Natural Line Shape

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The covariant methods of Feynman and Dyson are applied to the problem of line shape. It is shown that the line center depends almost completely on the form of the S_{Fe}' function, that is the Feynman-type Green's function for the electron interacting with an external field A_μ^e and with the quantized radiation field. A finite equation for S_{Fe}' is derived, from which the line center and shape may be calculated to any desired accuracy. The method is illustrated by two examples: the elastic scattering of photons by a one electron atom in its ground state and the emission of photons by the same type of atom following thermal excitation.

INTRODUCTION

THE shape of atomic spectral lines has been discussed by Weisskopf and Wigner.[1] Their results are inconclusive in three respects. In the first place, the time dependent formalism which they use leaves some doubt as to the correct choice of boundary conditions in a decay problem in which the excitation of the system (by electron bombardment, for instance, as in a discharge tube) is considered to be an independent, unspecified process. In the second place, although the line width found by these authors is finite and in agreement with experiment, the line center is shifted by an infinite energy, obviously corresponding to the infinite self-energy of an electron interacting with its own radiation field. Finally, within the Weisskopf-Wigner formalism, it would be extremely difficult to calculate a next approximation. This might conceivably be of some practical interest in an experiment such as the Lamb shift, where the accuracy of the measurement is a small fraction of the line width, and where it is not at all clear, beyond the lowest order, what the measured "energy" of the excited state corresponds to in the language of quantum-mechanical perturbation theory.

In order to discuss the problem in such a way that all our results will be finite we will make use of the computational techniques of Feynman[2] and Dyson.[3] The experiment which we shall discuss is the elastic scattering cross section for photons of frequency k of a one-electron atom in its ground state ψ_0; that is we shall calculate radiative corrections to the Kramers-Heisenberg dispersion formula. The emitted line shape can be obtained from this calculation by replacing the incoming photon by a time dependent external field whose frequency distribution corresponds roughly to that of the mode of excitation preceding the measured emission of photons.

The two questions that are of primary interest concern the symmetry of the line shape and the position of its center. The line center k_0 is here defined as the frequency corresponding to the maximum cross section in the neighborhood of a resonance E_n. In first approximation, of course, any line is symmetric about this point. One may, however, introduce, as a measure of asymmetry, the quantity

$$\delta=[\sigma(k_0+\Gamma)-\sigma(k_0-\Gamma)]/\sigma(k_0),$$

where Γ is the half-width of the line.

A convenient unit of an experimentally measurable order of magnitude is the Lamb unit, $\pounds\cong\alpha^3z^2(E-m)\cong\alpha^5z^4m$. In general, $\Gamma\cong\pounds$ for all but metastable states. We shall find that up to (but not including) terms of order $\alpha^3z^2\pounds$, the line center k_0 is shifted only by Lamb-shift-like effects, and that to this accuracy all the terms contributing to the shift (before renormalization) are in one to one correspondence with those predicted by stationary state perturbation theory, even though the "energy" of the "state" is only defined to within $\Gamma\approx\pounds$.

I. THE KRAMERS-HEISENBERG DISPERSION FORMULA

We shall begin by deriving the Kramers-Heisenberg dispersion formula within the framework of the S-matrix theory of Feynman and Dyson. This will immediately make it clear how radiative corrections must be calculated.

We shall work in the Furry[4] interaction representation; that is all electron operators ψ have their time dependence given by the external field A_μ^e, which we assume to be time independent:

$$[\gamma_\mu(\partial/\partial x_\mu-ieA_\mu^e(x))+m]\psi=0. \quad (1)$$

The stationary solutions of (1), $\psi_n(\mathbf{x})e^{-iE_nt}$, constitute a complete set of spinor functions of $\mathbf{x}$ at any one time.

The Feynman Green's function for the external field is given by

$$S_{Fe}(x_1,x_2)=S_{Fe}(\mathbf{x}_1,\mathbf{x}_2\cdot t_1-t_2)$$
$$=\epsilon(t_1,t_2)\langle V|P[\psi(x_1)\bar{\psi}(x_2)]|V\rangle, \quad (2)$$

where $|V\rangle$ is the exact vacuum state of the external field, $\epsilon(t_1,t_2)=\pm1$ according to whether $t_1>t_2$ or $t_1<t_2$,

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[1] V. Weisskopf and E. Wigner, Z. Physik **63**, 54 (1930); **65**, 18 (1930).

[2] R. Feynman, Phys. Rev. **76**, 749, 769 (1949).

[3] F. Dyson, Phys. Rev. **75**, 486, 1736 (1949).

[4] W. Furry, Phys. Rev. **81**, 115 (1950).

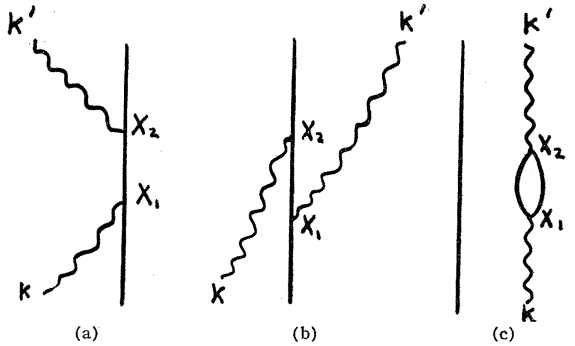

FIG. 1. (a) and (b): Kramers-Heisenberg scattering. (c): Delbrück scattering.

and P is Dyson's time ordering operator. We note, using (2), that

$$\begin{aligned} S_{Fe}(x_1, x_2) &= \sum_{n+} \psi_n(\mathbf{x}_1)\bar{\psi}_n(\mathbf{x}_2)e^{-iE_n(t_1-t_2)} \text{ for } t_1>t_2 \\ &= -\sum_{n-} \psi_n(\mathbf{x}_1)\bar{\psi}_n(\mathbf{x}_2)e^{-iE_n(t_1-t_2)} \text{ for } t_1<t_2 \\ &= \frac{1}{2\pi i}\sum_n \int_{-\infty}^{\infty} \frac{d\omega e^{i\omega(t_1-t_2)}}{E_n(1-i\epsilon)+\omega}\psi_n(\mathbf{x}_1)\bar{\psi}_n(x_2), \end{aligned} \tag{3}$$

where ϵ is to approach zero after the ω integration has been done. Finally, S_{Fe} satisfies the integral equation:

$$S_{Fe}(1,2) = S_F(1,2) - \int S_F(1,3)e\gamma_\mu A_\mu^e(3)S_{Fe}(3,2)dx_3. \tag{4}$$

The S-matrix element from a state with a photon of four-momentum $\mathbf{k}$, k to one of four-momentum $\mathbf{k}'$, k', the atom remaining in its ground state ψ_0, is

$$\begin{aligned} (k', 0|S|k, 0) = \sum_{n=0} \frac{(-i)^n}{n!}\int_{-\infty}^{\infty} dx_1\cdots dx_n \\ \times(k', 0|P[H_I(x_1)\cdots H_I(x_n)]|k, 0), \end{aligned} \tag{5}$$

where

$$H_I(x) = j_\mu(x)A_\mu(x), \tag{6}$$

with $j_\mu(x) = ie\bar{\psi}(x)\gamma_\mu\psi(x)$. The first nonvanishing approximation to (5) is represented by the three Feynman graphs, Figs. 1(a), (b), and (c), where of course the electron propagates from x_1 to x_2 according to S_{Fe}, not S_F. Figure 1(c) corresponds to the scattering of light by the external field A_μ^e and will not be discussed here. The matrix elements of 1(a) and 1(b) are

$$\begin{aligned} S_a &= \frac{2\pi e^2}{(kk')^{\frac{1}{2}}}\int_{-\infty}^{\infty} d\mathbf{x}_1 d\mathbf{x}_2 dt_1 dt_2 \bar{\psi}_0(\mathbf{x}_2)e^{-i\mathbf{k}'\cdot\mathbf{x}_2}\gamma_\mu e_\mu' \\ &\quad \cdot S_{Fe}(x_1, x_2)\gamma_\nu e_\nu e^{i\mathbf{k}\cdot\mathbf{x}_1}\psi_0(\mathbf{x}_1)e^{i(E_0+k')t_2}e^{-i(E_0+k)t_1} \\ &= \frac{2\pi e^2}{(kk')^{\frac{1}{2}}}\sum_n (0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda' e^{-i\mathbf{k}'\cdot\mathbf{x}}|\,n)(n|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{i\mathbf{k}\cdot\mathbf{x}}|\,0) \\ &\quad \times\int_{-\infty}^{\infty} dt_1 dt_2 e^{i(E_0+k')t_1}e^{-i(E_0+k)t_2}\frac{e^{i\omega(t_2-t_1)}}{2\pi i(E_n+\omega)}d\omega \end{aligned}$$

or

$$S_a = \frac{(2\pi)^2 e^2}{ki}\delta(k-k')\sum_n\left(0\left|\boldsymbol{\alpha}\cdot\hat{e}_\lambda'\frac{e^{-i\mathbf{k}'\cdot\mathbf{x}}}{E_n-E_0-k}\right|n\right) \times(n|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{i\mathbf{k}\cdot\mathbf{x}}|\,0).$$

Similarly,

$$\begin{aligned} S_a+S_b = -i\delta(k-k')(2\pi e)^2[k\textstyle\sum_n[0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda' e^{-i\mathbf{k}'\cdot\mathbf{x}}|\,n) \\ \times(n|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{i\mathbf{k}\cdot\mathbf{x}}|\,0)/(E_n-E_0-k) \\ +(0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{i\mathbf{k}\cdot\mathbf{x}}|\,n) \\ \times(n|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda' e^{-\mathbf{k}'\cdot\mathbf{x}}|\,0)/(E_n-E_0+k)], \end{aligned} \tag{7}$$

leading to a scattering cross section

$$d\sigma = (e^2/m)^2 d\Omega|H'|^2,$$

where

$$H' = m\sum_n\left\{\frac{(0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda' e^{-i\mathbf{k}'\cdot\mathbf{x}}|\,n)(n|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{i\mathbf{k}\cdot\mathbf{x}}|\,0)}{E_n-E_0-k} + \frac{(0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{i\mathbf{k}\cdot\mathbf{x}}|\,n)(n|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda' e^{-i\mathbf{k}'\cdot\mathbf{x}}|\,0)}{E_n-E_0+k}\right\}. \tag{8}$$

In nonrelativistic approximation $\boldsymbol{\alpha}$ is replaced by $\mathbf{p}/m$ in the sum over positive states. The negative energy sum leads in well-known fashion to the nonrelativistic A^2 term in the scattering cross section.

We may anticipate later results at this point to ask for the effect of nonresonant terms on the line shape near a resonance E_n, where the energy denominator in (8) must be replaced by

$$\frac{1}{E_n-E_0-k} \to \frac{1}{E_n-E_0-k-i\Gamma_n}.$$

One finds that the effect of a nonresonant level E_m is to shift the line center by

$$\delta k_0 \cong \alpha^6 z^4(E_n-E_0) \simeq \alpha^3 z^2 \mathcal{L},$$

and to distort the line shape by $\delta \simeq \alpha^3 z^2$. These orders of magnitude are the same whether or not the level E_m is removed from E_n by a fine structure splitting, since in that case the matrix element will be smaller by $\alpha^2 z^2$,

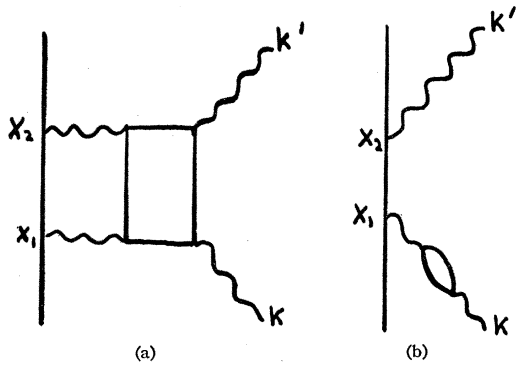

FIG. 2. Vacuum polarization corrections to scattering.

exactly compensating the smaller energy difference in the denominator.

The effect of the frequency variation of the matrix element

$$H'=(0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda \exp(i\mathbf{k}\cdot\mathbf{x})\,|n)$$

is even smaller, since parity allows only even or odd terms to appear for a given transition. One finds a shift

$$\delta k_0 \approx \alpha^e z^e (E_n - E_0) \approx \alpha^5 z^4 \mathfrak{L},$$

together with an asymmetry $\delta \approx \alpha^5 z^4$. Both of these corrections are much too small to be of interest at present.

II. GENERAL DISCUSSION OF RADIATIVE CORRECTIONS

When the photon frequency approaches any excitation energy of the atom (8) breaks down; for $k=E_n-E_0$ the scattering it predicts is infinite. We must therefore recalculate graph 1(a) together with its radiative corrections. These corrections can be of four types.

(1) Corrections due to vacuum polarization by the incoming and outgoing photons, such as shown in Figs. 2(a) and (b).

Aside from an unobservable renormalization of the photon wave functions, these graphs produce corrections considerably smaller than those discussed in I.

(2) Corrections to γ_μ, such as shown in Figs. 3(a) and 3(b). These are also small, and the same remarks apply as those of the preceding paragraph.

(3) Corrections to the incoming or out-going atom as in graph 3(c). These are important, but require no calculation. They replace $\psi_0(\mathbf{x})e^{-iE_0t}$ by $\langle v|\psi_H(x)|g\rangle = Z_2^{\frac{1}{2}}\psi_g(\mathbf{x})e^{-iE_0t}$, where ψ_H is a Heisenberg representation operator, $|V\rangle$ is the exact vacuum state and $|g\rangle$ the exact ground state of the atom, including all radiative corrections; $Z_2^{\frac{1}{2}}$ is the infinite (or zero) renormalization of probability amplitude discussed by Dyson. ψ_g is finite when it is expressed as a function of the renormalized mass and charge; once this is done it differs from ψ_0 by small corrections which are no longer of interest since they affect the resonant behavior even less than those discussed in I. In the future we shall therefore disregard these graphs and write $\psi_0 e^{-iE_0t}$ for the incoming, $\bar{\psi}_0 e^{iE_0t}$ for the outgoing atom, remembering that E_0 is the exact ground-state energy (which is of course a well-defined number).

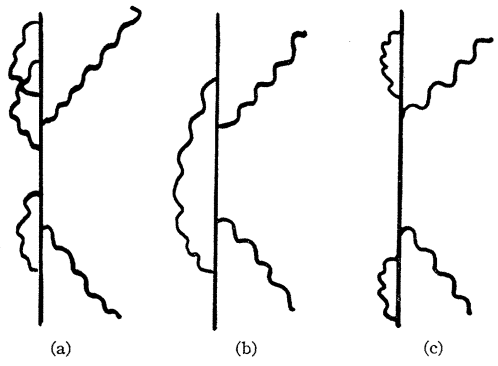

FIG. 3. (a) and (b): Radiative corrections to γ_μ. (c): Radiative corrections to ψ_0, $\bar{\psi}_0$ and E_0.

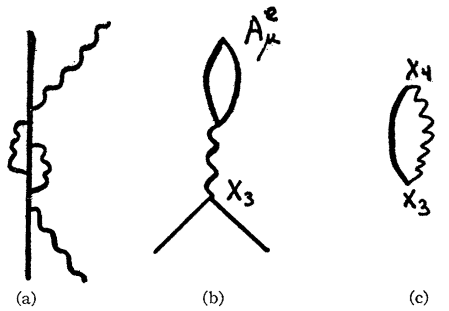

FIG. 4. (a): Radiative corrections to S_{Fe}'. (b): Vacuum polarization contribution to Σ_e. (c): Lowest order dynamic contribution to Σ_e.

(4) Finally we have corrections of the type shown in Fig. 4(a).

We note that these can be calculated in exactly the same manner as $(k'|S_A|k)$ in I, except that S_{Fe} must be replaced by S_{Fe}', where

$$S_{Fe}'(x_1, x_2)=\epsilon(1, 2)\langle 0|P[\psi_H(x_1)\bar{\psi}_H(x_2)]|0\rangle,$$

and where $|0\rangle$ is the exact vacuum state and ψ_H is in the Heisenberg representation.

III. CALCULATION OF S_{Fe}'

Dyson has shown that for $A_\mu^e=0$, S_F' satisfies an integral equation

$$S_F'(1-2)=S_F(1-2)+\int S_F(1-3)\Sigma(3-4)S_F'(4-2)d(34). \quad (9)$$

In fact it is in terms of the kernel of this equation, $\Sigma(3-4)$, that his renormalization procedure is defined.

When an external field is present, we may still write

$$S_{Fe}'(1, 2)=S_{Fe}(1, 2)+\int S_{Fe}(1,3)\sum_e(3,4)S_{Fe}'(4,2)d(34), \quad (10)$$

where $\sum_e$ is no longer a function of the difference x_3-x_4, but of $\mathbf{x}_3$, $\mathbf{x}_4$ and t_3-t_4.

$\sum_e$ will contain a whole new series of diagrams arising from vacuum polarization by the external field, of which the lowest order is shown in Fig. 4(b), and, after renormalization, is given by $\sum_p = iA_\mu^{e'}(x_3)\delta(x_3-x_4)$, where

$$A_\mu^{e'} \cong (e^2/15\pi m^2)\partial^2 A_\mu^e/\partial x_\nu^2$$

as shown by Schwinger.[5]

Otherwise the diagrams appearing in $\sum_e$ will be precisely those appearing in $\sum$, and can be renormalized appropriately.

[5] J. Schwinger, Phys. Rev. **76**, 790 (1949).

For instance, in lowest order one has, corresponding to the diagram of Fig. 4(c)

$$\sum_e = -\gamma_\mu S_{Fe}(x_3, x_4)\gamma_\nu D_{F\mu\nu}(x_3-x_4),$$
$$D_{F\mu\nu} = \langle 0|P[A_\mu(x_3)A_\nu(x_4)]|0\rangle, \quad (11)$$

or, using (4),

$$\sum_e = \gamma_\mu S_F(x_3-x_4)\gamma_\mu D_F(x_3-x_4)$$
$$-\int \gamma_\nu S_F(x_3-x_5)e\gamma_\mu A_\mu{}^e(x_5)$$
$$\times S_F(x_5+x_4)\gamma_\nu \cdot D_F(x_3-x_4)dx_5$$
$$+\int \gamma_\lambda S_F(3-5)e\gamma_\mu A_\mu{}^e(5)S_F(5-6)$$
$$\times\gamma_\nu A_\mu{}^e(6)S_{Fe}(6,4)\gamma_\lambda D_F(3-4)dx_5dx_6,$$

in which the divergences have been isolated in the first two terms, to which known methods apply. The last term is finite, and contains no renormalization. The same method can in principle be applied to any term in $\sum_e$, so that we may take $\sum_e(x_3, x_4)$ to be finite and known.

The equation we have to solve is thus

$$S_{Fe}'(1,2) = S_{Fe}(1,2) + \int S_{Fe}(1,3)\sum_e(3,4)S_{Fe}'(42)d(34). \quad (10)$$

To solve (10) we set

$$S_{Fe}'(1,2) = \frac{1}{2\pi i}\sum_n \int d\omega f_{nn}(\omega)e^{i\omega(t_1-t_2)}\psi_n(\mathbf{x}_1)\bar{\psi}_n(\mathbf{x}_2)$$
$$+\frac{1}{2\pi i}\sum_{n\neq m}\int d\omega f_{nm}(\omega)e^{i\omega(t_1-t_2)}\psi_n(\mathbf{x}_1)\bar{\psi}_m(\mathbf{x}_2), \quad (11)$$

where $f_{nn}(\omega)$ and $f_{nm}(\omega)$ are to be determined so that (10) is satisfied. So far (11) involves no approximations, since the ψ_n's form a complete set.

Substituting (11) into (10) we find, using (3), and taking the inner product with $\bar{\psi}_n(\mathbf{x}_1)\beta\cdots\beta\psi_n(\mathbf{x}_2)$,

$$\frac{1}{2\pi i}\int e^{i\omega(t_1-t_2)}d\omega f_{nn}(\omega)$$
$$=\frac{1}{2\pi i}\int \frac{e^{i\omega(t_1-t_2)}}{\omega+E_n}d\omega + \frac{1}{2\pi i}\int \frac{d\omega_1 e^{i\omega_1(t_1-t_2)}}{E_n+\omega_1}$$
$$\times\frac{d\omega_2 e^{i\omega_2(t_4-t_2)}}{2\pi i}dt_3dt_4d\mathbf{x}_3d\mathbf{x}_4\bar{\psi}_n(\mathbf{x}_3)$$
$$\cdot\sum_e(\mathbf{x}_3,\mathbf{x}_4,t_3-t_4)\{\psi_n(\mathbf{x}_4)f_{nn}(\omega_2)$$
$$+\sum_{m\neq n}\psi_m(\mathbf{x}_4)f_{mn}(\omega_2)\}, \quad (12)$$

or if we call

$$\int \bar{\psi}_n(\mathbf{x}_3)\sum_e(\mathbf{x}_3,\mathbf{x}_4,t_3-t_4)\psi_m(\mathbf{x}_4)d\mathbf{x}_3d\mathbf{x}_4 = H_{nm}(t_3-t_4), \quad (13)$$

(12) becomes

$$\int e^{i\omega(t_1-t_2)}d\omega f_{nn}(\omega)$$
$$=\int \frac{e^{i\omega(t_1-t_2)}}{E_n+\omega}d\omega + \frac{1}{i}\int \frac{d\omega e^{i\omega(t_1-t_2)}}{E_n+\omega}\cdot H_{nn}(-\omega)$$
$$\cdot f_{nn}(\omega) + \frac{1}{i}\int \frac{d\omega e^{i\omega(t_1-t_2)}}{E_n+\omega}\sum_{m\neq n}H_{nm}(-\omega)f_{mn}(\omega),$$

where

$$H_{nm}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t}H_{nm}(t),$$

or finally

$$f_{nn}(\omega) = \frac{1}{E_n+\omega} + \frac{1}{i}\frac{H_{nn}(-\omega)f_{nn}(\omega)}{E_n+\omega}$$
$$+\frac{1}{i}\sum_{m\neq n}\frac{H_{nm}(-\omega)f_{mn}(\omega)}{E_n+\omega}. \quad (14)$$

By taking the inner product with $\bar{\psi}_n\beta\cdots\beta\psi_m$, we obtain a second equation:

$$\frac{1}{2\pi i}\int d\omega f_{nm}(\omega)e^{i\omega(t_1-t_2)}$$
$$=\left(\frac{1}{2\pi i}\right)^2\int \frac{d\omega_3}{E_n+\omega_1}e^{i\omega_1(t_1-t_2)}d\omega_2 e^{i\omega_2(t_4-t_2)}$$
$$\cdot dt_3dt_4[H_{nm}(t_3-t_4)f_{mm}(\omega_2)$$
$$+\sum_{p\neq m}H_{np}(t_3-t_4)f_{pm}(\omega_2)], \quad (15)$$

$$f_{nm}(\omega) = \frac{-i}{E_n+\omega}[H_{nm}(-\omega)f_{mm}(\omega)$$
$$+\sum_{p\neq m}H_{np}(-\omega)f_{pm}(\omega)]. \quad (16)$$

In principle (16) and (14) determine S_{Fe}', and can be solved to any desired accuracy. In particular, if we neglect quadratic terms in $H_{nm}(n\neq m)$, corresponding to neglecting higher order Lamb shifts (but not higher order radiative corrections), we obtain a very simple solution of the expected type:

$$f_{nn} = 1/[E_n+\omega+W_{nn}(-\omega)+\cdots], \quad (17)$$

where

$$W_{nn} = iH_{nn}(-\omega) - \sum_{m\neq n}\frac{iH_{nm}(-\omega)iH_{mn}(-\omega)}{E_m+\omega}+\cdots,$$
$$f_{mn} = \frac{-iH_{mn}(-\omega)+\cdots}{[E_m+\omega+W_{mm}(-\omega)][E_n+\omega+W_{nn}(-\omega)]}. \quad (18)$$

IV. RESONANCE SCATTERING

We may now rederive Eq. (7). S_a becomes, if we neglect f_{mn} compared to f_{nn} (a neglect corresponding to a line shift $\delta k_0 \approx \alpha^9 z^6 \Delta E \approx \alpha^6 z^4 \mathfrak{L}$ and asymmetry $\delta \approx \alpha^6 z^4$).

$$S_a = \frac{2\pi e^2}{(kk')^{\frac{1}{2}}} \int_{-\infty}^{\infty} d\mathbf{x}_1 d\mathbf{x}_2 dt_1 dt_2 \bar{\psi}_0(x_2) e^{-i\mathbf{k}'\cdot\mathbf{x}_2} \gamma_\mu e_\mu' \cdot S_{Fe}'(x_1, x_2) \gamma_\nu e_\nu e^{i\mathbf{k}\cdot\mathbf{x}_1} \psi_0(\mathbf{x}_1) \times e^{i(E_0+k')t_1} e^{-i(E_0+k)t_2}$$

$$= \frac{1}{i}\frac{(2\pi e)^2}{k} \sum_n \frac{(0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda' e^{-\mathbf{k}'\cdot\mathbf{x}}|\,n)(n|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{i\mathbf{k}\cdot\mathbf{x}}|\,0)}{E_n - E_0 - k + W_{nn}(E_0+k)}, \quad (19)$$

and the resonance scattering is given by

$$d\sigma_n = (e^2/m)^2 d\Omega\, |(0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda' e^{-i\mathbf{k}'\cdot\mathbf{x}}|\,n)(n|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{i\mathbf{k}\cdot\mathbf{x}}|\,0)\cdot m|^2 \cdot 1/[(E_n - E_0 - k + \delta E_n(E_0+k))^2 + \Gamma_n^2(E_0+k)], \quad (20)$$

in the neighborhood of $k = E_n - E_0$, where δE_n and $-i\Gamma_n$ are the real and imaginary parts of $W_{nn}(E_0+k)$.

The line shape and center are therefore effectively determined by the energy denominator in (20). In the fourth-order term,

$$-\sum_{m\neq n} \frac{iH_{nm}(E_0+k) iH_{mn}(E_0+k)}{E_m - E_0 - k},$$

one may set $k + E_0 \cong E_n$ and obtain a shift of order of magnitude

$$\delta k_0 \approx z^3\alpha^5(E_n - E_0) \approx z\alpha^2 \mathfrak{L}.$$

The fourth-order renormalization term obtained by expanding

$$iH_{nn}(E_0+k) = iH_{nn}(E_n) + (E_0+k-E_n)(\partial/\partial E_n) iH_{nn}(E_n),$$

leaves the line shape symmetric but shifts its center by

$$\delta k_0 \approx z^4\alpha^6(E_n - E_0) \approx z^2\alpha^3 \mathfrak{L}.$$

To within present experimental accuracy, therefore, the entire observable effect arises from the term $iH_{nn}(E_n)$. This term is a power series in e^2 (but not in v/c as were the off-diagonal and renormalization terms). The first approximation in e^2 corresponds to the conventional Lamb-shift calculations. The shift due to the second approximation to $\sum_e$ is of order $e^2\mathfrak{L}$ and has been calculated by Berson, Kroll, and Weneser. Finally, the imaginary part of $iH_{nn}(E_n)$ is different from zero, and in lowest order is unaffected by the renormalization subtractions, which are real: i.e., the self-mass and the Z_2 renormalization, which subtracts a real multiple of $E_n - E_0 - k$ from $iH_{nn}(E_0+k)$, change iH_{nn} by a real number, so that $-i\Gamma_n$ may be computed in lowest order without renormalization. This is most easily done using the conventional sum over states which can easily be derived from (21). The Feynman prescription for going around poles will give an imaginary contribution to the sum from each state that has lower energy than E_n, this contribution being $-i/2$ times the transition probability per unit time from the state ψ_n to the state in question.

V. EMISSION LINE-SHAPE

We replace the incoming photon by an effective thermal excitation potential $V(x,t) = \int I(\omega) e^{-i\omega t} d\omega V(x)$. Then the probability of radiation of a photon of frequency k with the atom in its ground state is $|(k|S|0)|^2$ where

$$(k|S|0) = e\left(\frac{2\pi}{k}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} d\mathbf{x}_1 d\mathbf{x}_2 dt_1 dt_2 \bar{\psi}_0(\mathbf{x}_2) \times e^{-i\mathbf{k}\cdot\mathbf{x}_2} \gamma_\mu e_\mu S_{Fe}'(x_1, x_2) \beta V(\mathbf{x}_1) I(\omega) d\omega \times \psi_0(\mathbf{x}_1) e^{i(E_0+k)t_1} e^{-iE_0 t_2} e^{-i\omega t_2} \quad (21)$$

$$\approx \frac{1}{(k)^{\frac{1}{2}}} \sum_n (0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{-i\mathbf{k}\cdot\mathbf{x}}|\,n)(n|\,V(\mathbf{x})|\,0) \times \int dt_1 dt_2 d\omega d\nu e^{i(E_0+k)t_1} \times \frac{e^{-i(E_0+\omega)t_2} e^{i\nu(t_1-t_2)} I(\omega)}{E_n + \nu + W_{nn}(-\nu)} \quad (22)$$

$$= \frac{I(k)}{(k)^{\frac{1}{2}}} \sum_n \frac{(0|\,\alpha\cdot\hat{e}_\lambda e^{-i\mathbf{k}\cdot\mathbf{x}}|\,n)(n|\,V|\,0)}{E_n - E_0 - k + W_{nn}(E_0+k)}, \quad (23)$$

and the probability of radiation of a photon of frequency k is

$$P(k) \approx \frac{|I(k)|^2}{k} \left| \sum_n \frac{(0|\,\boldsymbol{\alpha}\cdot\hat{e}_\lambda e^{-i\mathbf{k}\cdot\mathbf{x}}|\,n)(n|\,V|\,0)}{E_n - E_0 - k + W_{nn}(E_0+k)} \right|^2. \quad (24)$$

When $k - E_n - E_0 \approx 0$, $1/W_{nn} \approx 1/[z^2\alpha^3(E_n - E_0)]$. Thus, if one of the terms in the sum is large, the others are very small, so that

$$P(k) \approx \frac{|I(k)|^2}{k} \sum_n \left| \frac{(0|H'|n)(n|V|0)}{(E_n - E_0 - k + \delta E_n)^2 + \Gamma_n^2} \right|, \quad (25)$$

where each term contributes only when k is very near resonance. If $I(k)$ is such as to excite many states, but varies slowly over the line width, this is the expected result.

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