted line shape, can also be obtained[8] with the help of (5.11). The asymptotic behavior for large times is found to depend very strongly on the excitation.

7. Persistent Effects and Dressing Transformation

When the "counter-rotating" terms that were omitted from the Hamiltonian to yield the exactly soluble model are reintroduced, drastic changes take place: these terms lead

to virtual transitions from the unperturbed ground state $|1;0\rangle$ to excited states with the emission of a photon, followed by the reverse transition in which the photon is absorbed. This produces persistent perturbation effects in the sense of Van Hove, i. e., both self-energy and cloud effects.

These effects are manifested in several ways: $|1;0\rangle$ is no longer the ground state of the interacting system (it gets "dressed by a photon cloud"), and the states $|1;1\beta, k\rangle$ are no longer asymptotically stationary, so that they cannot be employed as a basis to build up wave packets in the treatment of resonance scattering.

In order to deal with this situation, we first apply a dressing transformation in order to get rid of the persistent effects. After this is done, the resolvent operator method can in principle be employed as before, with the transformed Hamiltonian now generating the dynamics of "dressed" states of the system. However, exact results are no longer obtained: the transformation is defined order-by order in perturbation theory; we discuss the results obtained to second order. Mass renormalization must also be performed.

Attempts to perform such a transformation were made by Heitler, Arnous and collaborators in a series of papers[3], but they met with difficulties, because they attempted to solve the unphysical problem of dressing also excited atomic states. In their subsequent work[4,5], the transformation was suitably restricted, but no explicit expressions for it and for the transformed Hamiltonian were found; the treatment is also needlessly complicated. Coulter's dressing transformation[19] for an atom within a bounded volume also attempts

to satisfy unphysical requirements and it is not convergent in the infinite-volume limit.

Our procedure is based on a generalization of a dressing transformation proposed by Faddeev[12]. We transform

$$H = H_0 + \lambda V \quad , \tag{7.1}$$

where the coupling constant λ is the small perturbation parameter, into

$$H' = U H U^{-1} = H_0' + V', \tag{7.2}$$

where U is a unitary transformation,

$$U = \exp(iW) \quad , \quad W = W^{+} \quad , \tag{7.3}$$

and

$$V' = \sum_{n \geq 1} \lambda^n V'_n \quad , \quad W = \sum_{n \geq 1} \lambda^n W_n \, . \tag{7.4}$$

. Equating the coefficients of equal powers of λ , we get

$$V'_1 = V + i \left[W_1 , H_0 \right] \quad , \tag{7.5}$$

$$V'_2 = i \left[W_1, V \right] + \frac{i^2}{2!} \left[W_1, \left[W_1, H_0 \right] \right] + i \left[W_2, H_0 \right] ,$$

and so on.

We now choose W_1 so that $i \left[W_1, H_0 \right]$ cancels out (cf. (7.5)) those terms in V that lead to persistent effects, thus eliminating these effects to first order in λ . With this choice for W_1, we next choose W_2 in (7.6) so that the nondiagonal part of V'_2 is free from persistent effects (the diagonal part is incorporated into H_0'). In principle, this procedure can be continued up to arbitrarily high order in λ.

The terms that lead to persistent perturbation effects, according to (3.19), are those that lead to $\mathrm{Im}\,\Sigma_\alpha(E) \neq 0$ for non-dissipative states. They are readily recognized in the present problem as those terms that give rise to transitions from the ground state (such as the "counter-rotating" terms in V).

The choice of W_1, W_2 ,..... is clearly not unique. This non-uniqueness is inherent in any dressing transformation: transformations whose effects differ by an arbitrary admixture of transient terms (i. e., terms not conducive to persistent effects) are equivalent according to the above definition. In practice, our choice of W_1 , W_2, ... is guided by criteria of simplicity: their form is determined by that of the terms we wish to cancel out, with the insertion of suitable energy denominators to obtain the cancellation when the commutator with H_0 is taken.

8. Dressing Transformation for the Hydrogen Atom

For the sake of simplicity, and in order to facilitate the comparison with the usual treatment, we restrict our discussion of the dressing transformation for the hydrogen atom to the dipole approximation. The Hamiltonian of Sect. 2 is simplified to

$$H = H_0 + H_{I,1} + H_{I,2} + H_{ren} \quad , \tag{8.1}$$

$$H_0 = \sum_{n\geq 1} E_{On}\, |n\rangle\langle n| + \sum_{M=-1}^{1} \int_0^\infty k\, a_M^+(k)\, a_M(k)\, dk \quad , \tag{8.2}$$

$$H_{I,1} = \sum_{ijM} \lambda_{ijM}\, |i\rangle\langle j| \int_0^\infty \rho(k) \left[a_M(k) + a_M^+(k) \right] \sqrt{k}\, dk, \tag{8.3}$$

where $\rho(k)$ is a cutoff factor (usually taken in the form (4.9)) and

$$\lambda_{ijM} = -\frac{1}{m}\,(2\alpha/3\pi)^{1/2}\,\langle i\,|\,p_M\,|\,j\rangle \quad , \tag{8.4}$$

p_M being the spherical components[13] of $\underset{\sim}{p}$;

$$H_{I,2} = \lambda' \sum_{M=-1}^{1} (-1)^M \int_0^\infty dk \sqrt{k}\;\rho(k) \int_0^\infty dk' \sqrt{k'}\;\rho(k')$$

$$\times \left[a_M(k)\; a_{-M}(k') + (-1)^M\, a_M^{+}(k)\; a_M(k') + \text{h. c.}\right] , \tag{8.5}$$

where

$$\lambda' = \alpha/3\pi m \; . \tag{8.6}$$

We have already written $H_{I,2}$ in normally-ordered form, subtracting out a constant term. Finally, in order that m be the experimental mass of the electron, the usual nonrelativistic mass-renormalization counterterm H_{ren} is added. To second order (which is as far as we will carry out the calculation), it is given by

$$H_{ren,2} = (\Delta m/m)\;\; \underset{\sim}{p}^2/2m \quad , \tag{8.7}$$

$$\Delta m/m = 4\,\lambda' \int_0^\infty \rho(k)\; dk \; . \tag{8.8}$$

In order to apply the dressing transformation, some slight modifications in (7.6) are required, owing to the fact that, besides terms linear in the coupling constant ($H_{I,1}$), the Hamiltonian also contains quadratic terms ($H_{I,2}$, H_{ren}).

To first order, the "counter-rotating" terms that are responsible for persistent effects in (8.3) are those in $|\,i\rangle\langle 1\,|\,a_M^{+}(k)$ and their hermitean conjugates. To eliminate them, we choose

$$\lambda W_1 = i \sum_{i,M} \lambda_{i1M} \int_0^\infty dk\;\rho(k)\sqrt{k}\;\; \frac{|i\rangle\langle 1|a_M^{+}(k)}{E_{01} - E_{0i} - k} + \text{h.c.} \tag{8.9}$$

Applying a similar procedure to second order, we get for the transformed Hamiltonian

$$H' = H_0' + H_1' + H_2' \quad , \tag{8.10}$$

where H_1' is given by (8.3) with the counter-rotating terms connected with the ground state subtracted out, and H_2' is a sum of several terms that will not be written out here[8]; H_0' , which incorporates the diagonal contributions found in second order, is given by

$$H_0' = \sum_{n \geq 1} E'_{0n} \; |n\rangle\langle n| + \sum_{M=-1}^{1} \int_0^\infty k \; a_M^+(k) \; a_M(k) \; dk, \tag{8.11}$$

where

$$E'_{0n} = E_{0n} + 4\lambda' \langle n | \underset{\sim}{p}^2/2m | n \rangle \int_0^\infty \rho(k) \; dk, \quad n \neq 1, \tag{8.12}$$

$$E'_{01} = E_{01} + \mathcal{L}_1 \quad , \tag{8.13}$$

and

$$\mathcal{L}_1 = \sum_{n \neq 1, M} \lambda^2_{n1M} \; (E_{0n} - E_{01}) \int_0^\infty \frac{\rho(k) \; dk}{k + E_{0n} - E_{01}} \; . \tag{8.14}$$

When $\rho(k)$ is replaced by (4.9), $\mathcal{L}_1$ becomes identical with the nonrelativistic contribution to the ground-state Lamb shift, as computed by Bethe[20]. Thus, for the ground state, the dressing transformation cancels out the contribution from the mass-renormalization counterterm (cf. (8.12)), and it adds the Lamb-shift correction. Furthermore, the interaction terms H_1' and H_2' in (8.10) produce no persistent effects to second order. We can therefore apply the resolvent operator method, with H' as generator of the time evolution, to discuss decay and resonance fluorescence by procedures similar

to those described in Sect. 6. We confine ourselves to a description of the main results[8].

The time evolution of an initial excited state $|n\rangle|0)$ is determined, as in Sect. 6(a), by the analytic properties of $\mathscr{D}_{n;0}(z)$, the associated eigenvalue of the diagonal part of the resolvent. It is found in the second-order treatment that, in analogy with (6.2), the dominant exponentially-decaying term arises from an unphysical-sheet pole

$$z_n = E_n - \frac{i}{2}\Gamma_n = E_{On} + \mathscr{L}_n - \frac{i}{2}\sum_{j<n,M}\Gamma_{njM}\,, \qquad (8.15)$$

where $\mathscr{L}_n$ is the nonrelativistic contribution to the Lamb shift for state n and Γ_{njM} are the partial widths for the transitions to all lower levels.

Thus, the analogue of the energy correction (8.13) for excited states (cancellation of the mass-renormalization counterterm in (8.12) and Lamb-shift correction) appears, as it should, in the poles of the analytic continuation for the resolvent, and not through the dressing transformation, which should lead to the correct energy only for the ground state. This essential difference between ground and excited states was obscured in previous treatments where dressing transformations were attempted.

The discussion of resonance fluorescence also proceeds in analogy with Sect. 6(b). In order to treat the line shape problem, we consider, in particular, the differential cross-section for scattering of a photon with momentum $\underset{\sim}{k}$ and circular polarization λ from an atom in the ground state, leading to a photon with momentum $\underset{\sim}{k}'$ and circular polarization λ'. The result[8], obtained with the help of (3.22), is

given by a modified Kramers-Heisenberg dispersion formula :

$$\frac{d\sigma}{d\Omega} = r_o^2 \left| \hat{\underset{\sim}{\varepsilon}}_{\underset{\sim}{k}\lambda} \cdot \hat{\underset{\sim}{\varepsilon}}^{*}_{\underset{\sim}{k}'\lambda'} + \frac{1}{m} \sum_{n \neq 1} \frac{\langle 1 | \underset{\sim}{p} \cdot \hat{\underset{\sim}{\varepsilon}}_{\underset{\sim}{k}\lambda} | n \rangle \langle n | \underset{\sim}{p} \cdot \hat{\underset{\sim}{\varepsilon}}^{*}_{\underset{\sim}{k}'\lambda'} | 1 \rangle}{E_{01} - E_{on} - k} \right. \tag{8.16}$$

$$\left. + \frac{1}{m} \sum_{n \neq 1} \frac{\langle 1 | \underset{\sim}{p} \cdot \hat{\underset{\sim}{\varepsilon}}^{*}_{\underset{\sim}{k}'\lambda'} | n \rangle \langle n | \underset{\sim}{p} \cdot \hat{\underset{\sim}{\varepsilon}}_{\underset{\sim}{k}\lambda} | 1 \rangle}{E_{01}' + k - [E_{on}' + \Delta_n(E_{01}+k)] + \frac{i}{2}\Gamma_n(E_{01}+k)} \right|^2 ,$$

where r_o is the classical electron radius, $\hat{\underset{\sim}{\varepsilon}}_{\underset{\sim}{k}\lambda}$ and $\hat{\underset{\sim}{\varepsilon}}_{\underset{\sim}{k}'\lambda'}$ are polarization vectors of the incident and scattered photons, and Δ_n and Γ_n are defined in terms of the resolvent by (3.11). The first line of (8.16) contains the effects of Thomson scattering and of antiresonant terms. If the incident photon energy approaches a resonance associated with a given level n, the corrections Δ_n and Γ_n to the Kramers-Heisenberg formula in the corresponding term of the second line of (8.16) become important. In this case, $E_{On} + \Delta_n - \frac{i}{2}\Gamma_n$ is close to z_n (cf. (8.15)), so that the Lamb-shift correction and the linewidth are also properly taken into account in the resonance scattering cross-section.

9. Interaction Hamiltonian and Line Shape

We finally discuss the connection between the line shape and the choice of the interaction Hamiltonian. The problem is to compare the results obtained with the minimal coupling interaction Hamiltonian employed in (2.1), in dipole approximation, with those obtained from the interaction Hamiltonian

$$\bar{H}_I = - \underset{\sim}{e}\underset{\sim}{r} . \underset{\sim}{E}^{\perp}(\underset{\sim}{0}) , \tag{9.1}$$

which has been widely employed in quantum optics. The relation between these two Hamiltonians seems to have been first discussed by Göppert-Mayer[21] in a semiclassical context, and by Power and Zienau[22] for a quantized field; other recent discussions include that of Woolley[23]. The resonant term obtained from the two different interaction Hamiltonians yields different results for the line shape, and it was remarked by Lamb[2] that only the resonant term derived from (9.1) is in agreement with experiment for the Lamb-shift transition.

In Woolley's treatment, $\underset{\sim}{E}^{\perp} = -\partial \underset{\sim}{A} / \partial t$ is indeed the transverse electric field, while in Power and Zienau's treatment it is replaced by

$$\underset{\sim}{D}^{\perp} = (\underset{\sim}{E} + 4\pi \underset{\sim}{P})^{\perp} \quad , \tag{9.2}$$

where

$$\underset{\sim}{P} = e \underset{\sim}{r} \delta(\underset{\sim}{q}) \tag{9.3}$$

is the polarization operator in dipole approximation.

Both interpretations are possible, and the difference between them simply corresponds to regarding the transformation connecting the two Hamiltonians from the active or from the passive point of view[8].

In the active point of view[23], which will be adopted here, the new Hamiltonian $\bar{H}$ is connected with H (as given by (2.1), in dipole approximation) by

$$\bar{H} = \exp(-i\Sigma) \; H \; \exp(i\Sigma) \quad , \tag{9.4}$$

where[24]

$$\Sigma = e \underset{\sim}{r} . \underset{\sim}{A}(0) \tag{9.5}$$

leading to

$$\overline{H} = \frac{\underset{\sim}{p}^2}{2m} - \frac{e^2}{r} + \frac{1}{8\pi}\int d^3 r \left[(\underset{\sim}{E}^{\perp})^2 + (\underset{\sim}{\nabla} \times \underset{\sim}{A})^2 \right] - \underset{\sim}{e_r}.\underset{\sim}{E}^{\perp}(\underset{\sim}{0})$$

$$+ 2\pi \int \left[\underset{\sim}{p}^{\perp}(\underset{\sim}{q}) \right]^2 \quad d^3q \qquad , \qquad (9.6)$$

where the last term contributes to second-order (or higher--order) calculations, e.g., in the evaluation of the Lamb shift. Here, $\overline{H}$ is regarded as a new Hamiltonian, expressed in terms of the old canonical variabels, whereas, in the passive point of view[22], we would get the old Hamiltonian expressed in terms of new canonical variables.

Since the two Hamiltonians are connected by a unitary transformation, they must lead to equivalent results, provided that the state vectors are correspondingly transformed. If one tries to define the natural line shape in terms of the decay of a specified Weisskopf-Wigner initial state vector, without taking into account the transformation of this state vector (it can be shown[8] that this corresponds to adopting different definitions of the photon vacuum), the two Hamiltonians lead to different results, but one cannot say a priori which (if any) is to be preferred, because this depends on how realistic it is to regard the associated Weisskopf-Wigner state as being produced by the excitation process. An unambiguous definition of the line shape must include an account of the excitation process.

If we define the line shape in terms of resonance fluorescence, we must discuss the effect of the transformation (9.4) on the S-matrix. The exact S-matrix elements for transitions between corresponding physical states are indeed identi-

cal for H and $\bar{H}$. However, when they are defined in terms of the usual adiabatic hypothesis, this is true only after wave function renormalization[8], and the corresponding renormalization constants Z and $\bar{Z}$ (which represent the probability of finding the unperturbed ground state in the interacting ground state) are different. Since Z and $\bar{Z}$ differ from unity only by terms of order e^2, the Kramers-Heisenberg matrix element is the same for both Hamiltonians, as is well-known[25]. However, this need not apply to (8.16), which already includes partial summations over higher-order terms, embodied in the Δ_n and Γ_n corrections. It can be shown[8], nevertheless, that, for photon energies k within the resonance width associated with each given resonance denominator, these corrections also are the same, up to order e^2.

Let r be the resonant level, R the corresponding resonant term (the term n=r in the second line of (8.16)) , and B the background, i. e., the sum of all remaining terms in (8.16). The result just stated then implies that, to order e^2,

$$d\sigma/d\Omega = r_o^2|R + B|^2 = r_o^2|\bar{R} + \bar{B}|^2 . \qquad (9.7)$$

However, we have $R \neq \bar{R}$, $B \neq \bar{B}$. If, as is often done, one approximates the result by retaining only the resonant term, the results are indeed different, and the only way to find out which is the better approximation (apart from comparison with experiment) is to estimate the effect of the background terms.

Let us do this first for the Lyman-α line. In this case, we have

$$\bar{R}/R = k^2/(E_{02} - E_{01})^2 , \qquad (9.8)$$

where E_{02} is the energy of the 2p level. To compare the line shapes, we characterize them by two parameters: the photon energy k_0 at the peak of the curve and the asymmetry δ, defined by

$$\delta = \left[\left(\frac{d\sigma}{d\Omega}\right)_{k_0+\frac{\Gamma}{2}} - \left(\frac{d\sigma}{d\Omega}\right)_{k_0-\frac{\Gamma}{2}}\right] \Big/ \left(\frac{d\sigma}{d\Omega}\right)_{k_0} , \qquad (9.9)$$

where Γ is the linewidth associated with the 2p level.

In terms of these parameters, we find that

$$(\bar{k}_0 - k_0) / \Gamma = \frac{1}{2} \Gamma / k_0 , \qquad (9.10)$$

and that R is symmetric ($\delta = 0$), whereas for $\bar{R}$,

$$\delta = 2\Gamma / k_0 . \qquad (9.11)$$

Since $\Gamma / k_0 \simeq 4X10^{-8}$, both deviations are extremely small in this case. It may stil be asked, however, which one yields a better approximation.

In order to find out, one must compute B, the sum of all "background" terms. This can be done in closed form, with the help of the Coulomb Green's function, which has been employed by Gavrila[26] to compute the Kramers-Heisenberg matrix element.

The result[8] for the photon energy k_0' at the peak when both R and B are included is

$$(k_0' - k_0) / \Gamma \simeq -0.22 \Gamma / k_0 , \qquad (9.12)$$

and the corresponding asymmetry parameter is

$$\delta' \approx -1.8 \Gamma / k_0 . \qquad (9.13)$$

Comparing these results with (9.10) and (9.11), we see that the corrections associated with $\bar{R}$ have the wrong sign, so that, in this case, it is R that represents a better approximation.

As a final example, let us discuss the line shape for the Lamb-shift transition, i. e., for the induced decay from the metastable $2s_{1/2}$ state to the $2p_{1/2}$ state, in the presence of near-resonant microwave photons of frequency k_0 (followed by a Lyman-α transition to the ground state). This corresponds to a more recent version[27] of Lamb's experiment, which does not employ magnetic-field tuning of the $2s_{1/2} - 2p_{1/2}$ energy difference.

We make use of the fact that, up to second order, $\mathrm{Im}\ \Sigma_{2s} = 0$ (cf. (3.10)), so that the metastable $2s_{1/2}$ state may be treated as stable, to this order. However, to the same order, $\mathrm{Re}\ \Sigma_{2s} \neq 0$, so that one must correct the energy of the $2s_{1/2}$ state in order for it to behave as an asymptotically stationary state. This is achieved by adding a term to the unperturbed Hamiltonian (8.2) and then subtracting the same term from the interaction Hamiltonian. This term should be nondiagonal, so as to remove the degeneracy between the $2s_{1/2}$ and $2p_{1/2}$ states[28], and it must not affect the ground-state energy. A suitable choice is[8]

$$H_L = 8\pi\epsilon_0\ a_B^3\ \delta(\underset{\sim}{r}) - 8\epsilon_0\ |1\rangle\langle 1|\ , \qquad (9.14)$$

where a_B is the Bohr radius, and ϵ_0 is the (unrenormalized) nonrelativistic contribution to the Lamb shift of the $2s_{1/2}$ state.

This leads to the replacement

$$E_{02s} \longrightarrow E_{02s} + \epsilon \qquad (9.15)$$

in (8.12), where ϵ is the renormalized nonrelativistic contribution to the Lamb shift of the $2s_{1/2}$ state, whereas (8.13) remains unaffected. Corresponding modifications must be made in the dressing transformation to ensure that the $2s_{1/2}$ state (as well as the ground state) remains asymptotically stationary to second order.

A contact term similar to that in (9.14) appears in the usual treatment[29] of the nonrelativistic contribution to the Lamb shift. It has also been employed by Fried[30] as a phenomenological term in a treatment of the same problem based upon a semiclassical Hamiltonian.

Taking the above modifications into account, we find expressions[8] for the differential cross-section to second order that can be analysed in terms of resonant and background contributions, as in (9.7). We find that R is peaked at a photon energy

$$k_0 \approx \epsilon - \Gamma^2/8\epsilon \,, \qquad (9.16)$$

whereas $\bar{R}$ is peaked at

$$\bar{k}_0 \approx \epsilon + \Gamma^2/8\epsilon \,, \qquad (9.17)$$

while the corresponding asymmetries (9.9) are given by

$$\delta \approx -\Gamma/2\epsilon \quad , \quad \bar{\delta} \approx \Gamma/2\epsilon \,. \qquad (9.18)$$

Since $\Gamma/\epsilon \approx 10^{-1}$, we have $(\bar{k}_0 - k_0)/\epsilon \approx 2.5\text{X}10^{-3}$, which is about three orders of magnitude larger than the accuracy of present-day measurements of the Lamb shift.

Thus, the differences between R and $\bar{R}$ are easily detectable in this case.

The background contribution B can again be evaluated in closed form[31], with the help of the Coulomb Green's function. The results for k_0' and δ' when both R and B are included[8] agree with $\bar{k}_0$ and $\bar{\delta}$ of (9.17) and (9.18) up to terms of the order of $\epsilon\,(\Gamma/\epsilon)^4$ and $(\Gamma/\epsilon)^2$, respectively. This remains valid when fine and hyperfine structure contributions are taken into account.

Thus, in agreement with Lamb's remark[2], the resonant term derived from (9.1) indeed yields better results for the line shape in the Lamb-shift transition. However, this does not hold true in other cases, as shown by our discussion of the Lyman-α line. Similar conclusions were reached by Fried[30].

The line shape in the Lamb-shift transition, defined in terms of the usual minimal-coupling Hamiltonian of quantum electrodymanics, illustrates the need to go beyond the Weisskopf-Wigner approximation. In order to obtain agreement with experiment, one must take into account the effect of (virtual) transitions to all nonresonant levels. These background corrections to the line shape can be systematically evaluated by employing the Coulomb Green's function.

As the accuracy of Lamb-shift measurements increases, the evaluation of background corrections to the line shape becomes of comparable or possibly greater significance than that of higher-order radiative corrections to the resonant term, since the result of the measurement is directly affected by the line shape, which arises from the interference between resonant and background contributions.

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FIGURE CAPTIONS

Fig. 1. Transitions taken into account by the soluble N-level model. r = resonant level ; - - - - → absorption; ——→ emission.

Fig. 2. Equivalent path of integration for (6.1). The positive real axis is covered by a series of superimposed branch cuts associated with the threshold branch points, and the path winds around successive branch points; portions belonging to the same Riemann sheet are similarly represented. The pole z_r of (6.2) is indicated.

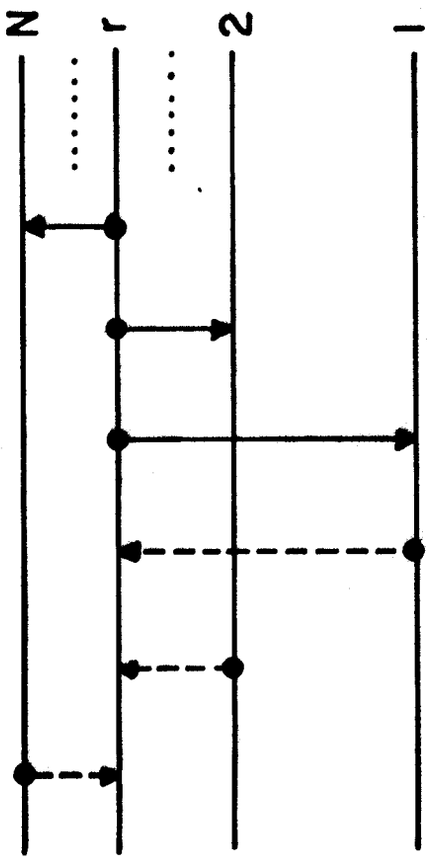

Fig. 1

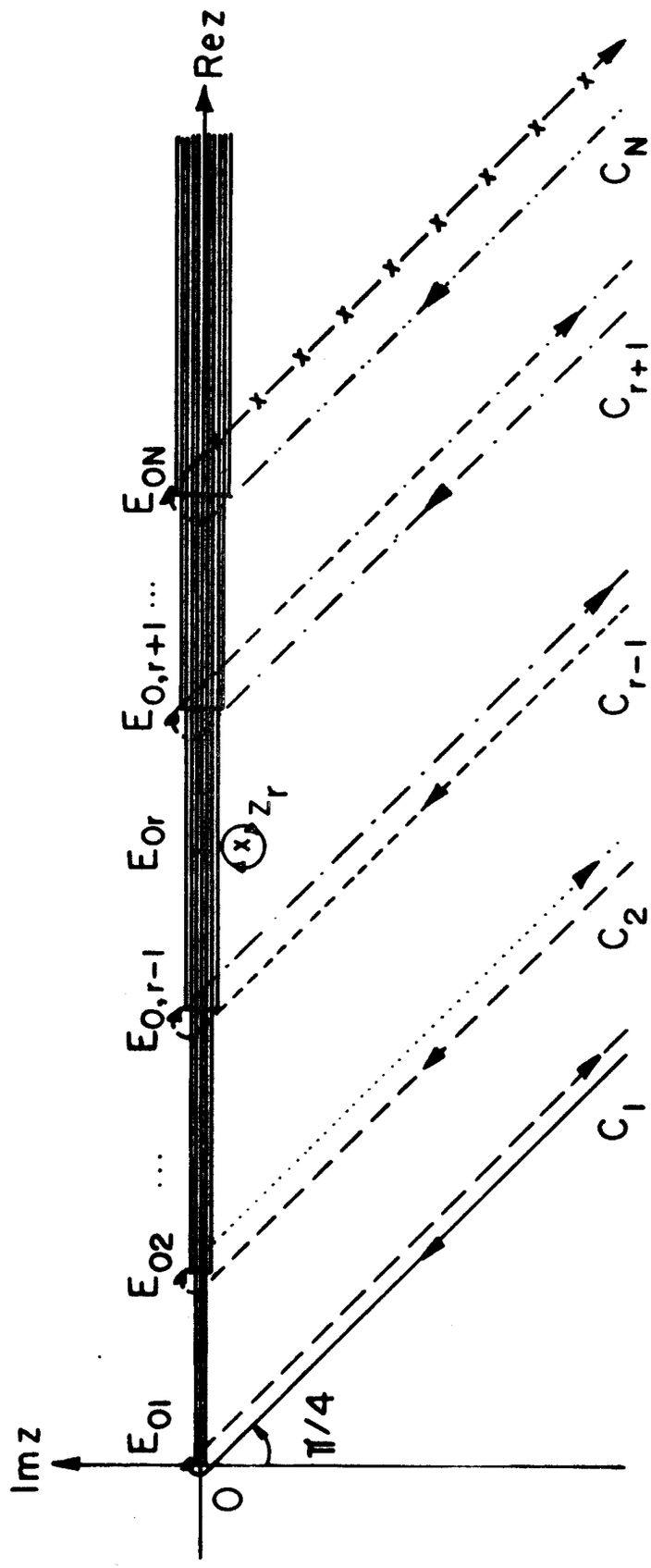

Fig. 2