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On the existence of Weisskopf–Wigner type theories

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Abstract. It is shown that certain features of the Weisskopf–Wigner theory of natural line width can be generalized for the construction of a systematic, mathematically and logically autonomous approximation scheme for treating the interaction of a bound electron with photons. This scheme is equipped with its own hierarchy of orders which are not ruled by powers of the coupling constant. Under very weak conditions on the bound electron all Weisskopf–Wigner theories of finite order exist as ordinary quantum theories on ordinary Hilbert spaces $\mathscr{H}_I$ and have strictly unitary time evolution operators $U_I(t)$, $t < \infty$. This implies in particular that in such theories the interaction of any finite number of states of the Dirac hydrogen atom with any bounded number of photons can never lead to divergencies. If an infrared catastrophe is banned by a small photon mass $\mu > 0$, Weisskopf–Wigner type theories of the interaction of an 'm-level atom', $m < \infty$, with any unbounded number of photons also exist and have strictly unitary time evolution operators. Some examples of novel applications of Weisskopf–Wigner type theories are given.

1. Introduction and discussion of results

The first successful attempt to obtain finite widths for emission lines of atoms was made by Weisskopf and Wigner (1930). Later it was believed (Low 1952, Källén 1958) that this theory leads to divergent line shifts related to the Lamb shift and this view has since been frequently stated (eg Ackerhalt *et al* 1973b, Louisell 1973). Consequently, a number of alternatives (Low 1952, Heitler and co-workers, in essence collected in Heitler 1954) have been worked out, based on perturbation theory with the removal of divergencies by renormalization techniques. We want to rehabilitate the original work of Weisskopf and Wigner by showing:

(i) Its 'basic idea', the 'important state hypothesis' (Källén 1958, Ernst and Stehle 1969), can be extended to a systematic, mathematically autonomous and self-reliant approximation scheme for the treatment of bound electrons with photons. This scheme, here called the Weisskopf–Wigner approximation (WWa), is equipped with its own hierarchy of orders which are *not* defined by powers of the coupling constant, but characterized by the property that the time evolution from $t = 0$ to any time $t < \infty$ in any (existing) WWa 'order' is described by a strictly unitary operator $U_I(t)$. The WWa is not restricted to the spontaneous emission processes which have mostly been treated up to now; it can also be used for cases with arbitrary numbers of incident photons which

can and must be described by finite, properly moving and spreading wavepackets. The 'lowest' (non-trivial) order of our WWa comprises the original Weisskopf–Wigner theory of spontaneous emission with a theory of resonance fluorescence with one incident photon.

(ii) To establish the—we believe, physically and mathematically most appealing—idea of the WWa we prove that any 'finite order' WWa *exists* under conditions which are always met when the atom is the Dirac hydrogen atom. This implies that WW type theories treating the interaction of any 'm-level atom', $m < \infty$, with any bounded number of photons will never lead to any infinities if the atomic eigenstates share certain properties, in essence the finite spatial extension, with the Dirac hydrogen atom.

(iii) If an 'infrared catastrophe' is banned by a small photon mass $\mu > 0$, the WW treatment of the interaction of any 'm-level atom', $m < \infty$, with any unbounded number of photons likewise will never lead to divergencies. Essential divergencies occur in WW theories, if at all, only by the inclusion of an infinite number of atomic states.

(iv) The existence of WWa does not affect the necessity of renormalization; it offers a chance for a novel, maybe more satisfying, form of it. We show, by an example (§ 5), how, in a certain Weisskopf–Wigner theory with an unbounded photon number, a 'bare', bound electron can 'dress' itself with bound(!), transverse(!) photons, thereby changing its 'state' as well as its eigen-energy. Since such dressing processes involve an unbounded number of photons, they could not be obtained in any finite order of perturbation theory.

(v) The use of the dipole (or similar) approximation(s) is strictly forbidden in Weisskopf–Wigner theories. We note without proof that the dipole approximation leaves calculated lifetimes practically untouched, but makes the line shifts, as given eg by Källén (1958), divergent, and the whole theory mathematically non-existent. Dangers arising from the dipole approximation have been noted earlier (Sauermann 1965, Ackerhalt *et al* 1973a, Moses 1973); its use is equivalent to the assumption of a 'pointlike' atom.

(vi) We note without proof: within finite order WW theories one may use perturbation expansions, but one *must* sum them up; otherwise the results in general will 'violate unitarity' by arbitrary amounts. In existing WW theories of infinite order the use of perturbation expansions is not, in general, allowed.

(vii) Weisskopf–Wigner theories owe their existence to a certain 'smoothness' and the finite spatial extension of atomic eigenstates and the inclusion of only a finite number of them. This means that the *electron* cannot propagate signals as required by strict causality. Signal propagation by *photons* is treated correctly in WW theories. In realistic cases the omitted electron retardation effects wash out strict causality by about 10^{-19} s.

(viii) We add, also without proof, that our existence theorems can be extended easily to all cases where $M < \infty$ non-overlapping 'm-level atoms' ($m < \infty$) interact with any number of photons. We thus obtain a wide base for various problems in modern 'super-radiance' and laser theory.

We demonstrate the principles of the WWa by the interaction of a Dirac one-electron atom with the transverse, quantized part of the electromagnetic field. In § 2 the corresponding equations of motion are 'derived', formally, from the usual non-existing operator expressions. The 'idea' of the WWa is described in § 3; there we also prove the existence of all finite order WWa. WW theories of infinite orders are treated in § 4 and in § 5, to illustrate the great flexibility of the WWa, we collect some interesting examples of WWa. Most of them have not been considered previously, to our knowledge.

2. Equations of motion for the interaction of a bound electron with the transverse electromagnetic field

To connect our work with the physical literature we first 'derive' the equations of motion in the usual formal way, thus introducing at least some necessary notation.

We consider a one-electron atom A, described by the Dirac equation for some given, stationary potential $V(\boldsymbol{x})$. Let $u_a(\boldsymbol{x})$ denote the normalized 'electron' eigensolutions to energy $E_a > 0$. The index $a \in Q_A$ comprises the quantum numbers which completely specify such an eigenstate; Q_A denotes the set of all these indices. By a suitable change of $V(\boldsymbol{x})$ at large distances we make the spectrum E_a discrete. This is inessential because in general we shall consider only finite sets of atomic states $u_a(\boldsymbol{x})$ which without loss can be identified with proper eigenstates. We subject this Dirac atom A to a process of second quantization by introducing for the electron field $\psi(\boldsymbol{x})$ in the Schrödinger picture the operator

$$\psi(\boldsymbol{x}) = \sum_{a \in Q_A} u_a(\boldsymbol{x}) b_a. \tag{1}$$

b_a 'annihilates an electron in the state $u_a(\boldsymbol{x})$' and satisfies with the corresponding creation operator $b_a^\dagger$ the usual Fermi anticommutation relations $[b_a, b_{a'}^\dagger]_+ = \delta_{aa'}$ etc. $\psi(\boldsymbol{x})$ 'acts' on the fermion Fock space $\mathscr{F}_A$ of the states

$$\sum_{\rho=0}^{\infty} \sum_{a_1 \in Q_A} \cdots \sum_{a_\rho \in Q_A} \alpha^{a_1 \ldots a_\rho} b_{a_1}^\dagger \ldots b_{a_\rho}^\dagger |v_e\rangle. \tag{2}$$

The $\alpha^{a_1 \ldots a_\rho}$ are antisymmetric c-number functions of the discrete variables $a_1, \ldots, a_\rho$ and are subject to the usual normalization conditions. $|v_e\rangle$ is the electron vacuum, defined by $b_a|v_e\rangle = 0$ for all a and $\langle v_e|v_e\rangle = 1$.

Since the scalar part of the Maxwell field has been already introduced as the c-number $V(\boldsymbol{x})$ and its longitudinal part is fixed by Coulomb gauge, we consequently quantize only its transverse part, the 'radiation field' R. The transverse part of the vector potential thus is given as the (Schrödinger) field operator

$$\boldsymbol{A}(\boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}^3\kappa \frac{\boldsymbol{\epsilon}(\kappa)}{(2\omega(\boldsymbol{k}))^{1/2}} (\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}} a_\kappa + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{x}} a_\kappa^\dagger) \tag{3}$$

where $\kappa = (\boldsymbol{k}, \lambda)$ comprises the continuous wavevector $\boldsymbol{k}$ and the discrete polarization indices $\lambda = 1, 2$ and $\int \mathrm{d}^3\kappa \ldots$ means integration over $\boldsymbol{k}$ *and* summation over λ. $\boldsymbol{\epsilon}(\boldsymbol{k}, \lambda)$ for $\lambda = 1, 2$ denotes two mutually orthogonal unit polarization vectors satisfying $\boldsymbol{\epsilon}(\boldsymbol{k}, \lambda)\boldsymbol{k} = 0$. a_κ and $a_\kappa^\dagger$ are the usual Bose annihilation and creation operators. $\omega(\boldsymbol{k})$ is defined as $(\mu^2 + \boldsymbol{k}^2)^{1/2}$ where $\mu \geqslant 0$ is a fictitious photon mass, introduced only to 'control' certain infrared problems. $\boldsymbol{A}(\boldsymbol{x})$ and all operators referring to R are formally defined on the space $\mathscr{F}_R$ of states of the form

$$\alpha_0|v_p\rangle + \sum_{n=1}^{\infty} \frac{1}{\sqrt{n!}} \int \mathrm{d}^3\kappa_1 \ldots \int \mathrm{d}^3\kappa_n \alpha_n(\kappa_1, \ldots, \kappa_n) a_{\kappa_1}^\dagger \ldots a_{\kappa_n}^\dagger |v_p\rangle. \tag{4}$$

$|v_p\rangle$ is the photon vacuum satisfying $a_\kappa|v_p\rangle = 0$, $\langle v_p|v_p\rangle = 1$, α_0 is some c-number and the $\alpha_n(\kappa_1, \ldots, \kappa_n)$ are Lebesgue square integrable c-number functions which are symmetric in the photon arguments $(\kappa_1, \ldots, \kappa_n)$. The scalar product $\langle\alpha|\alpha'\rangle$ on $\mathscr{F}_R$ is formally defined by applying the commutation relations in the usual way.

We couple A and R by assuming that the state space of the coupled system $A + R$ shall be the direct product $\mathscr{F}_A \otimes \mathscr{F}_R$ of the spaces $\mathscr{F}_A$ and $\mathscr{F}_R$, and that the coupling

hamiltonian density shall be the usual $eA(x)\psi^{\dagger}(x)\alpha\psi(x)$, where α is the Dirac vector. The total hamiltonian of $A+R$ thus shall be given by

$$H = \int \mathrm{d}^3\kappa\omega(\boldsymbol{k})a_\kappa^{\dagger}a_\kappa + \sum_{a\in Q_A} E_a b_a^{\dagger}b_a + e\int \mathrm{d}^3x A(x)\psi^{\dagger}(x)\alpha\psi(x), \tag{5}$$

to be understood as an operator on $\mathscr{F}_A \otimes \mathscr{F}_R$.

Equation (1) implies an extended important state hypothesis, namely the assumption that creation of electron–positron pairs plays no role in the theory to be constructed: we see that H commutes with the electron number operator $\Sigma_{a\in Q_A} b_a^{\dagger}b_a$, and so the number of electrons remains unchanged. This means that the time evolution of the system, if it exists, leaves the 'sections' $\mathscr{H}_A^{\rho} \otimes \mathscr{F}_R$ of $\mathscr{F}_A \otimes \mathscr{F}_R$ invariant, $\mathscr{H}_A^{\rho}$ being the ρ-electron subspace of $\mathscr{F}_A$. Therefore we lose nothing that has not been already lost by (1) if we consider only one electron, ie if we consider H only on the section $\mathscr{S} := \mathscr{H}_A^1 \otimes \mathscr{F}_R$ of $\mathscr{F}_A \otimes \mathscr{F}_R$. The considered states $|\alpha\rangle \in \mathscr{S}$ of $A+R$ thus are the vectors of the form

$$|\alpha\rangle = \sum_{a\in Q_A}\sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \int \mathrm{d}^3\kappa_1 \ldots \int \mathrm{d}^3\kappa_n \alpha_n^a(\kappa_1, \ldots, \kappa_n) a_{\kappa_1}^{\dagger} \ldots a_{\kappa_n}^{\dagger} b_a^{\dagger} |v_e\rangle |v_p\rangle. \tag{6}$$

The (one-electron) states of $A+R$ at different times t form a curve $|\alpha(t)\rangle$ in $\mathscr{S}$, determined by the Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\alpha(t)\rangle = H|\alpha(t)\rangle, \qquad |\alpha(t)\rangle \in \mathscr{S}, \tag{7}$$

and some initial condition at $t = 0$, say $|\alpha(0)\rangle = |\chi\rangle \in \mathscr{S}$. Equation (7) of course means a set of coupled equations of motion for the components $\alpha_n^a(t) := \alpha_n^a(\kappa_1, \ldots, \kappa_n; t)$ of $|\alpha(t)\rangle$. A somewhat tedious calculation shows that, with the atomic transition elements

$$M^*(a, b; \kappa) := \frac{e\epsilon(\kappa)}{[2\omega(\boldsymbol{k})(2\pi)^3]^{1/2}} \int \mathrm{d}^3x\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{x}} u_a^{\dagger}(x)\alpha u_b(x), \tag{8}$$

these purely c-number equations read explicitly:

$$\begin{aligned}
&\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) \\
&\quad = (\omega(\boldsymbol{k}_1) + \ldots + \omega(\boldsymbol{k}_n) + E_a)\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) \\
&\qquad + \sqrt{(n+1)} \sum_{b\in Q_A} \int \mathrm{d}^3\kappa M^*(a, b; \kappa)\alpha_{n+1}^b(\kappa, \kappa_1, \ldots, \kappa_n; t) \\
&\qquad + \frac{1}{\sqrt{n}} \sum_{\nu=1}^{n} \sum_{b\in Q_A} M(b, a; \kappa_\nu)\alpha_{n-1}^b(\kappa_1, \ldots, \kappa_{\nu-1}, \kappa_{\nu+1}, \ldots, \kappa_n; t).
\end{aligned} \tag{9}$$

These Schrödinger equations have to be solved simultaneously for all possible pairs $(a, n) \in Q_A \times \mathbb{N}_0 =: I_{\mathscr{S}}$ ($\mathbb{N}_0 = \{0, 1, 2, \ldots\}$) under the initial conditions

$$\alpha_n^a(\kappa_1, \ldots, \kappa_n; 0) = \chi_n^a(\kappa_1, \ldots, \kappa_n), \tag{10}$$

the χ_n^a being the components of any $|\chi\rangle \in \mathscr{S}$.

We prefer the Schrödinger picture to the Heisenberg picture because instead of nonlinear operator equations of motion on $\mathscr{F}_A \otimes \mathscr{F}_R$ here we have to solve only *linear* c number equations which in favourable situations can even be restricted to some

subspace, eg $\mathscr{S}$, of $\mathscr{F}_A \otimes \mathscr{F}_R$. In addition we may conceive approximations in dependence on the interesting initial state $|\chi\rangle$ and so even go into suitable subspaces of $\mathscr{S}$. All this is not possible in the Heisenberg picture because Heisenberg operators have the Schrödinger operators on $\mathscr{F}_A \otimes \mathscr{F}_R$ as initial values and so, in principle, solutions must hold on the whole state space $\mathscr{F}_A \otimes \mathscr{F}_R$.

The existence of solutions of (8) and (9), of course, depends on the integral kernels $M^*(a, b; \kappa)$. To get an idea of them we derive their decisive property. Since all $u_a(\boldsymbol{x})$ are square integrable, $u_b^\dagger(\boldsymbol{x})\alpha u_a(\boldsymbol{x})$ is absolutely integrable so that $\sqrt{(\omega(\boldsymbol{k}))}M(a, b; \kappa)$ is a uniformly continuous and thus bounded function of $\boldsymbol{k}$ which vanishes for large $|\boldsymbol{k}|$. If A is the Dirac hydrogen atom, the components of the spinor $u_a(\boldsymbol{x})$ (see eg Rose 1961) consist of a finite sum of terms of the form

$$CY_{l,m}(\vartheta, \varphi)r^{\gamma-1}\,\mathrm{e}^{-\lambda r}\sum_{i=0}^{L} c_i r^i \tag{11}$$

where $C, \lambda > 0$, γ, L, c_i are finite constants depending on a, (r, ϑ, φ) are the spherical coordinates of $\boldsymbol{x}$, and $Y_{l,m}(\vartheta, \varphi)$ is a spherical harmonic. In particular, for any a, $\gamma > 0$ satisfies an inequality

$$\gamma^2 \geqslant 1-(137, \ldots)^{-2}. \tag{12}$$

Therefore, $u_b^\dagger(\boldsymbol{x})\alpha u_a(\boldsymbol{x})$ for *any* $a, b \in Q_A$ will be even square integrable, and so the same holds for its Fourier transform $(\omega(\boldsymbol{k}))^{1/2}M(a, b; \kappa)$. But if $(\omega(\boldsymbol{k}))^{1/2}M(a, b; \kappa)$ is bounded at $\boldsymbol{k} = 0$ and square integrable, $M(a, b; \kappa)$ will also be square integrable, even for $\mu = 0$:

$$M(a, b; \kappa) \in \mathscr{L}^2(\mathbb{R}^3 \times \{1, 2\}) \qquad \text{for any } a, b \in Q_A. \tag{13}$$

This is the only property we shall need here.

We have checked relation (13) by a direct evaluation of the $M(a, b; \kappa)$ for all a, b of the Dirac hydrogen atom; we have found that for $|\boldsymbol{k}| \to \infty$ they fall off faster than required for square integrability. Similar calculations have also been done recently (Moses 1973) for the non-relativistic hydrogen atom.

3. The general idea of the Weisskopf–Wigner approximation (WWa) and the existence of finite order Weisskopf–Wigner theories

The formal solution $|\alpha(t)\rangle = \mathrm{e}^{-\mathrm{i}Ht}|\chi\rangle$ of (7) in practice does not help much, even if it should exist. We consider the WWa as a prospective method to 'derive information' from the equations of motion, maybe even to *define*, in a weaker sense than by the existence of the operator $\mathrm{e}^{-\mathrm{i}Ht}$, the solution of (7).

For this purpose we must first introduce some mathematical terminology. Let $\mathscr{H}_n^a$ denote the Hilbert space of the elements $\alpha_n^a = \alpha_n^a(\kappa_1, \ldots, \kappa_n)$, as introduced in § 2, the scalar product on $\mathscr{H}_n^a$ being defined by

$$\langle \alpha_n^a | \alpha_n'^a \rangle = \int \mathrm{d}^3\kappa_1 \ldots \int \mathrm{d}^3\kappa_n \alpha_n^{*a}(\kappa_1, \ldots, \kappa_n)\alpha_n'^a(\kappa_1, \ldots, \kappa_n). \tag{14}$$

The sector $\mathscr{S}$ can be understood as the orthogonal sum

$$\mathscr{S} = \bigoplus_{a \in Q_A} \bigoplus_{n=0}^{\infty} \mathscr{H}_n^a = \bigoplus_{(a,n) \in I\mathscr{S}} \mathscr{H}_n^a \tag{15}$$

with scalar product

$$\langle\alpha|\alpha'\rangle = \sum_{(a,n)\in I_{\mathscr{S}}} \langle\alpha_n^a|\alpha_n'^a\rangle. \tag{16}$$

For any finite or infinite subset of I of $I_{\mathscr{S}} = Q_A \times \mathbb{N}_0$ we define the Hilbert space

$$\mathscr{H}_I := \bigoplus_{(a,n)\in I} \mathscr{H}_n^a, \qquad \mathscr{H}_I \subset \mathscr{S}; \tag{17}$$

its elements $|\alpha_I\rangle$ consist of the sequence $\{\alpha_n^a, (a,n)\in I\}$ and the scalar product is given by

$$\langle\alpha_I|\alpha_I'\rangle = \sum_{(a,n)\in I} \langle\alpha_n^a|\alpha_n'^a\rangle. \tag{18}$$

The norm $\langle\alpha_I|\alpha_I\rangle^{1/2} \geqslant 0$ of a vector $|\alpha_I\rangle$ will be denoted by $\||\alpha_I\rangle\|$ and $|\alpha_I\rangle \in \mathscr{H}_I$ implies, as usual, $\||\alpha_I\rangle\| < \infty$.

The WW recipe for the construction of approximate solutions of (9), (10) consists of a simplification procedure Red(I) and a procedure Sum(I) which step by step 'corrects' the simplifications introduced by Red(I) and thus in a sense 'sums up' the WW 'expansion'.

Red(I) reads: '(i) Choose some I so that $|\chi\rangle \in \mathscr{H}_I$. It is obvious that any practically realizable initial condition $|\chi'\rangle$ can be approximated with any desired accuracy by a $|\chi\rangle$ which lies in one of the spaces $\mathscr{H}_I$. (ii) On the right-hand side of (9) put $\alpha_{n\pm1}^b(t) \equiv 0$ whenever $(b, n\pm1)\notin I$, and $\alpha_n^a(t) \equiv 0$, whenever $(a,n)\notin I$. (iii) Ignore all equations (9) where on the left-hand side stands an $(a,n)\notin I$.' The remaining 'reduced' equations of motion thus read

$$\begin{aligned}
&\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_n^a(\kappa_1,\ldots,\kappa_n;t) \\
&\quad = (\omega(\boldsymbol{k}_1)+\ldots+\omega(\boldsymbol{k}_n)+E_a)\alpha_n^a(\kappa_1,\ldots,\kappa_n;t) \\
&\qquad + \sum_{(b,n+1)\in I} \sqrt{(n+1)}\int \mathrm{d}^3\kappa M^*(a,b;\kappa)\alpha_{n+1}^b(\kappa,\kappa_1,\ldots,\kappa_n;t) \\
&\qquad + \sum_{(b,n-1)\in I} \frac{1}{\sqrt{n}} \sum_{\nu=1}^{n} M(b,a;\kappa_\nu)\alpha_{n-1}^b(\kappa_1,\ldots,\kappa_{\nu-1},\kappa_{\nu+1},\ldots,\kappa_n;t) \qquad (19) \\
&\qquad \alpha_n^a(\kappa_1,\ldots,\kappa_n;0) = \chi_n^a(\kappa_1,\ldots,\kappa_n)
\end{aligned}$$

and are to be solved simultaneously for all $(a,n)\in I$. Since on both sides appear only components of $|\alpha_I(t)\rangle$, by Red(I) we have reduced the 'exact' equations (9) for a curve $|\alpha(t)\rangle$ in $\mathscr{S}$ to a system of equations for the components of $|\alpha_I(t)\rangle \in \mathscr{H}_I \subset \mathscr{S}$. Equation (19) thus can be written in the form

$$\begin{aligned}
&\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\alpha_I(t)\rangle = H_I|\alpha_I(t)\rangle = (H_I^0 + H_I')|\alpha_I(t)\rangle \qquad (20) \\
&|\alpha_I(0)\rangle = |\chi\rangle
\end{aligned}$$

with H_I^0 defined as the multiplication operator $\alpha_n^a \to (\omega(\boldsymbol{k}_1)+\ldots+\omega(\boldsymbol{k}_n)+E_a)\alpha_n^a$ and H_I' as the integral and symmetrization operator given by the last two terms of (19).

Now let I be finite. Using the definition of Red(I) it is easily verified that $\langle\alpha_I|H_I'\alpha_I\rangle$ is *real* for any $|\alpha_I\rangle \in \mathscr{H}_I$ with $|\langle\alpha_I|H_I'\alpha_I\rangle| < \infty$; so H_I' is *symmetric* (or 'hermitean' in the physical nomenclature) on $\mathscr{H}_I$. Actually, if all $M(a,b;\kappa)$ occurring in (19) satisfy condition (13) we find $\|H_I'|\alpha_I\rangle\| < \infty$ for *any* $|\alpha_I\rangle \in \mathscr{H}_I$. So H_I' is defined *everywhere* on $\mathscr{H}_I$

and thus, by the Hellinger–Toeplitz theorem, it is bounded and self-adjoint (this actually is the mathematical point of the WWa). Since the multiplication operator H_I^0 is also a densely defined and self-adjoint, but not bounded, operator, the total hamiltonian H_I is also self-adjoint (eg Kato 1966, pp 190 and 278) on $\mathscr{H}_I$. It follows then by well established theorems of functional analysis (eg Kato 1966, p 483) that (for $t < \infty$ only!) there exists on $\mathscr{H}_I$ a strictly unitary time evolution operator

$$U_I(t) = \exp(-\mathrm{i}H_I t). \tag{21}$$

This means in particular that with square integrable atomic transition elements $M(a, b; \kappa)$ the Schrödinger equation (20) on $\mathscr{H}_I$ can always be solved uniquely (Kato 1966, p 481) with finite expressions for $|\alpha_I(t)\rangle$. If $|\chi\rangle$ is not from the domain of H_I^0 this solution of course must be constructed from 'neighbour solutions' in $\mathscr{H}_I$ by continuation by continuity. We emphasize that all this remains true for $\mu = 0$ as all the involved $M(a, b; \kappa)$ still satisfy (13).

When I is infinite, the existence of solutions of (19) cannot be proven so easily. A special case will be considered in § 4.

We now consider the convergence of the WWa, and its summation process Sum(I). Let $I = I_0 \subset I_1 \subset I_2 \subset \ldots$ be any sequence of subsets of $I_\mathscr{S}$ which tends to $I_\mathscr{S}$, ie which has the property that for any given (a, n) we can find a number $r_0 = r_0(a, n)$ such that $(a, n) \in I_r$ for $r \geqslant r_0$. The corresponding sequence of Hilbert spaces

$$\mathscr{H}_{I_0} \subset \mathscr{H}_{I_1} \subset \ldots$$

then in a sense tends to $\mathscr{S}$. Let us assume that the Schrödinger theories on $\mathscr{H}_{I_0}, \mathscr{H}_{I_1}, \ldots$ exist, as is the case with finite $I_0, I_1, \ldots$. We then get a sequence

$$U_{I_0}(t)|\chi\rangle, \qquad U_{I_1}(t)|\chi\rangle, \qquad \ldots \tag{22}$$

of solutions of approximate WW theories; if this sequence converges in $\mathscr{S}$, and if its limit is independent of the chosen $I_0, I_1, \ldots$, it is an excellent candidate for being the desired exact solution of (9). Since each element of the WW sequence (22) conserves the norm and scalar product, this limit, if it exists, will also conserve the norm and scalar product. We could also ask for a limit of the operators

$$U_{I_0}(t), \qquad U_{I_1}(t), \qquad \ldots \tag{23}$$

but this is obviously a much stronger requirement than the convergence of (22), which, from the physical point of view, is satisfactory already. Unfortunately not much is known about these convergence problems; some remarks are made in § 4.

Finally we introduce some convenient notation. The sequences $I \subset I_1 \subset \ldots$, $\mathscr{H}_I \subset \mathscr{H}_{I_1} \subset \ldots$ clearly define a well structured hierarchy of 'orders'. We therefore say that the WWa or WW theory obtained by Red(I_1) is of 'higher order' than the WW theory obtained by Red(I) if $I \subset I_1$. If I is finite (infinite), the corresponding WWa will be called 'of finite (infinite) order'. 'Lowest order' WW theories thus contain as few elements (a, n) as possible. The result of the considerations following (18) can be summed up by saying: *WW theories of finite order exist if and only if all involved atomic transition elements $M(a, b; \kappa)$ are square integrable.* The boundedness of the interaction hamiltonian obviously excludes the occurrence of *infinite* self-energy effects, but not the occurrence of such effects at all, see § 5.

4. On Weisskopf–Wigner theories of infinite order

The existence of a strong, unitary operator limit of (23) for $I_0, I_1, \ldots \to I_\mathscr{S}$ were practically equivalent to the existence of an exact operator theory on $\mathscr{S}$. This is unlikely to happen, because, despite (1), our interaction hamiltonian density in (5) is a product of three local field operators, as in relativistic quantum electrodynamics. But there remains at least some hope for the 'weaker' convergence of (22).

It is interesting, however, to localize these difficulties in the present theory: we show, that the inclusion of more and more photons does *not* lead to essential problems; it leads to no problems at all if an infrared catastrophe is banned by an arbitrary small photon mass $\mu > 0$. Essential divergencies in Weisskopf–Wigner type theories therefore arise solely, if at all, from the inclusion of *all* atomic states; we get finite results if only a finite number of atomic states $u_a(\boldsymbol{x})$ is allowed to interact with an arbitrary number of photons with $\mu > 0$. Theories of this type are interesting in quantum optics, eg for the interaction of an m-level atom with a coherent beam of light, because the latter allows no cut-off in the photon number.

For the above it is sufficient to look at the case in which I consists of all pairs $(a, n) \in I = Q \times \mathbb{N}_0$ where $Q \subset Q_A$ is some given, finite set of atomic indices. Then $\mathscr{H}_I$ is the orthogonal sum of a finite number of isomorphic Fock spaces $\mathscr{F}^a$, $a \in Q$, and the sums over $(b, n \pm 1) \in I$ in (19) become sums over $b \in Q$. The resulting WW theory then is of infinite order, in the sense of § 3. Using essentially a theorem of Rellich (eg Kato 1966, p 287) we show that for $\mu > 0$ the Hamilton operator $H_I = H_I^0 + H_I'$ is self-adjoint on $\mathscr{H}_I$ and thus, as in § 3, for $t < \infty$ generates a unique, unitary time evolution operator $U_I(t) = \exp(-\mathrm{i}H_I t)$. The sequences (22) thus remain existent also in infinite order WW theories of this type.

The multiplication operator H_I^0 with the dense domain

$$\mathscr{D}_I(H_I^0) = \{|\alpha_I\rangle, \|H_I^0|\alpha_I\rangle\| < \infty\}$$

is self-adjoint on $\mathscr{H}_I$. Because of $E_a > 0$ and $\omega(\boldsymbol{k}_1) + \ldots + \omega(\boldsymbol{k}_n) \geqslant \mu n$, for $\mu > 0$ we clearly have $\mathscr{D}_I(H_I^0) \subset \mathscr{D}_I(N) \subset \mathscr{H}_I$ and $\|H_I^0|\alpha_I\rangle\| \geqslant \mu\|N|\alpha_I\rangle\|$, where N is the photon number operator $\alpha_n^a \to n\alpha_n^a$ with domain $\mathscr{D}_I(N) = \{|\alpha_I\rangle, \|N|\alpha_I\rangle\| < \infty\}$.

We note an inequality which will be needed below. Let $(N+1)^{1/2}$ be the operator $\alpha_n^a \to \sqrt{(n+1)}\alpha_n^a$ with domain $\mathscr{D}_I((N+1)^{1/2}) \supset \mathscr{D}_I(N) \supset \mathscr{D}_I(H_I^0)$. Then for any

$$|\alpha_I\rangle \in \mathscr{D}_I(H_I^0)$$

and to any $\epsilon > 0$ there exists a number b', namely a $b' < \infty$ satisfying $b' > \max(1, (2\epsilon)^{-1})$ such that

$$\|(N+1)^{1/2}|\alpha_I\rangle\| \leqslant \epsilon\|N|\alpha_I\rangle\| + b'\||\alpha_I\rangle\| \leqslant \frac{\epsilon}{\mu}\|H_I^0|\alpha_I\rangle\| + b'\||\alpha_I\rangle\|. \tag{24}$$

Such an estimate has been used by Nelson (1964) in the case $\mathscr{H}_I = \mathscr{F}_R$. We prove it for our case. With $b' > 1$, $2\epsilon b' > 1$ we have

$$\begin{aligned}
&\|(N+1)^{1/2}|\alpha_I\rangle\|^2 \\
&\quad = \sum_{(a,n)\in I} (n+1)\|\alpha_n^a\|^2 < \sum_{(a,n)\in I} (\epsilon^2 n^2 + 2\epsilon b' n + b'^2)\|\alpha_n^a\|^2 \\
&\quad = \sum_{(a,n)\in I} \|(\epsilon n + b')\alpha_n^a\|^2 = \|(\epsilon N + b')|\alpha_I\rangle\|^2 \leqslant (\epsilon\|N|\alpha_I\rangle\| + b'\||\alpha_I\rangle\|)^2.
\end{aligned}$$

$\|\alpha_n^a\|$ denotes the norm of an element α_n^a of $\mathscr{H}_n^a$, in accordance with (14). The second inequality in (24) then follows from $\|H_I^0|\alpha_I\rangle\| \geqslant \mu\|N|\alpha_I\rangle\|$.

We now look at the interaction hamiltonian H_I'. By the triangle and the Schwarz inequality we get

$$\begin{aligned}\|H_I'|\alpha_I\rangle\|^2 &\leqslant \sum_{(a,n)\in I}\left[\sum_{b\in Q}\left(\|\sqrt{(n+1)}\int \mathrm{d}^3\kappa M^*(a,b;\kappa)\alpha_{n+1}^b(\kappa,*,\ldots,*)\| \right.\right.\\ &\qquad \left.\left.+\|\sqrt{n}M(b,a)\alpha_{n-1}^b\|\right)\right]^2\\ &\leqslant \sum_{(a,n)\in I}\left(\sum_{b\in Q} m(a,b)(\|\sqrt{n}\alpha_n^b\|+\|\sqrt{(n+1)}\alpha_n^b\|)\right)^2 \qquad (25)\end{aligned}$$

where $m(a,b)$ is the $\mathscr{L}^2$ norm of $M(a,b;\kappa)$. If $M(a,b;\kappa)$ for $a,b\in Q$ is square integrable, the first, the annihilation part of H_I', is well defined on $\mathscr{D}_I(N^{1/2})$. The creation part of H_I' is well defined on $\mathscr{D}_I((N+1)^{1/2}) \subset \mathscr{D}_I(N^{1/2})$ if and only if $m(a,b)<\infty$ for $a,b\in Q$. This implies that H_I' is well defined on the dense set

$$\mathscr{D}_I((N+1)^{1/2}) \subset \mathscr{D}_I(H_I') = \{|\alpha_I\rangle, \|H_I'|\alpha_I\rangle\| < \infty\}.$$

Further it is easily seen that $\langle\alpha_I|H_I'|\alpha_I\rangle$ is real so that H_I' is a symmetric operator on $\mathscr{H}_I$. With $\|\sqrt{n}\alpha_n^b\| < \|\sqrt{(n+1)}\alpha_n^b\|$ and further with the use of the Schwarz inequality we obtain for any $|\alpha_I\rangle \in \mathscr{D}_I((N+1)^{1/2})$:

$$\begin{aligned}\|H_I'|\alpha_I\rangle\|^2 &\leqslant 4\sum_{(a,n)\in I}\left(\sum_{b\in Q} m(a,b)\|\sqrt{(n+1)}\alpha_n^b\|\right)^2 \leqslant 4\left(\sum_{a,b\in Q} m^2(a,b)\right)\left(\sum_{(b,n)\in I}\|\sqrt{(n+1)}\alpha_n^b\|^2\right)\\ &= C^2\|(N+1)^{1/2}|\alpha_I\rangle\|^2. \qquad (26)\end{aligned}$$

By means of (24) we get

$$\|H_I'|\alpha_I\rangle\| \leqslant C\frac{\epsilon}{\mu}\|H_I^0|\alpha_I\rangle\| + Cb'\||\alpha_I\rangle\|. \qquad (27)$$

Choosing ϵ smaller than μC^{-1}, because of $\mathscr{D}_I(H_I') \supset \mathscr{D}_I((N+1)^{1/2}) \supset \mathscr{D}_I(N) \supset \mathscr{D}_I(H_I^0)$ we can satisfy the conditions of the theorem of Rellich, so that H_I is proved to be self-adjoint on $\mathscr{H}_I$.

5. Physical aspects of the Weisskopf–Wigner idea and some examples of unusual WW theories

The simplification of the 'exact' equations (9) to the approximate equations (19), and their 'correction' by going to the limits (22) or (23), if possible, are the essential ideas of the WWa. We emphasize in particular the great flexibility of this idea, characterized by the free choice of I, which allows its adaptation to various physical problems and permits the 'exploitation' of other 'smallnesses' than the coupling constant, such as energy barriers, approximate selection rules, etc. Indeed we frequently face a situation where from physical arguments we can hope that the tentative solution of (9) in essence will remain in some given Hilbert space $\mathscr{H}_I$ if initially it was in $\mathscr{H}_I$. The important state hypothesis of Weisskopf and Wigner is actually such an exploited approximate selection rule (see example 2). We give some examples where I is chosen by various arguments.

Example 1.

The greatest simplicity is achieved in the lowest order WWa, when I contains only one given element (a, n). Red(I) then reduces equation (9) to

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) = (\omega(\boldsymbol{k}_1) + \ldots + \omega(\boldsymbol{k}_n) + E_a)\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) \tag{28}$$

with the trivial solution describing n freely moving photons, in no way disturbed by the atom. The same trivial behaviour is obtained if I consists of pairs $(a, n_0 + 2\nu)$ with n_0 fixed and $\nu = 0, 1, 2, \ldots$.

Example 2.

If I contains two given elements we get non-trivial theories only if their photon numbers n differ by one, eg $I = \{(b, n), (a, n+1)\}$. This choice of I is 'natural' in situations where one can accept the important state hypothesis of Weisskopf and Wigner: that only two atomic states $u_b(\boldsymbol{x})$, $u_a(\boldsymbol{x})$, say with $E_b > E_a$, are 'important' for the interaction with photons, and that in a transition $u_b(\boldsymbol{x}) \rightleftarrows u_a(\boldsymbol{x})$ precisely one photon will be emitted or absorbed. The corresponding WWa equations of motion read

$$\begin{aligned}
&\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) \\
&\quad = (\omega(\boldsymbol{k}_1) + \ldots + \omega(\boldsymbol{k}_n) + E_a)\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) \\
&\qquad + \sqrt{(n+1)} \int \mathrm{d}^3\kappa M^*(a, b; \kappa)\alpha_{n+1}^b(\kappa, \kappa_1, \ldots, \kappa_n; t) \\
&\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\alpha_{n+1}^b(\kappa_1, \ldots, \kappa_{n+1}; t) \\
&\quad = (\omega(\boldsymbol{k}_1) + \ldots + \omega(\boldsymbol{k}_{n+1}) + E_b)\alpha_{n+1}^b(\kappa_1, \ldots, \kappa_{n+1}; t) \\
&\qquad + \frac{1}{\sqrt{(n+1)}} \sum_{\nu=1}^{n+1} M(a, b; \kappa_\nu)\alpha_n^b(\kappa_1, \ldots, \kappa_{\nu-1}, \kappa_{\nu+1}, \ldots, \kappa_{n+1}; t).
\end{aligned} \tag{29}$$

These equations are well suited eg for the analysis (to be given elsewhere) of directivity effects in the 'stimulated' emission of a photon under n simultaneously incident photons, or in resonance fluorescence with $n+1$ simultaneously incident photons. For $n = 0$ equations (29) are identical with the Schrödinger form of the original WW equations of motion as given by Källén (1958). As a curiosity we note that the $\{(b, n), (a, n+1)\}$ theory remains existent for $E_b < E_a$; it then leads to problems related with example 3.

Example 3.

Weisskopf–Wigner theories can also be used to attack certain self-energy problems of bound electrons. If we treat the atom as a 'one-level atom', but allow the photon number n to assume any value, we get a non-trivial theory with

$$I = \{(a, n), n = 0, 1, 2, \ldots\},$$

$\mathscr{H}_I = \mathscr{F}^a$ and the WW equations of motion

$$\begin{aligned} i\frac{d}{dt}\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) &= (\omega(\boldsymbol{k}_1) + \ldots + \omega(\boldsymbol{k}_n) + E_a)\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) \\ &\quad + \sqrt{(n+1)} \int d^3\kappa M^*(a, a; \kappa)\alpha_{n+1}^a(\kappa, \kappa_1, \ldots, \kappa_n; t) \\ &\quad + \frac{1}{\sqrt{n}} \sum_{\nu=1}^{n} M(a, a; \kappa_\nu)\alpha_{n-1}^a(\kappa_1, \ldots, \kappa_{\nu-1}, \kappa_{\nu+1}, \ldots, \kappa_n; t) \\ &\quad n = 0, 1, 2, \ldots . \end{aligned} \tag{30}$$

It is easily verified that the stationary, coherent state in $\mathscr{F}^a$,

$$\alpha_n^a(\kappa_1, \ldots, \kappa_n; t) = \exp[-i(E_a - \Delta_a)t](-1)^n \frac{\exp(-\frac{1}{2}\bar{n}_a)}{\sqrt{n!}} \frac{M(a, a; \kappa_1)}{\omega(\boldsymbol{k}_1)} \ldots \frac{M(a, a; \kappa_n)}{\omega(\boldsymbol{k}_n)} \tag{31}$$

with

$$\Delta_a = \int d^3\kappa \frac{|M(a, a; \kappa)|^2}{\omega(\boldsymbol{k})}, \qquad \bar{n}_a = \int d^3\kappa \frac{|M(a, a; \kappa)|^2}{\omega^2(\boldsymbol{k})} \tag{32}$$

is a solution of (30). Δ_a and $\bar{n}_a$ are finite for any state $u_a(\boldsymbol{x})$ of the Dirac atom even for $\mu = 0$; the example proves that the condition $\mu > 0$ of § 5 is not always necessary for the existence of finite results. Equation (31) clearly defines an eigensolution of the Schrödinger equation (30) to the eigenvalue $E_a - \Delta_a$; the interaction of the one-level atom with the radiation field thus *shifts the considered level of the atom* and modifies, in the sense of Friedrichs (1953), the ground state in $\mathscr{F}^a$ which no longer is the ordinary vacuum state $\alpha_n^a = \delta_{n0}$. In a similar way to the case when the radiation field interacts with a given, prescribed, *classical* source (Friedrichs 1953, Cook 1961), we express this by saying that the source 'dresses' itself with bound photons. But here the source consists of a prescribed quantum state $u_a(\boldsymbol{x})$ of the electron, and the dress consists of bound transverse(!) photons in a coherent state of the Fock space $\mathscr{F}^a$. We emphasize that Glauber's coherent states (Glauber 1963) are identical with Friedrichs' 'modified vacuum states' (Friedrichs 1953), namely the eigenstates of a_κ in $\mathscr{F}^a$.

It is interesting that, when applied to the $2S_{1/2}$–$2P_{1/2}$ states with due regard for their spin degeneracy, these shifts remove the $2S_{1/2}$–$2P_{1/2}$ energy degeneracy of the Dirac hydrogen atom by an amount which agrees to within 1% with the observed Lambshift. Such applications of the WW theory will be considered elsewhere.

Example 4.

Quite different WWa's of finite or infinite order are obtained if we assume that any finite or infinite number of atomic states $u_a(\boldsymbol{x})$, but only few photons, say $n = 0$ and $n = 1$, will be important. We then get

$$\begin{aligned} i\frac{d}{dt}\alpha_0^a(t) &= E_a\alpha_0^a(t) + \sum_{b \in Q} \int d^3\kappa M^*(a, b; \kappa)\alpha_1^b(\kappa; t) \\ i\frac{d}{dt}\alpha_1^b(\kappa; t) &= (\omega(\boldsymbol{k}) + E_b)\alpha_1^b(\kappa; t) + \sum_{a \in Q} M(a, b; \kappa)\alpha_0^a(t) \end{aligned} \tag{33}$$

where Q is some finite or infinite subset of Q_A.

This theory is important because, when *all* atomic states are included, its state space $\mathscr{H}_I$ contains all states which also occur in second-order perturbation treatments of self-energy effects (cf eg Heitler 1954). The choice of I is thus motivated by the smallness of the coupling constant, but we see here that this principle definitely violates physical self-consistency. A theory with all atomic states, but only few photons, 'provides room in its state space' for only a few photons in the final states. It therefore excludes the often more probable cascade transitions to the ground state as well as 'dressing processes' of the type of example 3, which frequently require many photons, but not necessarily much energy. It is also not self-consistent to include all one-electron states, say of energy greater than about 10^{20} electron–positron pair masses, but not to include even one single such pair.

It is one of the most prospective features of the WWa that it provides more or less 'natural' means to avoid such inconsistencies. The conservation of unitarity, though only on subspaces of $\mathscr{S}$, is another feature which favourably distinguishes the WWa from perturbation theory.

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