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A graphical representation of Weisskopf–Wigner type theories

E Grimm and V Ernst

Sektion Physik der Universität München, Theoretische Physik, 8000 München 2, Theresienstrasse 37, West Germany

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Abstract. It is shown that the usual (non-existing) Hamiltonian operator H' governing the interaction of a one-electron atom with transverse photons, can be written as the sum of a finite number of self-adjoint and bounded 'partial' interaction Hamiltonians L, where each L has a well defined physical meaning. The simplest of the well known Weisskopf–Wigner type theories which are used occasionally, are defined by a single L and practically all model Hamiltonians used in quantum optics are closely related either to a single L or to sums of very few L. The systematic 'Weisskopf–Wigner approximation scheme' introduced previously consists of special sequences of partial sums of L. We equip the system of partial sums of L with a system of graphs where each graph defines uniquely a certain Weisskopf–Wigner theory and visualises its physical content in a comparable way to a Feynman graph. Finally some applications are given.

1. Introduction and discussion of the main results

We have shown recently (Grimm and Ernst 1974, 1975, to be referred to as I and II) that the idea of the important state hypothesis, first used by Dirac (1927) and Weisskopf and Wigner (1930), can be appreciably generalised. This has led us to a self-reliant hierarchy of Weisskopf–Wigner approximations or ww theories for the treatment of the interaction of a one-electron atom A with the radiation field R of transverse photons. The idea of this approach is essentially to consider an increasing number of the possible states of A + R as 'important' till the 'exact' theory is reached in the formal limit, when all possible states are admitted as 'important' (see below, however). The corresponding mathematical scheme is characterised by the existence of a unitary time-evolution operator $U_I(t)$ in any finite-order ww theory, and, under certain conditions, in some infinite-order ww theories as well. The unitarity of $U_I(t)$ excludes 'infinities' in the corresponding ww theories.

In the present paper we describe a modification of this approach which offers a number of advantages. The first of these advantages is as follows. The usual interaction Hamiltonian H' of the system A + R is basically the restriction of the 'minimal' interaction Hamiltonian $e\int \mathrm{d}^3x\, A^\mu(x)\bar{\psi}(x)\gamma_\mu\psi(x)$ of quantum electrodynamics (QED) to transverse photons and to one bound electron (cf § 2 with the necessary notation etc). We show in § 3 that H' can be written in the form:

$$H' = \sum_{n=0}^{\infty}\sum_{b=0}^{\infty}\sum_{a=0}^{\infty} L[(b,n)\rightleftarrows(a,n+1)]. \tag{1}$$

$L[(b, n) \rightleftarrows (a, n+1)]$ is a *self-adjoint* and *bounded* partial Hamiltonian operator on the Hilbert space $\mathscr{S}_1$ of the interacting system A+R for any $(n, b, a) \in \mathbb{N}_0 \times \mathbb{N}_0 \times \mathbb{N}_0 (\mathbb{N}_0 := \{0, 1, \ldots\})$. So any partial sum Σ of any finite number of L is again a self-adjoint and bounded partial interaction Hamiltonian on $\mathscr{S}_1$. The sum of the 'free' Hamiltonian H^0 and any Σ is again self-adjoint. Results of I can be reformulated in the sense that $H^0 + \Sigma$ is self-adjoint again if the photons are equipped with any mass $\mu > 0$ and if Σ is obtained from equation (1) by restricting the sums over b and a (but not n) to any finite domain $0, \ldots, A$.

The decisive advantage of the expansion (1) is that each L may be interpreted *physically*: $L[(b, n) \rightleftarrows (a, n+1)]$ is the interaction Hamiltonian of a class of well defined physical processes, namely the 'transitions' from any state of R with n photons and A in the eigenstate $u_b(\boldsymbol{x})$ to any state of R with $n+1$ photons and A in the state $u_a(\boldsymbol{x})$, and *vice versa*. For example, the simplest ww theory (e.g. Källén 1958, II) of a transition $u_b(\boldsymbol{x}) \rightleftarrows u_a(\boldsymbol{x})$ under emission or absorption of one photon is obtained by retaining only one single term $L[(b, 0) \rightleftarrows (a, 1)]$ in equation (1). Such crudest, lowest-order ww theories allow the prediction of natural lifetimes of atomic states and of linewidths in spontaneous emission and resonance fluorescence which, in all cases considered so far, agree with experience. In particular, all selection rules of the Dirac atom can be explained by such crude one-term ww theories. It is shown (§ 5) that practically all model Hamiltonians used in atomic physics and quantum optics are related with one, or at most several terms of equation (1).

A third advantage therefore is that partial sums Σ can be interpreted correspondingly. They refer to compound processes, i.e. to sums of the elementary one-term processes contained in Σ. However, in general these processes must compete with each other because, due to unitarity of $U_I(t) = U_\Sigma(t)$ the sum of all transition probabilities is equal to one for any Σ. The addition of a new L to a given Σ always opens a new 'reaction channel' for A+R because the new processes are now acknowledged, but they must of course compete with those already contained in Σ. This can lead to novel 'melting effects' (§ 6).

It is in fact the main purpose of this paper to give an easy access to higher-order ww theories. We achieve this by introducing in § 4 a graphical representation of the ww theories defined by the partial sums Σ of equation (1). Each ww theory which is so defined will be described by a certain graph which, comparable to a Feynman graph, visualises the essential features of the ww theory represented. We set up rules (§ 4) which allow us to write down immediately the equations of motion of this ww theory. As the essential physical content is displayed by the graph we can thus write down ww theories for any purpose. To become acquainted with this graphical language, we discuss in § 5 the graphs of several known ww theories. In § 6 we apply this method to a ww theory which describes a special case of the above competition. In § 7 this will lead us to the simplest 'infinities' that can occur in ww theories of infinite order. We compare them with certain divergences known from second-order perturbation QED.

It is natural to ask for the 'convergence' of the expansion (1). In comparable models of Nelson (1964), Eckmann (1970), Gross (1973), Fröhlich (1973), Schroeck (1973, 1975) with 'unrenormalised' Hamiltonians H_{ur} sharing the existence of a persistent electron vacuum with our $H^0 + H'$, it was essentially shown that H_{ur} can be written in the form $H_{\text{ur}} = H_{\text{ren}} - E_C$ where H_{ren} is self-adjoint and bounded from below and E_C is some infinite constant. This is achieved in all cases by modifying H_{ur} by some cut-off procedure C to get a self-adjoint 'cut-off Hamiltonian' H_{ur}^C, and by then removing the

cut-off. Taking partial sums Σ of equation (1) certainly resembles a cut-off because our cut-off Hamiltonians $H^0+\Sigma$ are also self-adjoint and bounded from below. But there is a fundamental difference in that we know that each Σ defines a class of characteristic processes which retain an autonomous physical meaning even if they have to compete with other processes which are 'admitted' as more and more of the L are taken into account. We repeat that even the crudest one-term ww approximations lead to agreement with experience whereas the finite cut-offs used in the constructive field theory are not closely comparable to experience and *must* be removed. The necessity of including *all* terms of equation (1) is not so obvious. In fact, it may be questioned by physical arguments derived from the direct interpretation of the Σ, as follows.

Consider a single one-electron atom A. The 'diameters' of the eigenstates of the non-relativistic hydrogen atom tend to infinity as the ionisation limit is approached from below (e.g. Weizel 1958). The same can be expected of our A in the limit $a \to \infty$, cf § 2. But we never observe one single atom as measurements are always made on some ensemble of atoms; for example, active atoms in a laser, or atomic beam, or interstellar matter, etc. Whichever situation we consider we must admit that the states $u_a(\boldsymbol{x})$ with a greater than some 'overlap value' a^* cannot play a decisive role, because the states of two atoms would finally overlap. However then the *two* electrons are subject to the Pauli principle which plays no role at all in our case. But we know that only the $L[(b, n) \rightleftarrows (a, n+1)]$ with $a > a^*$ and/or $b > a^*$, whatever a^* might be, can lead to divergences. Divergences in our theory therefore always come from physical processes which can never occur or play any role in any real situation considered. In other words the model reaches its limits of applicability long before infinities can occur. In our case it is the authority of the Pauli principle that comes into play before infinities can appear. Rephrasing this again, the 'surrounding effects' upon A are always more important than the physical processes that cause divergences in the atom–photon interaction. The only realistic conclusion to draw from this can be that terms $L[(b, n) \rightleftarrows (a, n+1)]$ with a and/or b greater than a^* *must* be omitted, in which case no infinities can occur at all.

This does not question the need for some renormalisation which in the present case must deal with the proper handling of the phenomena of 'bound' photons characteristic of ww theories (I, II). We are content here to collect some of the facts which must be taken into account in any renormalisation.

2. Formal definition of the Hamiltonians of our problem

We inspect first the necessary background material and introduce the inevitable notation etc.

As in I we consider a slightly modified one-electron Dirac atom A with a complete set of 'electron' eigenstates $u_a(\boldsymbol{x})$ corresponding to a discrete, unbounded energy spectrum $E_a > 0$. It will be convenient to assume that the eigenstates are numbered throughout so that each number $a = 0, 1, 2, \ldots$ corresponds to precisely one $u_a(\boldsymbol{x})$, and to assume $E_b \geqslant E_a$ for $b > a$. A shall interact with R by the transverse part $e\dot{\boldsymbol{A}}\boldsymbol{J}$ of the usual minimal coupling density $eA_\mu J^\mu$ of QED. To control certain infrared problems we equip the photons with an arbitrary mass $\mu \geqslant 0$, as in I. Since the total Hamiltonian resulting from this assumption commutes with the electron number operator, the theory 'decays' to a countable number of sub-theories, one for each number of electrons. As in

I we consider the one-electron theory defined on the Hilbert space:

$$\mathscr{S}_1 := \mathscr{H}_{\mathrm{el}}^1 \otimes \mathscr{F}_{\mathrm{p}} = \bigoplus_{a=0}^{\infty} \bigoplus_{n=0}^{\infty} \mathscr{H}_n^a. \tag{2}$$

$\mathscr{H}_{\mathrm{el}}^1$ is the Hilbert space spanned by the electron solutions of the Dirac equation, $\mathscr{F}_{\mathrm{p}}$ is the Fock space of transverse photons, and $\mathscr{H}_n^a$ denotes the Hilbert space of all states of n photons with A in the state $u_a(\boldsymbol{x})$. The elements of $\mathscr{H}_n^a$ will be denoted by $|\alpha_n^a\rangle$ or $\alpha_n^a(\kappa_1, \ldots, \kappa_n)$, whichever is the more convenient. $\alpha_n^a(\kappa_1, \ldots, \kappa_n)$ is a c-number for $n = 0$, while for other values of n it is a c-number-valued, symmetric, square integrable function of n arguments $\kappa_1, \ldots, \kappa_n$, where $\kappa = (\boldsymbol{k}, \lambda)$ comprises wavevector $\boldsymbol{k} \in \mathbb{R}^3$ and polarisation index $\lambda \in \{1, 2\}$. Norm and scalar products on $\mathscr{H}_n^a$ are defined by

$$\langle \beta_n^a | \alpha_n^a \rangle := \int \mathrm{d}^3\kappa_1 \ldots \int \mathrm{d}^3\kappa_n \, \beta_n^a(\kappa_1, \ldots, \kappa_n)^* \alpha_n^a(\kappa_1, \ldots, \kappa_n), \tag{3}$$

the symbol $\int \mathrm{d}^3\kappa \ldots$ comprising the elementary Lebesgue integration over $\boldsymbol{k} \in \mathbb{R}^3$ and the summation over $\lambda \in \{1, 2\}$. 'Square integrability' is defined accordingly. *Finite* direct sums of $\mathscr{H}_n^a$ are defined as usual (e.g. Achieser and Glasman 1968) whereas the infinite direct sum in equation (2) is understood to be the Hilbert space completion of the set of arrays $\{\alpha_n^a(\kappa_1, \ldots, \kappa_n)\}$ with a finite number of elements $\alpha_n^a(\kappa_1, \ldots, \kappa_n)$ (Prugovecki 1971). An element of $\mathscr{S}_1$ will be denoted by $|\alpha\rangle$ or $\{\alpha_n^a(\kappa_1, \ldots, \kappa_n)\}$, the latter being short for the set $\{\alpha_n^a(\kappa_1, \ldots, \kappa_n); (a, n) \in \mathbb{N}_0 \times \mathbb{N}_0\}$ of 'components' $\alpha_n^a(\kappa_1, \ldots, \kappa_n)$ of $|\alpha\rangle$.

Under the above assumptions on the interaction of A and R we find formally, as in I, the equations of motion:

$$\begin{aligned} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) &= (\omega(\kappa_1) + \ldots + \omega(\kappa_n) + E_a)\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) \\ &\quad + (n+1)^{1/2} \sum_{b=0}^{\infty} \int \mathrm{d}^3\kappa \, M^*(a, b; \kappa)\alpha_{n+1}^b(\kappa, \kappa_1, \ldots, \kappa_n; t) \\ &\quad + n^{-1/2} \sum_{b=0}^{\infty} \sum_{\nu=1}^{n} M(b, a; \kappa_\nu)\alpha_{n-1}^b(\kappa_1, \ldots, \kappa_{\nu-1}, \kappa_{\nu+1}, \ldots, \kappa_n; t) \end{aligned} \tag{4}$$

where $\omega(\kappa) := \omega(|\boldsymbol{k}|) := (\boldsymbol{k}^2 + \mu^2)^{1/2}$. $M(a, b; \kappa)$ is the complex conjugate of:

$$M^*(a, b; \kappa) := \frac{e\boldsymbol{\epsilon}(\kappa)}{(2\omega(\kappa)(2\pi)^3)^{1/2}} \int \mathrm{d}^3x \, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}} u_a^+(\boldsymbol{x})\boldsymbol{\alpha} u_b(\boldsymbol{x}), \tag{5}$$

where e is the electromagnetic coupling constant, $\boldsymbol{\epsilon}(\kappa)$ denotes two unit polarisation vectors orthogonal to $\boldsymbol{k}$ and to each other for $\lambda = 1, 2$, and $\boldsymbol{\alpha}$ is the usual vector of Dirac matrices. We showed in I that $M^*(a, b; \kappa)$ is square integrable in the sense of equation (3) for any couple $u_a(\boldsymbol{x})$, $u_b(\boldsymbol{x})$ of eigenstates of the Dirac atom with the pure Coulomb potential. We shall assume that this holds throughout the paper because it guarantees the boundedness and self-adjointedness of the terms in (1). Equations (4) have to be solved simultaneously for all pairs $(a, n) \in \mathbb{N}_0 \times \mathbb{N}_0$ under initial conditions

$$\alpha_n^a(\kappa_1, \ldots, \kappa_n; 0) = \chi_n^a(\kappa_1, \ldots, \kappa_n), \tag{6}$$

the $\chi_n^a(\kappa_1, \ldots, \kappa_n)$ being the components of any unit vector $|\chi\rangle \in \mathscr{S}_1$.

The right-hand side of (4) defines, formally, the total Hamiltonian H to be considered. The first term on the right-hand side defines the Hamiltonian H^0 of the non-interacting system. It can obviously be written as a *direct sum* of multiplication operators on $\mathscr{H}_n^a$:

$$H^0 = \bigoplus_{a=0}^{\infty} \bigoplus_{n=0}^{\infty} (\omega(\kappa_1) + \ldots + \omega(\kappa_n) + E_a). \tag{7}$$

Since all these operators are self-adjoint, but not bounded, H^0 is also self-adjoint and not bounded. (Each multiplication operator 'generates' on $\mathscr{H}_n^a$ a one-parameter group of unitary operators; the direct sum of these unitary operators is unitary on $\mathscr{S}_1$ so that, by the theorem of Stone (e.g. Yosida 1968), there exists a self-adjoint generator H^0. This is the precise *definition* of H^0 by equation (7).

The second and the third terms on the right-hand side define formally the interacting Hamiltonian H' to be analysed here.

3. Representation of the interaction Hamiltonian H' by an infinite sum of bounded self-adjoint operators

We show now that H' can be written in the form of equation (1).

For this we *define* an operator $L[(b, n) \rightleftarrows (a, n+1)]$ by

$$L[(b, n) \rightleftarrows (a, n+1)] := i_n^b I[(b, n) \leftarrow (a, n+1)] p_{n+1}^a + i_{n+1}^a S[(a, n+1) \leftarrow (b, n)] p_n^b, \tag{8}$$

where p_n^a is the 'projector' that maps any element $\{\alpha_n^a(\kappa_1, \ldots, \kappa_n)\}$ of $\mathscr{S}_1$ onto its component $\alpha_n^a(\kappa_1, \ldots, \kappa_n)$ in the space $\mathscr{H}_n^a$, and i_n^a is the injection operator which identifies any element $\alpha_n^a(\kappa_1, \ldots, \kappa_n)$ of $\mathscr{H}_n^a$ with that vector $\{\beta_m^b(\kappa_1, \ldots, \kappa_m)\}$ of $\mathscr{S}_1$ which has components $\beta_m^b(\kappa_1, \ldots, \kappa_m) = 0$ for all $(b, m) \neq (a, n)$, and the component $\alpha_n^a(\kappa_1, \ldots, \kappa_n)$ for $(b, m) = (a, n)$. We have the formal relation

$$p_n^a i_m^b = \delta_{ab} \delta_{nm}. \tag{9}$$

Also $I[(b, n) \leftarrow (a, n+1)]$ is the integral operator which maps $\mathscr{H}_{n+1}^a$ into $\mathscr{H}_n^b$ by

$$\alpha_{n+1}^a(\kappa_1, \ldots, \kappa_{n+1}) \mapsto \beta_n^b(\kappa_1, \ldots, \kappa_n)$$

$$:= (n+1)^{1/2} \int \mathrm{d}^3\kappa \, M^*(b, a; \kappa) \alpha_{n+1}^a(\kappa, \kappa_1, \ldots, \kappa_n), \tag{10}$$

$S[(a, n+1) \leftarrow (b, n)]$ is the multiplication and symmetrisation operator which maps $\mathscr{H}_n^b$ into $\mathscr{H}_{n+1}^a$ by

$$\alpha_n^b(\kappa_1, \ldots, \kappa_n) \mapsto \beta_{n+1}^a(\kappa_1, \ldots, \kappa_{n+1})$$

$$:= (n+1)^{-1/2} \sum_{\nu=1}^{n+1} M(b, a; \kappa_\nu) \alpha_n^b(\kappa_1, \ldots, \kappa_{\nu-1}, \kappa_{\nu+1}, \ldots, \kappa_{n+1}). \tag{11}$$

$L[(b, n) \leftrightarrows (a, n+1)]$ is obviously defined *everywhere* on $\mathscr{S}_1$ if all $M(a, b; \kappa)$ are square integrable, as assumed. We claim that it is also *symmetric*, i.e. that $\langle \alpha | L[(b, n) \leftrightarrows (a, n+1)] | \alpha \rangle$ is real for any $|\alpha\rangle = \{\alpha_n^a(\kappa_1, \ldots, \kappa_n)\} \in \mathscr{S}_1$.

(*Proof.* By the definition (8) we have

$$\langle\alpha|L[(b,n)\leftrightarrows(a,n+1)]|\alpha\rangle$$
$$=\langle\alpha|i_n^b I[(b,n)\leftarrow(a,n+1)]p_{n+1}^a|\alpha\rangle+\langle\alpha|i_{n+1}^a S[(a,n+1)\leftarrow(b,n)]p_n^b|\alpha\rangle$$
$$=\int \mathrm{d}^3\kappa_1\ldots\int \mathrm{d}^3\kappa_n\,\alpha_n^b(\kappa_1,\ldots,\kappa_n)^*(n+1)^{1/2}\int \mathrm{d}^3\kappa\,M^*(b,a;\kappa)$$
$$\times\alpha_{n+1}^a(\kappa,\kappa_1,\ldots,\kappa_n)+\int \mathrm{d}^3\kappa_1\ldots\int \mathrm{d}^3\kappa_{n+1}\alpha_{n+1}^a(\kappa_1,\ldots,\kappa_{n+1})^*$$
$$\times(n+1)^{-1/2}\sum_{\nu=1}^{n+1}M(b,a;\kappa_\nu)\alpha_n^b(\kappa_1,\ldots,\kappa_{\nu-1},\kappa_{\nu+1},\ldots,\kappa_{n+1}).\qquad(12)$$

It poses no problem to verify that the second term is the complex conjugate of the first term so that the sum is real.)

But, if $L[(b,n)\leftrightarrows(a,n+1)]$ is *defined everywhere* on $\mathscr{S}_1$ and is *symmetric*, it is *bounded* and *self-adjoint on* $\mathscr{S}_1$, by well known theorems (e.g. Yosida 1968).

Finally we have to show that the sum H' of the L, as defined in equation (1), is identical with the interaction terms on the right-hand side of equation (4). For this we compute formally the expression $p_n^a H'|\alpha\rangle$ for any $|\alpha\rangle\in\mathscr{S}_1$. We have

$$p_n^a H'|\alpha\rangle=\sum_{n'=0}^{\infty}\sum_{a'=0}^{\infty}\sum_{b'=0}^{\infty}p_n^a L[(b',n')\leftrightarrows(a',n'+1)]|\alpha\rangle\qquad(13)$$
$$=\sum_{a'=0}^{\infty}I[(a,n)\leftarrow(a',n+1)]p_{n+1}^{a'}|\alpha\rangle+\sum_{b'=0}^{\infty}S[(a,n)\leftarrow(b',n-1)]p_{n-1}^{b'}|\alpha\rangle.\qquad(14)$$

The last expressions have been obtained using equation (9). They are easily identified, formally, with the interaction terms on the right-hand side of equation (4).

It is clear that all procedures carried out are permitted if the sum in equation (1) converges. Otherwise we have carried out only formal procedures. Still, because of its transparence, we take the sum (1) as the final definition of H'; the L are well defined (and harmless) operators.

4. Graphical representation of Weisskopf–Wigner theories

To learn more about the physical content of the partial sums of equation (1) we work out a graphical representation which is at least as illustrative as the representation of certain elements of the S matrix by Feynman graphs.

For this we consider first a two-dimensional array of 'circles', one for each pair (a,n) (figure 1, considered without the lines (a)–(f)). Each circle (a,n) represents, *firstly*, the Hilbert space $\mathscr{H}_n^a$; a given set $I=\{(a,n)\}$ of circles represents the Hilbert space

$$\mathscr{H}_I:=\bigoplus_{(a,n)\in I}\mathscr{H}_n^a,\qquad(15)$$

and the full array of all circles represents the Hilbert space $\mathscr{S}_1$ of our theory. *Secondly*, the circle (a,n) symbolises the multiplication operator on $\mathscr{H}_n^a$ with the function

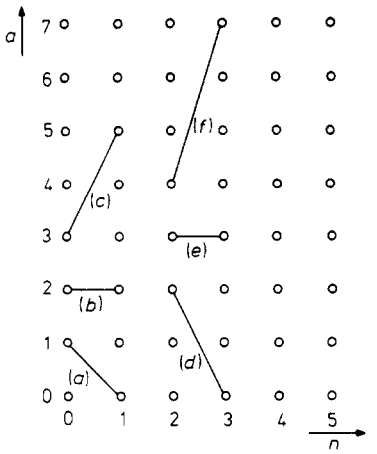

Figure 1. Section from the full array of 'circles' with 'lines' inserted for the following simplest WW theories: ordinary Bohr transitions are represented by (*a*) in the presence of no photons and by (*d*) in the presence of two photons; WW theories of the self-interactions of the states $u_2(x)$ and $u_3(x)$ are represented by (*b*) in the presence of no photons and by (*e*) in the presence of two photons; (*c*) and (*f*) correspond to virtual transitions in the presence of no photons and two photons, respectively.

$(\omega(\kappa_1)+\ldots+\omega(\kappa_n)+E_a)$. Correspondingly a set $I=\{(a,n)\}$ represents the direct sum:

$$H_I^0 := \bigoplus_{(a,n)\in I} (\omega(\kappa_1)+\ldots+\omega(\kappa_n)+E_a) \tag{16}$$

of such operators, and all the circles together represent the Hamiltonian H^0 of the non-interacting system.

Now choose some circle (b, n) in the column n and connect it by a straight line with some circle $(a, n+1)$ in the column $n+1$. This line represents the operator $L[(b, n)\rightleftarrows(a, n+1)]$. If more lines are inserted in this way, we get the graphs of the partial sums Σ of H'; H' itself is obtained by so inserting *all* possible lines. Note that only circles in 'immediate neighbour columns' are to be connected. Figures 1–5 provide examples of various graphs constructed in this way. Superfluous circles may be omitted, as is the case in figures 2–5.

Consider now some given graph, with a given number of lines inserted according to the above rule. Denote with I the set of all circles which are connected to at least one other circle. It may happen now that, starting from one circle of I, one can reach any circle of I by going along the given lines, or it may be that one cannot reach *any* circle of I. In the former case the graph 'on I' will be called 'connected', in the latter case 'disconnected'. Figures 1, 3(*D*), and 4 show examples of disconnected graphs, while all the other graphs in the figures are connected. A disconnected graph consists obviously of connected sub-graphs. We shall see that disconnected graphs represent *independent* theories on *orthogonal* Hilbert spaces so that only connected graphs need to be considered.

Finally, a connected graph may be 'complete' if, given I, it contains *all* lines that can be inserted by the above rules, or it may be 'incomplete' if some lines are omitted which do not yet lead to a disconnected graph. In figure 3, (*A*) shows a complete graph, while (*B*) and (*C*) are incomplete graphs.

The identification of the 'lines' of a graph with well defined terms $L[(a, n) \leftrightarrows (b, n+1)]$ of equation (1) define the meaning of a graph completely. The following 'rules' allow us to write down the time-dependent Schrödinger equation of the corresponding theory. Consider some given graph on some given I and choose some circle (a, n) of I, before proceeding as follows.

(1) For the circle (a, n) write down the expression:

$$\left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}+\omega(\kappa_1)+\ \ldots\ +\omega(\kappa_n)+E_a\right)\alpha_n^a(\kappa_1, \ldots, \kappa_n; t). \tag{17}$$

(2) For each line entering this circle from the left-hand side write down the expression:

$$n^{-1/2}\sum_{\nu=1}^{n} M(b, a; \kappa_\nu)\alpha_{n-1}^b(\kappa_1, \ldots, \kappa_{\nu-1}, \kappa_{\nu+1}, \ldots, \kappa_n; t), \tag{18}$$

b being the number of the circle this line 'is coming from', *and sum* over all entering lines, i.e. over the corresponding b.

(3) For each line 'leaving' (a, n) to the right write down the expression

$$(n+1)^{1/2}\int \mathrm{d}^3\kappa\, M^*(a, b; \kappa)\alpha_{n+1}^b(\kappa, \kappa_1, \ldots, \kappa_n; t) \tag{19}$$

and sum over all 'leaving' lines, i.e. over b.

(4) Sum the expressions for the circle (a, n), for the entering and leaving lines, and put this sum equal to zero.

(5) Write down this equation for any circle $(a, n) \in I$, and consider all these equations simultaneously.

(6) Rules (1)–(5) define a theory in terms of elements $|\alpha_n^a\rangle$ of the spaces $\mathscr{H}_n^a$. If necessary, they may be identified with the elements of $\mathscr{S}_1$ with the same $\mathscr{H}_n^a$-components, and with vanishing components elsewhere. So we obtain a theory on $\mathscr{S}_1$.

The equations given by these rules define the time-dependent Schrödinger equation of the Weisskopf–Wigner theory represented by the graph considered. The reader will have no problems in 'deriving' these equations. For example, the one-line graphs (a), (b), (c) of figure 1 represent the equations of motion considered in II; the graphs of figure 3 show the corresponding equations of motion of Ernst (1976a, b), and so on.

If the graph was *complete* the sum over all entering lines would equal the sum over all $(b, n-1) \in I$ and the sum over all leaving lines would equal the sum over all $(b, n+1) \in I$. The resulting equations of motion are then identical with those of a ww theory on $\mathscr{H}_I$ as considered in I. If the graph was *disconnected*, the resulting system of equations will also consist of independent sub-systems which are not connected with each other. They are actually defined on *orthogonal* subspaces $\mathscr{H}_I$ of $\mathscr{S}_1$.

5. The physical interpretation of a graph

We can now see quite well the physical meaning of an 'isolated line' $(b, n) \rightleftarrows (a, n+1)$ connecting the circles (b, n) and $(a, n+1)$. It represents the interaction Hamiltonian $L[(b, n) \rightleftarrows (a, n+1)]$ of a class of mechanisms where, influenced by the presence of n photons anywhere in space, the atom A makes a transition from the state $u_b(\boldsymbol{x})$ to the state $u_a(\boldsymbol{x})$ and thereby emits a photon in any state. It also represents the inverse mechanisms, where, in the presence of $n+1$ photons in any state anywhere in space, A

makes a transition $u_a(x) \to u_b(x)$ and thereby absorbs a photon. Figure 1 shows the three typical cases that are possible.

Case 1. For $b < a$ and hence $E_b \leqslant E_a$ the line $(b, n) \leftrightarrows (a, n+1)$ will rise from left to right like (c) and (f). This line represents a 'virtual' process because A either 'jumps' to a state of higher energy under *emission* or, in the inverse process, it jumps to a state of lower energy under *absorption* of a photon. Both processes, however, are *real*, and comparable to quantum mechanical barrier penetration effects. We have shown in II that they are related with 'bound photons'.

Case 2. For $b = a$ we get a self-interaction line like (b) and (e) because A now makes the transitions $u_a(x) \leftrightarrows u_a(x)$ under emission or absorption of a photon. It is clear that primarily this photon will be of zero frequency. These processes are also virtual (II) and thus related with photon-binding effects.

Case 3. For $b > a$ we get, in general, lines of ordinary Bohr transitions like (a) and (d), where, under the influence of n photons anywhere in space, A jumps from a state of higher energy to one of lower energy, and thereby emits a photon. Similarly, in the presence of $n+1$ photons, A jumps to a state of higher energy and thereby absorbs a photon. These ordinary transitions occur if an only if $E_b - E_a$ is not too small; otherwise the transition is again virtual, cf II. In particular, transitions between different states of the same energy are always virtual.

The lines may of course be linked together. So we get graphs of compound theories describing two or more photon 'cascades', competing cascades, round trips and many other chains of single processes, as described for simple cases in figure 2.

The graphs (A)–(D) of figure 3 are an excellent illustration of the changes of the mathematical and physical structures involved in various 'orders' of the familar rotating wave approximation, as applied to the interaction of a two-level atom A with photons. Graph (A) represents the complete WW theory, defined by the important state hypothesis that A be a two-level atom. In this approximation the self-interaction of the two states and the virtual transitions between them are still included. Virtual transitions are omitted, but self-interaction is retained in graph (B). This is motivated in the sense

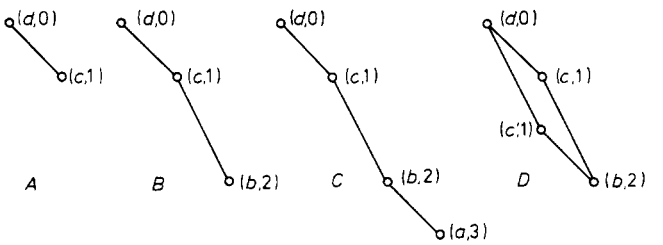

Figure 2. Graphs of simple WW theories involving only ordinary Bohr transitions. (A) The simplest WW theory as treated e.g. by Källén (1958) and in II; (B) Graph of a WW theory describing the spontaneous two-photon cascade $u_d(x) \to u_c(x) \to u_b(x)$, the two-photon resonance fluorescence process $u_b(x) \to u_c(x) \to u_d(x) \to u_c(x) \to u_b(x)$, the one-photon resonance fluorescence $u_b(x) \to u_c(x) \to u_b(x)$ in the presence of another photon, etc; (C) Graph of a theory describing the three-photon cascade $u_d(x) \to u_c(x) \to u_b(x) \to u_a(x)$ and any other process obtained by any 'trip' in the scheme $u_d(x) \leftrightarrows u_c(x) \leftrightarrows u_b(x) \leftrightarrows u_a(x)$. (D) Graph of a two-channel theory of competing cascades $u_d(x) \to u_c(x) \to u_b(x)$ and $u_d(x) \to u_{c'}(x) \to u_b(x)$ and several other chains of processes.

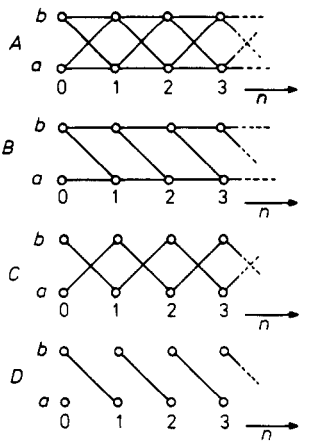

Figure 3. Graphs of ww theories of the interaction of a 'two-level' atom with transverse photons in various states of the rotating wave approximation.

of the rotating wave approximation because the omitted terms are 'more anti-resonant' than those retained. Self-interaction is omitted, but virtual transitions are retained in graph (C). In dipole approximation this theory corresponds to the 'spin formalism' used frequently in quantum optics (e.g. Agarwal 1971, 1973) which cannot account for the self-interaction. Graph (D) is the incomplete and disconnected graph obtained from graph (A) by retaining *only* the resonant terms. The omission of all anti-resonant terms is equivalent to the omission of level shifts of the order of magnitude of Lamb shifts (Ernst 1976a). The equations of motion corresponding to graph 3(D) can be solved approximately (Ernst 1976b). The decay of the graph in the transitions (C)→(D), (B)→(D) displays the deep-lying decay of the total interaction process between A and photons into many *independent* partial processes (represented by the *isolated* lines of (D)). This has been interpreted as the actual reason for the common experience that atoms cannot be used as 'linear detectors' for electromagnetic field strengths at optical or higher frequencies. Graph (D) tells us indeed that A interacts *in independent processes* with the n-photon components of the state of R; so it is insensitive to photon-number uncertainties to which any linear detector *must* be sensitive (cf Ernst 1976a).

We learn further that two standard assumptions of quantum optics, namely 'two-level atoms' and the rotating wave approximation, correspond to certain orders of the hierarchy of ww theories. For example, practically all existing theories (e.g. Kimble and Mandel 1976) of the dynamical Stark effect contain assumptions equivalent to graph 3(D).

The characteristics of the ww theory represented by figure 4 are bound transverse photons in a fully coherent state (I, Ernst 1976a); a generalisation to non-relativistic more-electron atoms leads to a prospective quantum theory of the self-energy of these electrons and of the Coulomb force acting between them (to be published later).

Under the conditions of § 2 the mean number of bound *transverse* photons is small compared with one. Therefore one expects and finds that the main contributions to the corresponding binding energies come from the first line $L[(a, 0) \rightleftarrows (a, 1)]$ of figure 4. So one must expect that the lines included in figure 5(A) account mainly for the binding

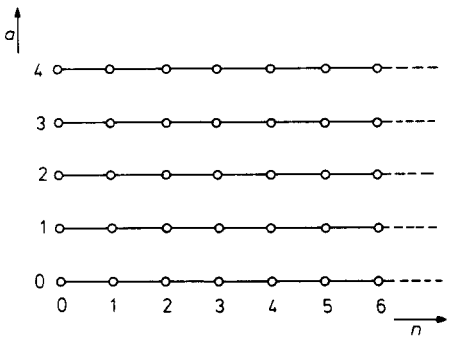

Figure 4. Graphs of all self-interaction processes of the states of an atom. A single 'horizontal cascade' leads to a coherent state of bound photons with binding energies causing shifts of the atomic levels of the order of Lamb shifts, cf I, Ernst (1976a). The theory defined by all horizontal cascades is the 'direct sum' of those corresponding to the single theories.

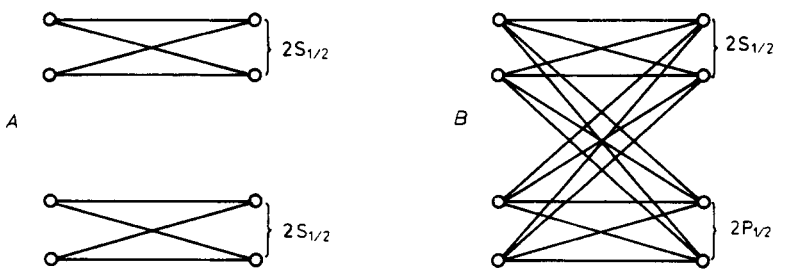

Figure 5. Graphs of the ww theories of the two-level complexes $2S_{1/2}$ and $2P_{1/2}$ and of the four-level complex $2S_{1/2}+2P_{1/2}$.

energies of transverse photons bound to the $2S_{1/2}$ and $2P_{1/2}$ two-level complexes. The *difference* of these binding energies is about 1064 MHz, to be compared with the experimental $2S_{1/2}$–$2P_{1/2}$ Lamb shift separation of approximately 1057 MHz (II). The full ww theory of the $2S_{1/2}$–$2P_{1/2}$ four-level complex, figure 5(*B*), leads to the following results (Grimm 1976). The familar $2S_{1/2}$–$2P_{1/2}$ degeneracy of the Dirac atom is removed at around 1064 MHz, while the spin degeneracy of both $2S_{1/2}$ and $2P_{1/2}$ is retained.

6. A Weisskopf–Wigner theory of competing ordinary and virtual transitions

We now discuss in detail the ww theory defined by figure 6(*a*). We are mainly interested in its dependence on the number of lines $A+1<\infty$ which are included. The figure immediately illustrates that there is a special case of ordinary Bohr transitions if $A<B$, and that virtual transitions come into play if $A>B$. We look here at the resulting 'competition', cf § 1. The limit as $A\to\infty$ and another more important reason for our interest in this particular ww theory are given in § 7.

The rules of § 4 provide the time-dependent Schrödinger equation of this ww theory (we assume $\mu = 0$ and put $\omega(\kappa) = |\boldsymbol{k}| = k$):

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_0^B(t) = E_B\alpha_0^B(t) + \sum_{a=0}^{A}\int \mathrm{d}^3\kappa\, M^*(B, a; \kappa)\alpha_1^a(\kappa; t), \tag{20a}$$

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_1^a(\kappa; t) = (E_a + k)\alpha_1^a(\kappa; t) + M(B, a; \kappa)\alpha_0^B(t), \qquad a = 0, 1, \ldots, A. \tag{20b}$$

The Hilbert space of the theory is $\mathscr{H}_I = \mathscr{H}_0^B \oplus \mathscr{H}_1^0 \oplus \ldots \oplus \mathscr{H}_1^A$ with elements $|\alpha_I\rangle = \{\alpha_0^B; \alpha_1^0(\kappa), \ldots, \alpha_1^A(\kappa)\}$. The Hamiltonian H_I^0, for the case with no interaction, is obtained by putting $M(B, a; \kappa) = 0$ for any a. The total Hamiltonian $H_I^0 + \Sigma$ is given by the right-hand side of equation (20).

It is frequently convenient to compare the spectra of H_I^0 and $H_I^0 + \Sigma$. In our case H_I^0 has a continuous spectrum extending from $E = E_0$ to $E = \infty$ and an eigenstate $|(B, 0)\rangle = \{1; 0, \ldots, 0\}$ at $E = E_B$. We assume, in general, $E_B > E_0$ (cf figure 6(*b*)). We are interested in the perturbation of this spectrum by Σ. It is shown in § 8 that H_I^0 and $H_I^0 + \Sigma$ have the same continuous spectrum (figure 6(*c*)). The theorem says nothing about the eigenvalues of $H_I^0 + \Sigma$ which must be analysed separately.

For reasons of comparison we first compute the correction δE_B^A of the energy E_B of the eigenstate of H_I^0 by formally applying the perturbation theory to equation (20). First-order corrections vanish, so to second order we get:

$$\begin{aligned} -\delta E_B^A &= \sum_{|z\rangle}\frac{|\langle(B, 0)|\Sigma|z\rangle|^2}{E_{|z\rangle} - E_B} \\ &= \sum_{a=0}^{A}\sum_{\kappa}\frac{|\langle(B, 0)|L[(B, 0)\rightleftarrows(a, 1)]|a, \kappa\rangle|^2}{k + E_a - E_B} \\ &= \sum_{a=0}^{A}\frac{(2\pi)^3}{V}\sum_{\kappa}{}'\frac{|M(B, a; \kappa)|^2}{k + E_a - E_B}. \end{aligned} \tag{21}$$

The sum over $|z\rangle$ covers all eigenstates of H_I^0 except $|(B, 0)\rangle$. To make the formula applicable at all we have introduced the usual 'box normalisation' with a box of volume V, (e.g. Källén 1958). The $|z\rangle$ are then given as states $|a, \kappa\rangle$ with A in the state $u_a(\boldsymbol{x})$ and the photon in the 'mode' κ, a plane wave eigenstate of the box of energy $k = |\boldsymbol{k}|$. Hence $E_{|z\rangle} = k + E_a$. The required element $\langle|L\ldots|\rangle$ is given by $((2\pi)^3/V)^{1/2}M(B, a; \kappa)$, as may be seen from a comparison with Källén (1958). The last expression is ready for the usual transition to a 'continuum of modes', $V \to \infty$. To define the resulting integral properly we include the usual $\mathrm{i}\epsilon$. So we get

$$-\delta E_B^A = \sum_{a=0}^{A}\int \mathrm{d}^3\kappa\frac{|M(B, a; \kappa)|^2}{k + E_a - E_B + \mathrm{i}\epsilon} = \sum_{a=0}^{A}\int_0^\infty \mathrm{d}k\frac{m(B, a; k)}{k + E_a - E_B + \mathrm{i}\epsilon} = \sum_{a=0}^{A}(\epsilon_{Ba} - \mathrm{i}\Gamma_{Ba}) \tag{22}$$

with the definitions

$$m(A, b; k) := k^2\sum_{\lambda=1}^{2}\int \mathrm{d}^2\Omega\,|M(A, b; \kappa)|^2, \qquad \epsilon_{Ba} := \mathrm{P}\int_0^\infty \mathrm{d}k\frac{m(B, a; k)}{k + E_a - E_B},$$

$$\Gamma_{Ba} := \pi m(B, a; E_B - E_a)\theta(E_B - E_a). \tag{23}$$

$\int \mathrm{d}^2\Omega$ denotes the integration over the angles in $\boldsymbol{k}$-space, P denotes the Cauchy principal value if $E_B > E_a$, and $\theta(x)$ is the step function $\theta(x) = 1$ for $x > 0$, $\theta(x) = 0$ for

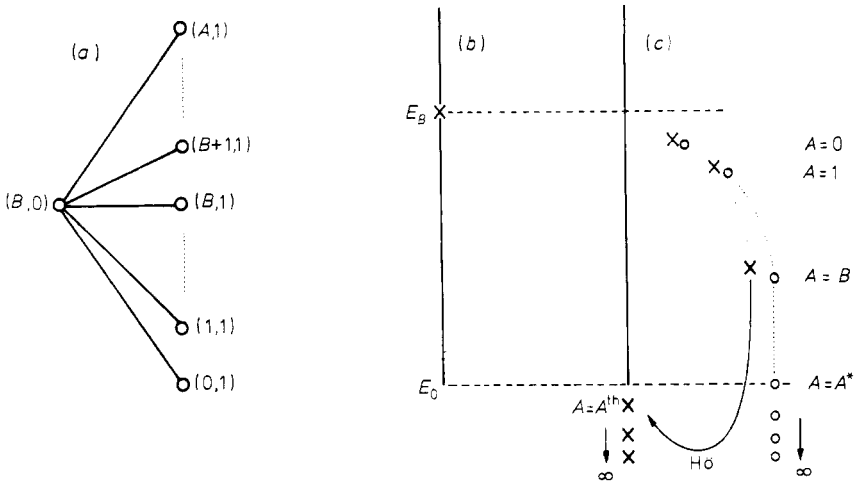

Figure 6. (*a*) Graph of a WW theory of competing ordinary and virtual transitions in the presence of no photons. (*b*) Spectrum of the 'free' Hamiltonian H_I^0 of this theory. (*c*) Spectrum of the total Hamiltonian of this theory in dependence of the number $A+1$ of lines included in (*a*). The crosses mark the positions of the 'exact' (complex or real) eigenvalues, the circles mark the eigenvalues as obtained in second-order perturbation theory. The scales are arbitrary. In reality we have, in general, $\epsilon_{Ba} \gg \Gamma_{BA}$.

$x \leqslant 0$. Both the integrals $\int_0^\infty \mathrm{d}k\, m(B, a; k)$ and $\int_0^\infty \mathrm{d}k\, m(B, a; k)/k$ exist (II) so that all terms in equation (22) are finite. ϵ_{Ba} is typically of the order of magnitude of Lamb shifts, and Γ_{Ba} is the decay constant of the transition $u_B(\boldsymbol{x}) \to u_a(\boldsymbol{x})$ as obtained in typical WW theories, e.g. Källén (1958).

In figure 6(*c*) the positions of the complex energies $E_B^A = E_B + \delta E_B^A$ are marked by circles denoted with the value of A. As $\epsilon_{Ba} > 0$, the E_B^A move with increasing A for $A > B$ on a parallel to the real E axis in the direction of $-\infty$. For $A \approx A^*$ the complex eigenvalue 'passes' the lower end of the continuous spectrum and diverges for $A \to \infty$, cf § 7. If $u_B(\boldsymbol{x})$ is one of the states $2S_{1/2}$, $2P_{1/2}$ the value of A^* is of the order of about 10^6, according to the figures given in II.

The above transition is a continuum of modes and the inclusion of $\mathrm{i}\epsilon$, though widely used in literature, is somewhat heuristic because the general formula (21) applies only to real perturbations of *isolated* eigenvalues. But we can solve the 'exact' equations (20) and so compare the exact result with equation (22).

The case $A = 0$ of equation (20) is identical with the simplest, ordinary WW theory (Källén 1958, II) of the transition $u_B(\boldsymbol{x}) \to u_0(\boldsymbol{x})$ if $E_B - E_0 \gg \epsilon_{B0}$, cf II. In a very good secondary approximation to the exact solution of equation (20) the decaying state can be represented by the same complex eigenvalue E_B^0 as obtained above. Weisskopf and Wigner (1930) have shown that the same is true for small A, say $A \leqslant A_1 < B$. In figure 6(*c*) we have therefore plotted exact eigenvalues, marked with crosses, near the corresponding perturbation circles. For small A the transitions from $u_B(\boldsymbol{x})$ to states of lower energies can be considered to be approximately independent of each other: Melting effects (§ 1) arising from their competition are still very small. Their complete absence gives the characteristics of equation (22) because $\epsilon_{Ba} - \mathrm{i}\Gamma_{Ba}$ is a typical quantity related to the *isolated* line $L[(B, 0) \rightleftarrows (a, 1)]$.

This agreement between exact and second-order perturbation results is restricted to small A. We shall see below that the crosses move (somehow) with increasing A

towards the lower end of the continuous spectrum, 'jump' up to the real E axis at some $A = A^{\text{th}}$, and then move along on this axis to $E = -\infty$. In a theory of Höhler (1958) with comparable mathematical structure the lower end of the continuous spectrum is approached on a path marked in figure 6(*c*) with an arrow Hö. A similar path can also be expected in our case but we shall be content to prove that the exact E_B^A becomes real for $A \geqslant A^{\text{th}} > A^*$. In § 7 we shall show convincingly that E_B^A diverges for $A \to \infty$.

To prove the jump up to the real axis, we make the usual *ansatz*:

$$\{\alpha_0^B(t); \alpha_1^0(\kappa; t), \ldots, \alpha_1^A(\kappa; t)\} = \exp(-\mathrm{i}t(E_0 - X))\{\beta_0^B; \beta_1^0(\kappa), \ldots, \beta_1^A(\kappa)\} \tag{24}$$

for a real eigenvalue at $E = E_0 - X$, where $X \geqslant 0$ is the distance ('gap') between this eigenvalue and the lower end of the continuous spectrum. Inserting equation (24) into equation (20) and putting $E_a - E_0 =: \Delta_a \geqslant 0$, and $E_B - E_0 =: \Delta_B \geqslant 0$ we get

$$(X + \Delta_B)\beta_0^B = -\sum_{a=0}^{A} \int \mathrm{d}^3 M^*(B, a; \kappa)\beta_1^a(\kappa), \tag{25a}$$

$$(X + \Delta_a + k)\beta_1^a(\kappa) = -M(B, a; \kappa)\beta_0^B, \qquad a = 0, 1, \ldots, A. \tag{25b}$$

As $(X + \Delta_a + k) > 0$ we can solve (25*b*) with respect to $\beta_1^a(\kappa)$ and insert this into equation (25*a*). As $\beta_0^B = 0$ leads only to the trivial solution we assume $\beta_0^B \neq 0$. So we get

$$(X + \Delta_B) = \sum_{a=0}^{A} \int_0^{\infty} \mathrm{d}k \frac{m(B, a; k)}{X + \Delta_a + k} =: F_B^A(X). \tag{26}$$

$F_B^A(X)$ exists for any $A < \infty$ as a monotonically decreasing function of X at $X \geqslant 0$. Therefore only one solution $X = X_B^A$ of equation (26) *can* exist; it *will* exist if and only if

$$\Delta_B \leqslant F_B^A(0). \tag{27}$$

The accidental case $\Delta_B = F_B^A(0)$ need not be considered. X_B^A satisfies $\Delta_B + X_B^A < F_B^A(0)$. We show in § 7 that $F_B^A(0)$ diverges for $A \to \infty$. Condition (27) is therefore always satisfied if A is larger than some threshold A^{th}. If the continuation of $F_B^A(X)$ to negative X is defined by adding a term $\mathrm{i}\epsilon$ we get $F_B^A(-\Delta_B) = -\delta E_B^A$. This means that the terms $a \geqslant B$ in $F_B^A(0)$ are smaller than the corresponding terms in $-\delta E_B^A$. As the few complex terms $a < B$ do not count in this connection we have, in general, $A^{\text{th}} > A^*$. For $B = 0$ we have $A^{\text{th}} = 0$: in this case an eigenstate of $H_I^0 + \Sigma$ always exists outside the continuous spectrum.

We should consider also the corresponding eigenstate. Equation (25*b*) yields

$$\beta_1^a(\kappa) = -\beta_0^B M(B, a; \kappa)/(X_B^A + \Delta_a + k) \tag{28}$$

with a constant β_0^B with arbitrary phase, but a modulus defined by the normalisation condition:

$$1 = |\beta_0^B|^2 + \sum_{a=1}^{A} \int \mathrm{d}^3\kappa \, |\beta_1^a(\kappa)|^2 = |\beta_0^B|^2(1 + D_B^A), \tag{29}$$

$$D_B^A := \sum_{a=0}^{A} \int_0^{\infty} \mathrm{d}k \, m(B, a; k)/(X_B^A + \Delta_a + k)^2 \leqslant (X_B^A + \Delta_B)/X_B^A. \tag{30}$$

The last inequality is obtained by replacing $(X_B^A + \Delta_a + k)^2$ by $X_B^A(X_B^A + \Delta_a + k)$ and using equation (26). It means that $\bar{n}_B^A := 1 - |\beta_0^B|^2$ satisfies

$$0 < \bar{n}_B^A < (X_B^A + \Delta_B)/(2X_B^A + \Delta_B) < 1. \tag{31}$$

where $\bar{n}_B^A$ is the mean number of photons in the eigenstate. If the system is in this eigenstate, these photons can be considered as 'bound' (I, II) because within the given theory they cannot be 'removed' from the atom, as any eigenstate of $H_I^0+\Sigma$ is clearly stable under the interaction Σ. $X_B^A+\Delta_B$ is the corresponding 'binding energy' which increases monotonically with A. We have namely

$$X_B^{A+1}-X_B^A=\left(\int_0^\infty \mathrm{d}k\,\frac{m(B,A+1;k)}{X_B^{A+1}+\Delta_{A+1}+k}\right)\times\left(1+\sum_{a=0}^{A}\int_0^\infty \mathrm{d}k\,\frac{m(B,a;k)}{(X_B^A+\Delta_a+k)(X_B^{A+1}+\Delta_a+k)}\right)^{-1} \tag{32}$$

which is obtained by substituting for X_B^{A+1} and X_B^A in accordance with equation (26), computing the difference under the sum over a and under the k integral, and solving the resulting equation with respect to $X_B^{A+1}-X_B^A$. As $X_B^{A+1}>X_B^A$ the sum in the denominator is smaller than D_B^A. So we get $N(X_B^A+\Delta_B)/(2X_B^A+\Delta_B)<X_B^{A+1}-X_B^A<N$ where N is the numerator in equation (32).

It is remarkable that the 'contribution' $X_B^{A+1}-X_B^A$ of the $(1+A)$th line is always *smaller* than the 'binding energy' of this line if it is considered alone as in II. This can be shown by a derivation similar to equation (32). It seems that $\bar{n}_B^A$ does not increase, in general, with increasing A, but we shall not look at this in detail.

We learn that the second-order perturbation theory gives correct results if and only if A is small. Also, as bound photons and proper eigenstates are the characteristics of virtual transitions (II) the appearance of a proper eigenstate of $H_I^0+\Sigma$ for $A>A^{\text{th}}$ means that sufficiently many virtual transitions (in our case) always win the competition with few ordinary Bohr transitions. In fact, the jump up to the real axis leaves not the slightest trace of the characteristics of ordinary Bohr transitions, i.e. the decay of the state $|(B,0)\rangle$ and the natural linewidths for the transitions $u_B(\boldsymbol{x})\to u_a(\boldsymbol{x})$, $a<B$. Melting effects, which vanish in second-order perturbation theory, are very strong for large A. However, the discussion of § 1 on the convergence of equation (1) applies, *mutatis mutandis*, to the present case. From the physical point of view the results for large A therefore must not be taken seriously, cf § 7.

7. The first divergences in a Weisskopf–Wigner theory

We consider now the limit as $A\to\infty$ which is not covered by the existence theorems of I. We show that both $F_B^A(0)$ and X_B^A diverge, and compare this ww divergence with well known infinities of QED.

As $-\mathrm{Re}\,E_B^A=\mathrm{Re}\,F_B^A(-\Delta_B)>F_B^A(0)$ for large A, as $F_B^A(X)$ decreases monotonically with increasing $X>0$, and as $X_B^A+\Delta_B=F_B^A(X_B^A)$ we get $-\mathrm{Re}\,E_B^A>F_B^A(0)>X_B^A+\Delta_B$ for large A. The 'exact' correction $X_B^A+\Delta_B$ of E_B is thus always smaller than the correction in second-order perturbation theory. The divergence of $F_B^A(0)$ and X_B^A is therefore not trivial and must be proved.

To find lower bounds for X_B^A we use the following identity on the right-hand side of equation (26) with any $\bar{X}>0$:

$$\frac{1}{X+k+\Delta_a}=\frac{1}{\bar{X}+k+\Delta_a}-\frac{X-\bar{X}}{(\bar{X}+k+\Delta_a)(X+k+\Delta_a)} \tag{33}$$

to obtain

$$\Delta_B+\bar{X}+(X-\bar{X})\Big(1+\sum_{a=0}^{A}\int_0^\infty \mathrm{d}k\,\frac{m(B,a;k)}{(\bar{X}+k+\Delta_a)(X+k+\Delta_a)}\Big)=F_B^A(\bar{X}). \tag{34}$$

Using equation (33) once more we get

$$(\Delta_B+X)(1+L_B^A(\bar{X}))=F_B^A(\bar{X})+(X-\bar{X})^2G_B^A(\bar{X},X)+L_B^A(\bar{X})(\Delta_B+\bar{X}) \tag{35}$$

with the abbreviations

$$L_B^A(\bar{X}):=\sum_{a=0}^{A}\int_0^\infty \mathrm{d}k\,\frac{m(B,a;k)}{(\bar{X}+k+\Delta_a)^2}, \tag{36}$$

$$G_B^A(\bar{X},X):=\sum_{a=0}^{A}\int_0^\infty \mathrm{d}k\,\frac{m(B,a;k)}{(\bar{X}+k+\Delta_a)^2(X+k+\Delta_a)}. \tag{37}$$

The solution $X=X_B^A$ of equation (35) is of course identical with the solution of equation (26). As the last two terms on the right-hand side are not negative we get the first inequality for any $\bar{X}>0$:

$$F_B^A(\bar{X})/(1+L_B^A(\bar{X}))<\Delta_B+X_B^A<F_B^A(\bar{X}). \tag{38}$$

The second inequality holds for $\bar{X}<X_B^A$ and is a trivial consequence of the monotonic nature of $F_B^A(X)$.

We show below that $F_B^A(X)$ diverges linearly like $\int^\infty \mathrm{d}k$ for any $X\geqslant 0$ whereas $L_B^A(X)$ has a *maximum* logarithmic divergence like $\int^\infty \mathrm{d}k/k$ for any $X\geqslant 0$. The former case includes the divergence of $F_B^A(0)$ whereas both cases prove that X_B^A has a minimum divergence like $(\int^\infty \mathrm{d}k)/(\int^\infty \mathrm{d}k/k)$.

To prove these statements we put $F_B^A(X)=M_B^A(X)-L'^A_B(X)$ with

$$M_B^A(X):=\sum_{a=0}^{A}\int_0^\infty \mathrm{d}k\,\frac{m(B,a;k)}{X+k},\qquad L'^A_B(X)=\sum_{a=0}^{A}\int_0^\infty \mathrm{d}k\,\frac{m(B,a;k)}{(X+k)(X+k+\Delta_a)}. \tag{39}$$

$M_B^A(X)$ diverges linearly. To show this we substitute equation (23) and equation (5) to obtain:

$$M_B^A(X)=\frac{e^2}{2(2\pi)^3}\int \mathrm{d}^3\kappa\,\frac{1}{k(k+X)}\int \mathrm{d}^2x\int \mathrm{d}^3x'\,u_B^+(\boldsymbol{x})(\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}}$$
$$\times\Big(\sum_{a=0}^{A}u_a(\boldsymbol{x})u_a^+(\boldsymbol{x}')\Big)\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}'}(\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha})u_B(\boldsymbol{x}'). \tag{40}$$

$\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}'}(\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha})u_B(\boldsymbol{x}')$ is for any $\boldsymbol{k}$ in the Hilbert space of 'electron' solutions of the Dirac equation. Therefore, the sum over a acts upon it in the limit $A\to\infty$ like $\delta(\boldsymbol{x}-\boldsymbol{x}')$. The integration over $\boldsymbol{x}'$ can be carried out immediately, the exponentials cancel and we find that $(\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha})^2=1$, and the integral over x yields 1. The remaining integral over κ diverges linearly, as stated. To show that $L'^A_B(X)$ has a maximum logarithmic divergence we enlarge the right-hand side of equation (39) by putting $\Delta_a=0$ in the denominator. Then inserting equation (23) and equation (5) as above, putting $u_a^+(\boldsymbol{x}')\Delta_a=u_a^+(\boldsymbol{x}')(E_a-E_0)=u_a^+(\boldsymbol{x}')(H^{\mathrm{D}}-E_0)$ where H^{D} is the Hamiltonian of the Dirac equation, carrying out the sum over a and the integration over $\boldsymbol{x}'$ as above we

find:

$$L_B^{\infty}(X) \leqslant \frac{e^2}{2(2\pi)^3} \int \mathrm{d}^3\kappa \frac{1}{k(k+X)^2} \int \mathrm{d}^3x\, u_B^+(\boldsymbol{x})(\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha})\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}}(H^{\mathrm{D}} - E_0)\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}}(\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha})u_B(\boldsymbol{x}). \tag{41}$$

The contribution from E_0 can be evaluated as above and diverges logarithmically. To get the contribution from H^{D} we put $H^{\mathrm{D}}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}}\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha}u_B(\boldsymbol{x}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}}(-\boldsymbol{k}\boldsymbol{x} + H^{\mathrm{D}})\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha}u_B(\boldsymbol{x})$. The exponentials then cancel as before. The contribution from $\boldsymbol{k}\boldsymbol{x}$ vanishes from symmetry arguments. The remaining integral over $\boldsymbol{x}$ satisfies

$$\begin{aligned}
&\left| \int \mathrm{d}^3x\, u_B^+(\boldsymbol{x})(\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha}) H^{\mathrm{D}} (\boldsymbol{\epsilon}(\kappa)\boldsymbol{\alpha}) u_B(\boldsymbol{x}) \right| \\
&\qquad = \left| \sum_{i,k=1}^{3} \epsilon_i(\kappa)\epsilon_k(\kappa) \int \mathrm{d}^3x\, u_B^+(\boldsymbol{x})\alpha_i H^{\mathrm{D}} \alpha_k u_B(\boldsymbol{x}) \right| \\
&\qquad \leqslant \sum_{i,k=1}^{3} \left| \int \mathrm{d}^3x\, u_B^+(\boldsymbol{x})\alpha_i H^{\mathrm{D}} \alpha_k u_B(\boldsymbol{x}) \right|.
\end{aligned} \tag{42}$$

$\epsilon_i(\kappa)$ and α_i are the Cartesian components of $\boldsymbol{\epsilon}(\kappa)$ and $\boldsymbol{\alpha}$. As $\boldsymbol{\epsilon}(\kappa)^2 = 1$ the components of $\boldsymbol{\epsilon}(\kappa)$ are bounded by 1. The last integrals exist, so $L'^{A}_B(X)$ has a maximum logarithmic divergence as stated. One can also show that it has a *minimum* logarithmic divergence, but this is not needed here. It now follows that $F_B^A(X)$ diverges 'linearly', because the logarithmical divergence of $L'^{A}_B(X)$ does not count beside the linear one of $M_B^A(X)$.

To show that $L_B^A(X)$ has a maximum logarithmic divergence we enlarge the right-hand side of equation (36) by putting $\Delta_a = 0$. The resulting upper bound can be treated as equation (40), except that $(k+X)$ is replaced by $(k+X)^2$ which also accounts for the weaker divergence. By the same argument we find that $G_B^A(\bar{X}, X)$ converges, but this is not relevant here.

The reader will have observed that equations (40) and (41) resemble certain 'divergences' known from QED. A comparison with Heitler (1954) shows that the limit $A \to \infty$ of our δE_B^A agrees with the contribution of the transverse photons and 'electron' solutions of the Dirac equation to the (divergent) 'corrections' of E_B obtained if second-order perturbation theory is applied to the *full* Hamiltonian. This means that only the very few terms $L[(B,0) \rightleftarrows (a,1)]$ of equation (1) which contribute to the present limit $A \to \infty$ determine familar divergences of QED which are usually removed by renormalisation. This is why the present WW theory deserves attention. It displays the structure of certain divergences of QED. Firstly, a glance at figure 6(*c*) shows that second-order perturbation divergences contain an infinite methodical error. Secondly, the (smaller) WW divergences cannot be renormalised by an infinite, real mass term $\delta m\bar{\psi}\psi$ because this would not re-introduce the decay constants which are necessary to obtain emission and absorption lines at all. Thirdly, the continuous spectrum is stable under those terms of equation (1) which contribute at all to the second-order perturbation divergences of QED considered here. Fourthly, these divergences arise from physical processes which cannot play any role in any given physical situation, cf § 1.

We learn that there are fundamental differences between perturbation theory and the WW approach, despite some occasional overlapping. The WW approach elucidates the problems of the atom–photon interaction from other angles and so provides a true alternative to perturbation theory. Let us consider an example.

At the end of § 6 we had to admit that the results for large A must not be taken too seriously. In fact, instead of too many virtual terms $L[(B,0) \rightleftarrows (a,1)]$, we would have

been better had we included some ordinary Bohr terms $L[(A,1)\leftrightarrows(B,2)]$, because, given $A>B$, the term $L[(A,1)\rightleftarrows(B,2)]$ is always 'more important' than any $L([B,0)\rightleftarrows(a,1)]$ with sufficiently large a. We 'allow' thereby that the atom may return to the state $u_B(\boldsymbol{x})$ under proper emission of a photon *if* it has jumped virtually, i.e. under emission of a photon, to a state $u_A(\boldsymbol{x})$ of higher energy E_A. This type of reasoning is not possible if perturbation theory is applied systematically to the full interaction Hamiltonian H'. In this case, the ordering principle is violated if only a part of the terms $L[(B,0)\rightleftarrows(a,1)]$ is included, and this cannot be permitted without allowing that contributions from higher orders can be more important than non-vanishing lower-order effects.

8. The stability of the continuous spectra in a class of Weisskopf–Wigner theories

We show finally that H_I^0 and $H_I^0+\Sigma$ have indeed the same continuous spectrum. This is a special case of the following theorem to be proved below.

Theorem. H_I^0, the Hamiltonian of the case of no interaction, and $H_I^0+\Sigma$ have the same continuous spectrum if Σ is the sum of any finite number of terms of (1) of the form $L[(b,0)\rightleftarrows(a,1)]$.

Proof. Consider any set of such lines. Denote the circles $(b,0)$ which are connected with at least one circle $(a,1)$ by $(b^1,0),\ldots,(b^n,0)$ and the circles $(a,1)$ which are connected with at least one $(b,0)$ by $(a^1,1),\ldots,(a^m,1)$. The corresponding ww theory is defined essentially on the Hilbert space $\mathcal{H}_I=\mathcal{H}_0^{b^1}\oplus\ldots\oplus\mathcal{H}_0^{b^n}\oplus\mathcal{H}_1^{a^1}\oplus\ldots\oplus\mathcal{H}_1^{a^m}$ with elements

$$|\alpha_I\rangle=\{\alpha_0^{b^1},\ldots,\alpha_0^{b^n};\alpha_1^{a^1}(\kappa),\ldots,\alpha_1^{a^m}(\kappa)\}. \tag{43}$$

The rules of § 4 yield the Schrödinger equation (again for $\mu=0$):

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_0^{b^q}(t)=E_{b^q}\alpha_0^{b^q}(t)+\sum_{r=1}^{m}\int \mathrm{d}^3\kappa\, M^*(b^q,a^r;\kappa)D^{qr}\alpha_1^{a^r}(\kappa;t), \qquad q=1,\ldots,n, \tag{44a}$$

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_1^{a^p}(\kappa;t)=(E_{a^p}+k)\alpha_1^{a^p}(\kappa;t)+\sum_{s=1}^{n}M(b^s,a^p;\kappa)D^{sp}\alpha_0^{b^s}(t), \qquad p=1,\ldots,m. \tag{44b}$$

D^{ij} is unity if the graph of Σ contains the line $L[(b^i,0)\rightleftarrows(a^j,1)]$, and zero if this is not the case. The spectrum of H_I^0 consists obviously of the union of the eigenvalues at $E=E_{b^1},\ldots,E_{b^n}$ and the union of continuous spectra extending from $E_{a^1},\ldots,E_{a^m}$ to $+\infty$. The 'continuous spectrum', the 'essential spectrum' and the 'absolutely continuous spectrum', all in the sense of Kato (1966), agree in the present case.

We note that $\Sigma|\alpha_I\rangle$ is for any $|\alpha_I\rangle\in\mathcal{H}_I$ of the form

$$\begin{aligned}\Sigma|\alpha_I\rangle=\Big\{&\sum_{r=1}^{m}\int \mathrm{d}^3\kappa\, M^*(b^1,a^r;\kappa)D^{1r}\alpha_1^{a^r}(\kappa),\ldots,\sum_{r=1}^{m}\int \mathrm{d}^3\kappa\, M^*(b^n,a^r;\kappa)D^{nr}\alpha_1^{a^r}(\kappa);\\ &\sum_{s=1}^{n}M(b^s,a^1;\kappa)D^{s1}\alpha_0^{b^s},\ldots,\sum_{s=1}^{n}M(b^s,a^m;\kappa)D^{sm}\alpha_0^{b^s}\Big\}\\ =&\sum_{s=1}^{n}\Big[\Big(\sum_{r=1}^{m}\int \mathrm{d}^3\kappa\, M^*(b^s,a^r;\kappa)D^{sr}\alpha_1^{a^r}(\kappa)\Big)|C_0^s\rangle+\alpha_0^{a^s}|C_1^s\rangle\Big]\end{aligned} \tag{45}$$

with Hilbert vectors from $\mathcal{H}_I$ defined for $s = 1, \ldots, n$ by

$$|C_1^s\rangle := \{0, \ldots, 0; M(b^s, a^1; \kappa)D^{s1}, \ldots, M(b^s, a^m; \kappa)D^{sm}\}, \tag{46}$$

$$|C_0^s\rangle := \{0, \ldots, 0, 1, 0, \ldots 0; 0, \ldots, 0\}. \tag{47}$$

The 1 is inserted at the sth position. Equation (45) means that the range $R(\Sigma)$ of Σ is spanned by the $2n$ vectors $|C_1^s\rangle$, $|C_0^s\rangle$. $R(\Sigma)$ is therefore contained in a subspace of $\mathcal{H}_I$ whose dimension is at most $2n$, i.e. finite. This means that Σ is *degenerate* and thus *compact* (Kato 1966, p 160). As Σ is defined everywhere on $\mathcal{H}_I$ (II) and is self-adjoint, it is also *compact relative to* H_I^0 (Kato 1966, p 194) and H_I^0 and $H_I^0 + \Sigma$ have the same essential spectrum (Kato 1966, p 244) which in our case agrees with the continuous spectrum.

We may go a little further than this in the following way. As Σ is compact, it has a discrete spectrum of eigenvalues. Non-vanishing eigenvalues are of finite multiplicity. The eigenvalue 0 has an infinite multiplicity because all vectors of $\mathcal{H}_I$ which are orthogonal to the subspace spanned by the $|C_1^s\rangle$ and $|C_0^s\rangle$ are eigenvectors to this eigenvalue. As the eigenvectors corresponding to non-vanishing eigenvalues are in $R(\Sigma)$, and the dimension of $R(\Sigma)$ is not greater than $2n$, Σ has at most $2n$ non-vanishing eigenvalues, each one being counted by its multiplicity. Σ is therefore in the *trace class* (Kato 1966, p 521) which means that H_I^0 and $H_I^0 + \Sigma$ have the same absolutely continuous spectrum (Kato 1966, p 540) which again agrees with the continuous spectrum. Moreover, *there exists a wave operator* (which defines the physical 'spectrum of observable emission and absorption lines').

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