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A quantum theory of the self-energy of non-relativistic fermions and of the Coulomb–Yukawa force acting between them

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Abstract. The idea of the systematic Weisskopf–Wigner approximation as used sporadically in atomic physics and quantum optics, is extended here to the interaction of a field of non-relativistic fermions with a field of relativistic bosons. It is shown that the usual (non-existing) interaction Hamiltonian of this system can be written as a sum of a countable number of self-adjoint and bounded partial Hamiltonians. The system of these Hamiltonians defines the order hierarchy of our approximation scheme. To demonstrate its physical utility we show that in a certain order it provides us with a satisfactory quantum theory of the 'self-energy' of our fermions. This is defined as the binding energy of bosons bound to the fermions and building up the latter's 'individual Coulomb or Yukawa fields' in the sense of expectation values of the corresponding field operator. In states of more than one fermion the bound photons act as a mediating agent between the fermions; this mechanism closely resembles the Coulomb or Yukawa 'forces' used in conventional non-relativistic quantum mechanics.

1. Introduction

In the following we treat once more the old problem of the interaction of two quantised fields. We want to analyse the potentials of two ideas which in general have not yet been tested in quantum field theory, it seems.

Let us first describe the physical problem. We consider a 'Schrödinger field' S of non-relativistic, scalar fermions of mass $M>0$ and charge $-e<0$, called 'electrons'. Let $\psi(\boldsymbol{x}, t)$ and $\psi\dagger(\boldsymbol{x}, t)$ denote the Heisenberg operators of the field amplitudes of S which satisfy for any t the usual equal-time *anticommutation* relations

$$\{\psi(\boldsymbol{x}, t), \psi\dagger(\boldsymbol{y}, t)\} = \delta(\boldsymbol{x}-\boldsymbol{y}), \qquad \{\psi\dagger(\boldsymbol{x}, t), \psi\dagger(\boldsymbol{y}, t)\} = \{\psi(\boldsymbol{x}, t), \psi(\boldsymbol{y}, t)\} = 0. \tag{1a}$$

(Natural units $\hbar = c = 1$ are used throughout.) S shall interact with a 'radiation field' R of relativistic, scalar bosons each of mass $\mu \geqslant 0$, to be referred to as 'photons'. Let $E(\boldsymbol{x}, t)$ and $A(\boldsymbol{x}, t)$ be the Heisenberg operators of the canonical momentum and position amplitudes of R, respectively. They have the same dimensions as the electric field strength and the vector potential of electrodynamics and play an analogous role in the Hamilton formalism, hence the notation. We assume they satisfy for any t the equal-time *commutation* relations

$$[E(\boldsymbol{x}, t), A(\boldsymbol{y}, t)] = -\mathrm{i}\delta(\boldsymbol{x}-\boldsymbol{y}), \qquad [E(\boldsymbol{x}, t), E(\boldsymbol{y}, t)] = [A(\boldsymbol{x}, t), A(\boldsymbol{y}, t)] = 0. \tag{1b}$$

The 'mixed' equal-time commutators must vanish in all cases:

$$[\psi^\dagger(\boldsymbol{x}, t), E(\boldsymbol{y}, t)] = [\psi^\dagger(\boldsymbol{x}, t), A(\boldsymbol{y}, t)] = [\psi(\boldsymbol{x}, t), E(\boldsymbol{y}, t)] = [\psi(\boldsymbol{x}, t), A(\boldsymbol{y}, t)] = 0. \tag{1c}$$

S and R interact in the presence of a given, prescribed, static, integrable and square integrable, real 'charge density' $Zej(\boldsymbol{x})$, where Z is an arbitrary, real number and $j(\boldsymbol{x})$ satisfies $\int \mathrm{d}^3x j(\boldsymbol{x}) = 1$ if $Q := Ze \int \mathrm{d}^3x j(\boldsymbol{x}) \neq 0$. Z and $j(\boldsymbol{x})$ remain unspecified if $Q = 0$. The Heisenberg equations of motion of the interacting system (S, R, $Zj(\boldsymbol{x})$) are assumed to read

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi(\boldsymbol{x}, t) = \left(-\frac{\Delta}{2M} - eA(\boldsymbol{x}, t)\right)\psi(\boldsymbol{x}, t), \tag{2a}$$

$$(\Box - \mu^2)A(\boldsymbol{x}, t) = eZj(\boldsymbol{x}) - e\psi^\dagger(\boldsymbol{x}, t)\psi(\boldsymbol{x}, t) \tag{2b}$$

where $\Delta = \nabla^2$ is the Laplace operator and $\Box := \Delta - \partial^2/\partial t^2$. For $e = 0$ the system (S, R, $Zj(\boldsymbol{x})$) decays into independent subsystems S, R, $Zj(\boldsymbol{x})$ which are governed by the Schrödinger equation for free electrons, the Klein–Gordon equation for free photons, and $\mathrm{d}j(\boldsymbol{x})/\mathrm{d}t = 0$, respectively. We see from (2*b*) that for $e > 0$ the 'external' charge $Zj(\boldsymbol{x})$ as well as the electron field S play the role of 'sources' of the photon field R. Equation (2*a*) tells us that the position amplitude $A(\boldsymbol{x}, t)$ of R plays the role of 'potential' for the field S of electrons.

Formally, the equations (2) can be obtained as the Hamilton equations of motion corresponding to the Hamiltonian

$$\begin{aligned} H &= H(\psi^\dagger, \psi, E, A) \\ &:= \int \mathrm{d}^3x \psi^\dagger(\boldsymbol{x})\left(-\frac{\Delta}{2M}\right)\psi(\boldsymbol{x}) + \tfrac{1}{2}\int \mathrm{d}^3x [E(\boldsymbol{x})^2 + (\nabla A(\boldsymbol{x}))^2 + \mu^2 A(\boldsymbol{x})^2] \\ &\quad + e\int \mathrm{d}^3x [Zj(\boldsymbol{x}) - \psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x})]A(\boldsymbol{x}). \end{aligned} \tag{3}$$

H is a functional of the Schrödinger operators $\psi^\dagger(\boldsymbol{x}), \psi(\boldsymbol{x}), E(\boldsymbol{x}), A(\boldsymbol{x})$ of the corresponding field amplitudes which satisfy

$$\{\psi(\boldsymbol{x}), \psi^\dagger(\boldsymbol{y})\} = \delta(\boldsymbol{x} - \boldsymbol{y}), \qquad \{\psi^\dagger(\boldsymbol{x}), \psi^\dagger(\boldsymbol{y})\} = \{\psi(\boldsymbol{x}), \psi(\boldsymbol{y})\} = 0, \tag{4a}$$

$$[E(\boldsymbol{x}), A(\boldsymbol{y})] = -\mathrm{i}\delta(\boldsymbol{x} - \boldsymbol{y}), \qquad [E(\boldsymbol{x}), E(\boldsymbol{y})] = [A(\boldsymbol{x}), A(\boldsymbol{y})] = 0, \tag{4b}$$

$$[\psi^\dagger(\boldsymbol{x}), E(\boldsymbol{y})] = [\psi^\dagger(\boldsymbol{x}), A(\boldsymbol{y})] = [\psi(\boldsymbol{x}), E(\boldsymbol{y})] = [\psi(\boldsymbol{x}), A(\boldsymbol{y})] = 0. \tag{4c}$$

These operators are *given*, once and for all (cf § 2), and serve as 'initial values' of the corresponding Heisenberg operators. Therefore the equations (2) must be solved under the initial conditions

$$\psi^\dagger(\boldsymbol{x}, 0) = \psi^\dagger(\boldsymbol{x}), \qquad \psi(\boldsymbol{x}, 0) = \psi(\boldsymbol{x}), \qquad E(\boldsymbol{x}, 0) = E(\boldsymbol{x}), \qquad A(\boldsymbol{x}, 0) = A(\boldsymbol{x}). \tag{5}$$

Only this one particular solution of (2) can be considered as 'physical', provided that solutions exist at all. It is easy to write it down in a formal way. The expressions

$$\begin{aligned} \psi^\dagger(\boldsymbol{x}, t) &:= U^\dagger(t)\psi^\dagger(\boldsymbol{x})U(t), & \psi(\boldsymbol{x}, t) &:= U^\dagger(t)\psi(\boldsymbol{x})U(t), \\ E(\boldsymbol{x}, t) &:= U^\dagger(t)E(\boldsymbol{x})U(t), & A(\boldsymbol{x}, t) &:= U^\dagger(t)A(\boldsymbol{x})U(t) \end{aligned} \tag{6}$$

satisfy (1) and (2) if a unitary time evolution operator $U(t)$ exists which satisfies

$$i\frac{d}{dt}U(t)=HU(t), \qquad U(0)=1. \tag{7}$$

From the mathematical point of view we know (e.g., Kato 1966, p 478) that $U(t):=e^{-itH}$ exists if H is self-adjoint, and conversely, that a self-adjoint generator H exists if the unitary time evolution operator $U(t)$ exists (Stone's theorem, see e.g., Yosida 1968). However, it is probably futile to search for this ideal solution because H seems to be hopelessly non-existent as an operator on a Hilbert space. On the other hand we know that field theories contain 'a lot of truth'. This forces us to formulate some compromise, and it is in the tricky details of this compromise where we want to test the power of the ideas we are announcing initially.

The first idea consists of the introduction of an external *charge* $Zej(\boldsymbol{x})$ instead of an external *field*, e.g. the classical Coulomb–Yukawa field

$$V(\boldsymbol{x}):=-\frac{Ze}{4\pi}\int d^3x'\frac{j(\boldsymbol{x}')}{|\boldsymbol{x}-\boldsymbol{x}'|}\exp(-\mu|\boldsymbol{x}-\boldsymbol{x}'|) \tag{8}$$

of this charge. We show in an appendix that the present theory can be considered as a special case of *three* interacting quantum fields in which one field is degenerated so strongly that its quanta neither move nor show any reaction upon the quanta of the other fields. Such a theory leads immediately to external charges like $Zej(\boldsymbol{x})$, but not to external fields like $V(\boldsymbol{x})$. This difference is essential (cf §§ 3, 6, 8) because in connection with the second idea to be tested it allows us to suggest a solution of the self-energy problem for our electrons. It is fairly well known (e.g. Glauber 1951, Friedrichs 1953, Cook 1961) that an external charge 'dresses' itself with 'bound' (Cook 1961) photons in a coherent state (Friedrichs 1953, Glauber 1963a, b), this state being such that $V(\boldsymbol{x})$ is obtained as the expectation value of $A(\boldsymbol{x})$ in it (cf § 6). We show in § 7 that in a similar way also the *electrons* 'dress themselves with bound photons' which build up their 'individual Coulomb–Yukawa fields' in the sense of expectation values of $A(\boldsymbol{x})$ in the state of the bound photons. The binding energy of these photons is the self-energy of the electron (see § 10 for a comparison with other definitions). In addition, the photons bound to the electrons act as a mediating agent *between* any two electrons as well as between any electron and the external charge. This action resembles closely (§§ 7, 9) the conventional Coulomb–Yukawa 'force'. It is clear, however, that any bound photon is simultaneously bound to any electron as well as to the external charge. This simultaneous photon binding causes the 'binding of the electrons to the external charge' which means the formation of an 'atom'. We get a satisfactory 'screening' of the external charge by the electrons bound to it by means of bound photons (§ 8). In the case of a 'neutral' atom the usual infrared problem also disappears (§ 8).

However, these self-energy and binding effects obviously do not yet exhaust the set of *all* phenomena which are described by our model. Therefore they must be determined and classified in accordance with some 'ordering principle' which defines a classification scheme for the effects described by our model. This brings into play the second idea to be tested here, the use of the 'Weisskopf–Wigner approximation scheme' which has been systematised by Grimm and Ernst (1974, 1977) and Stelzer *et al* (1977) for the interaction of real atoms and real, transverse photons. We show that

the idea of this approximation scheme can be extended to our interacting fields (§§ 4, 5).

We proceed as follows. As H commutes with the electron number operator S (cf § 2) it 'decays' necessarily into a 'direct' sum (e.g. Achieser and Glasman 1968)

$$H = \bigoplus_{s=0}^{\infty} H^s \tag{9a}$$

of Hamiltonians H^s which act formally on the eigenspaces $\mathcal{H}^s$ of S for the eigenvalues $s = 0, 1, 2, \ldots$. This corresponds to the decomposition

$$\mathcal{H} = \bigoplus_{s=0}^{\infty} \mathcal{H}^s \tag{9b}$$

of the Hilbert space $\mathcal{H}$ of (S, R, $Zej(\boldsymbol{x})$) in terms of these eigenspaces. The sector $\mathcal{H}^s$ is basically the Hilbert space of the vectors which describe s electrons in any state in the presence of any number of photons in any state. H is self-adjoint on $\mathcal{H}$ if all H^s are self-adjoint on their sectors, but this can certainly not be hoped for. So we shall be content with the following mathematical surrogate.

We show first (§§ 3, 4) that any H^s can be written in the form

$$H^s = W^s(\bar{H}_0^s + \bar{H}_w^s)(W^s)^\dagger \tag{10}$$

where W^s is unitary on $\mathcal{H}^s$ for $\mu > 0$, and at least 'formally well defined and formally unitary' for $\mu = 0$ (cf § 6). It transforms from the conceptual level of external charges to the auxiliary level of external fields like $V(\boldsymbol{x})$ whose introduction is convenient. On this level $\bar{H}_0^s$ is an unbounded, but still self-adjoint operator, and $\bar{H}_w^s$ is the critical interaction Hamiltonian. The core of the Weisskopf–Wigner approach (cf Grimm and Ernst 1977) consists of the fact that $\bar{H}_w^s$ can be 'expanded' formally like

$$\bar{H}_w^s = \sum_{\rho=1}^{\infty} L_\rho^s \tag{11}$$

where each term L_ρ^s is a *self-adjoint* and even *bounded* 'partial interaction Hamiltonian' on $\mathcal{H}^s$. If Σ^s denotes any partial sum of a finite number of L_ρ^s, $\bar{H}_0^s + \Sigma^s$ is self-adjoint again. By including in Σ^s an increasing number of L_ρ^s we thus can 'gradually exhaust' the information contained in $\bar{H}_w^s$ without ever meeting any divergence. This allows us to *define* the auxiliary total Hamiltonian $\bar{H}_{ex}^s$ of the 'exact' theory as the potential limit of $\bar{H}_0^s + \Sigma^s$ as more and more terms are included in Σ^s.

We now have the prospect of two directions in which to continue. It is natural to analyse the convergence of the operator sequence $\bar{H}_0^s + \Sigma^s$ against the hypothetical 'exact' $\bar{H}_{ex}^s$. However, for practically the same reasons as discussed by Grimm and Ernst (1977), Stelzer *et al* (1977), and Ernst (1978) the potential results are hardly worth the effort that is probably needed to get them. The unrealistic features of our model also do not suggest we should do too much work in this direction. We prefer therefore an evaluation of the physical content of the theories which are defined by certain partial sums Σ^s. It is namely anything but trivial that these Σ^s define reasonable, 'natural' classes of physical phenomena which deserve attention and interest even if the convergence problems of (11) are not yet solved. The above self-energy and photon binding effects provide an example of such a class which is defined by one particular Σ^s (cf § 6). This proves that the 'expansion' (11) employs and reveals 'natural structures' which provide a natural classification scheme for the phenomena

described by the model. It allows us to reveal at least 'partial truths' about interacting fields which have not yet been obtained by any other method. In particular, it appears to offer the prospect of an alternative to perturbation theory (cf § 10).

The models of Nelson (1964), Fröhlich (1973), and Schroeck (1973, 1975) are the closest analogues of the present model, but they have been treated from quite different aspects. Our model resembles many features of the covariant Gupta–Bleuler form of quantum electrodynamics. An extension of the present formalism in that direction seems to be possible and work is in progress to this end.

2. State space and operators of the interacting fields S and R

We define first the general mathematical framework in which the problem of our interacting fields will be formulated.

It is well known that the anticommutation or commutation relations of a free Fermi or Bose field can be represented easily on corresponding Fermi or Bose Fock spaces which then serve as 'state spaces' of these physical systems. In our case this means that the Schrödinger operators $\psi^\dagger(\boldsymbol{x})$, $\psi(\boldsymbol{x})$ of S which satisfy (4*a*), are constructed on a Fermi Fock space $\mathscr{F}_S$ whereas the Schrödinger operators $E(\boldsymbol{x})$, $A(\boldsymbol{x})$ of R which satisfy (4*b*), are constructed on a Bose Fock space $\mathscr{F}_R$. Following first principles of quantum mechanics (see e.g. Jauch 1968) the state space $\mathscr{H}$ of the system (S, R) obtained by conceptually uniting the fields S and R, is the tensor product $\mathscr{H} := \mathscr{F}_S \otimes \mathscr{F}_R$ of the state spaces of the 'isolated' systems S and R. This holds independently of their potential interaction, and independently of this we also require the mixed commutation relations (4*c*). We show in the appendix that these requirements remain reasonable in the presence of an external charge $Zj(\boldsymbol{x})$.

As far as possible, all operators of (S, R, $Zj(\boldsymbol{x})$) should be defined on $\mathscr{H}$. Therefore we begin the discussion with the construction of a realisation of $\mathscr{H}$. For this we consider first the set $\mathscr{V}$ of double sequences

$$\alpha := \{\alpha(X^s; K^n);\ n, s = 0, 1, 2, \dots\} \tag{12}$$

of 'components $\alpha(X^s; K^n)$ of α' with the following properties: X^0, K^0 stand for the empty sets $\varnothing$, $\varnothing$ and $\alpha(X^0; K^0) := \alpha(\varnothing; \varnothing)$ is a complex number. K^n is short for the set $\boldsymbol{k}_1, \dots, \boldsymbol{k}_n$ of n photon variables $\boldsymbol{k}_\nu \in \mathbb{R}^3$, $\nu = 1, \dots, n$. $\alpha(X^0; K^n) := \alpha(\varnothing; \boldsymbol{k}_1, \dots, \boldsymbol{k}_n)$ is for any $n \geqslant 1$ a complex valued, *symmetric* function of the $\boldsymbol{k}_\nu$ which is defined almost everywhere (AE) on an $\mathbb{R}^{3n}$. X^s is short for the set $\boldsymbol{x}_1, \dots, \boldsymbol{x}_s$ of $s \geqslant 1$ electron variables $\boldsymbol{x}_\sigma \in \mathbb{R}^3$, $\sigma = 1, \dots, s$. $\alpha(X^s; K^0) := \alpha(\boldsymbol{x}_1, \dots, \boldsymbol{x}_s; \varnothing)$ is for any $s \geqslant 1$ an *antisymmetric*, complex-valued function of the $\boldsymbol{x}_\sigma$ which is defined AE on an $\mathbb{R}^{3s}$. Finally, $\alpha(X^s; K^n) := \alpha(\boldsymbol{x}_1, \dots, \boldsymbol{x}_s; \boldsymbol{k}_1, \dots, \boldsymbol{k}_n)$ is for $s \geqslant 1$, $n \geqslant 1$ a complex-valued function of the $\boldsymbol{x}_\sigma$ and the $\boldsymbol{k}_\nu$ which is antisymmetric in the $\boldsymbol{x}_\sigma$, symmetric in the $\boldsymbol{k}_\nu$, and defined AE on $\mathbb{R}^{3s} \times \mathbb{R}^{3n}$. We make a linear vector space of $\mathscr{V}$ by defining the sum $\alpha + \alpha'$ of two elements by $(\alpha + \alpha')(X^s; K^n) := \alpha(X^s; K^n) + \alpha'(X^s; K^n)$ and the product $c\alpha$ of $\alpha \in \mathscr{V}$ with $c \in \mathbb{C}$ by $(c\alpha)(X^s; K^n) := c\alpha(X^s; K^n)$, both of course for any $s, n = 0, 1, 2, \dots$. We shall frequently have to deal with quantities which are defined only on $\mathscr{V}$ which is not a Hilbert space.

Consider now elements $\alpha \in \mathscr{V}$ with the following properties: $\alpha(X^0; K^0)$ as above, $\alpha(X^0; K^n)$ *square integrable* in the $\boldsymbol{k}_\nu$ in the elementary Lebesgue sense on $\mathbb{R}^{3n}$ (if

nothing else is stated explicitly, all integrals occurring in this work are to be understood in this sense), $\alpha(X^s; K^0)$ square integrable in the $\boldsymbol{x}_\sigma$ on $\mathbb{R}^{3s}$, and $\alpha(X^s; K^n)$ square integrable on $\mathbb{R}^{3s} \times \mathbb{R}^{3n}$ for any $s \geq 1$, $n \geq 1$. The components $\alpha(X^s; K^n)$ of α are now elements of well defined Hilbert spaces $\mathcal{H}^{sn}$ of square integrable functions or of the trivial Hilbert space $\mathcal{H}^{00} = \mathbb{C}$. We take $\mathcal{H}^{sn}$ as the representative of the abstract Hilbert space $\mathcal{H}_S^s \otimes \mathcal{H}_R^n$ of a system of s electrons and n photons. A realisation of the Hilbert space $\mathcal{H} = \mathcal{F}_S \otimes \mathcal{F}_R$ of our system (S, R, $Zj(\boldsymbol{x})$) is defined as the direct sum

$$\mathcal{H} := \bigoplus_{s=0}^{\infty} \bigoplus_{n=0}^{\infty} \mathcal{H}^{sn} = \left(\bigoplus_{s=0}^{\infty} \mathcal{H}_S^s \right) \otimes \left(\bigoplus_{n=0}^{\infty} \mathcal{H}_R^n \right) = \mathcal{F}_S \otimes \mathcal{F}_R. \tag{13a}$$

This means that $\mathcal{H}$ is the subset of all $|\alpha\rangle \in \mathcal{V}$ which satisfy

$$\| |\alpha\rangle \|^2 := \sum_{s=0}^{\infty} \sum_{n=0}^{\infty} \| \alpha(X^s; K^n) \|^2 < \infty, \tag{13b}$$

with $\| \ldots \|$ denoting the usual norm on $\mathcal{H}^{sn}$. The Dirac ket bracket $| \ldots \rangle$ is restricted to elements of $\mathcal{H}$. In terms of these quantities the s-electron sectors $\mathcal{H}^s$ in (9b) are given as the Hilbert spaces

$$\mathcal{H}^s := \bigoplus_{n=0}^{\infty} \mathcal{H}^{sn} = \mathcal{H}_S^s \otimes F_R. \tag{14}$$

In general we shall not distinguish between abstract Hilbert spaces and their particular realisations.

We consider now the operators to be used. Following Friedrichs (1953) we formally define $\psi(\boldsymbol{x})$ and $\psi^\dagger(\boldsymbol{x})$ by

$$(\psi(\boldsymbol{x})\alpha)(X^s; K^n) := (s+1)^{1/2} \alpha(\boldsymbol{x}, X^s; K^n), \tag{15a}$$

$$(\psi^\dagger(\boldsymbol{x})\alpha)(X^s; K^n) := \frac{1}{s^{1/2}} \sum_{\sigma=1}^{s} (-1)^\sigma \delta(\boldsymbol{x} - \boldsymbol{x}_\sigma) \alpha(X^s \backslash \boldsymbol{x}_\sigma; K^n) \tag{15b}$$

for any $s \geq 0$, $n \geq 0$. $(\boldsymbol{x}, X^s)$ is short for the set $(\boldsymbol{x}, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_s)$ of $s+1$ electron variables and $(X^s \backslash \boldsymbol{x}_\sigma)$ for the set $(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\sigma-1}, \boldsymbol{x}_{\sigma+1}, \ldots, \boldsymbol{x}_s)$. The right-hand side of (15b) is zero for $s = 0$. It poses no problems to show that these operators satisfy (4a). They are defined only as distributions on $\mathcal{V}$, but certain functionals of them may lead to well-defined operators on $\mathcal{H}$. For example, if in the first expression

$$S := \int \mathrm{d}^3 x \psi^\dagger(\boldsymbol{x}) \psi(\boldsymbol{x}) := \bigoplus_{s=0}^{\infty} s \tag{16}$$

for the operator S of the number of electrons we first apply $\psi(\boldsymbol{x})$ as defined by (15a), then $\psi^\dagger(\boldsymbol{x})$ as defined in (15b), then integrate over all $\boldsymbol{x}$, we obtain $(S\alpha)(X^s; K^n) = s\alpha(X^s; K^n)$. In agreement with this we may finally define S as the direct sum of the operators of multiplication with the numbers s as indicated by the last expression for S. This decomposition corresponds of course to the decomposition (9b) of $\mathcal{H}$.

Using the similar symbols $(\boldsymbol{k}, K^n) := (\boldsymbol{k}, \boldsymbol{k}_1, \ldots, \boldsymbol{k}_n)$, $(K^n \backslash \boldsymbol{k}_\nu) := (\boldsymbol{k}_1, \ldots, \boldsymbol{k}_{\nu-1}, \boldsymbol{k}_{\nu+1}, \ldots, \boldsymbol{k}_n)$ we define photon annihilation and creation operators $a(\boldsymbol{k})$, $a^\dagger(\boldsymbol{k})$ by

$$(a(\boldsymbol{k})\alpha)(X^s; K^n) := (n+1)^{1/2} \alpha(X^s; \boldsymbol{k}, K^n), \tag{17a}$$

$$(a^\dagger(\boldsymbol{k})\alpha)(X^s; K^n) := \frac{1}{n^{1/2}} \sum_{\nu=1}^{n} \delta(\boldsymbol{k} - \boldsymbol{k}_\nu) \alpha(X^s; K^n \backslash \boldsymbol{k}_\nu). \tag{17b}$$

These operators satisfy by definition the usual commutation relations $[a(\boldsymbol{k}), a^{\dagger}(\boldsymbol{k}')] = \delta(\boldsymbol{k}-\boldsymbol{k}')$ etc. We use them and the abbreviation $\omega(\boldsymbol{k}) := (\boldsymbol{k}^2+\mu^2)^{1/2}$ to define formally the Sehrödinger operators of the field amplitudes of R by

$$E(\boldsymbol{x}) := -\frac{\mathrm{i}}{(2\pi)^{3/2}} \int \mathrm{d}^3k (\tfrac{1}{2}\omega(\boldsymbol{k}))^{1/2} (\mathrm{e}^{\mathrm{i}\boldsymbol{k}.\boldsymbol{x}} a(\boldsymbol{k}) - \mathrm{e}^{-\mathrm{i}\boldsymbol{k}.\boldsymbol{x}} a^{\dagger}(\boldsymbol{k})), \tag{18a}$$

$$A(\boldsymbol{x}) := \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}^3k \frac{1}{(2\omega(\boldsymbol{k}))^{1/2}} (\mathrm{e}^{\mathrm{i}\boldsymbol{k}.\boldsymbol{x}} a(\boldsymbol{k}) + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}.\boldsymbol{x}} a^{\dagger}(\boldsymbol{k})). \tag{18b}$$

These operators satisfy of course (4*b*) and (4*c*), the latter together with (15). If, as above, we understand (18) as prescriptions to apply on an arbitrary $|\alpha\rangle \in \mathscr{H}$ first (17), then multiply by the functions $e^{\pm \mathrm{i}\boldsymbol{k}.\boldsymbol{x}}$, subtract or add the results, multiply by the functions of $\omega(\boldsymbol{k})$ indicated, integrate over $\boldsymbol{k}$, and finally multiply by the numbers in front of the integrals, we get unique expressions for $E(\boldsymbol{x})|\alpha\rangle$, $A(\boldsymbol{x})|\alpha\rangle$. However, they are in general not elements of $\mathscr{H}$, but only well defined elements of $\mathscr{V}$. This holds at least for a dense set of $|\alpha\rangle \in \mathscr{H}$, and this is sufficient to carry out unique and meaningful algebraic procedures with $E(\boldsymbol{x})$, $A(\boldsymbol{x})$.

Introducing now the abbreviation

$$\tilde{j}(\boldsymbol{k}) := \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}^3x \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}.\boldsymbol{x}} j(\boldsymbol{x}) \tag{19}$$

and 'computing' in the above sense the Hamiltonian H we find

$$\begin{aligned}(H\alpha)(X^s; K^n) = {} & (\omega(\boldsymbol{k}_1)+\ldots+\omega(\boldsymbol{k}_n))\alpha(X^s; K^n) - \frac{1}{2M}(\Delta_1+\ldots+\Delta_s)\alpha(X^s; K^n) \\ & + Ze\Big((n+1)^{1/2} \int \mathrm{d}^3k \frac{\tilde{j}(\boldsymbol{k})^*}{(2\omega(\boldsymbol{k}))^{1/2}} \alpha(X^s; \boldsymbol{k}, K^n) \\ & + \frac{1}{n^{1/2}} \sum_{\nu=1}^{n} \frac{\tilde{j}(\boldsymbol{k}_\nu)}{(2\omega(\boldsymbol{k}_\nu))^{1/2}} \alpha(X^s; K^n \backslash \boldsymbol{k}_\nu)\Big) \\ & - \frac{e}{(2\pi)^{3/2}} \sum_{\sigma=1}^{s} \Big((n+1)^{1/2} \int \mathrm{d}^3k \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{k}.\boldsymbol{x}_\sigma}}{(2\omega(\boldsymbol{k}))^{1/2}} \alpha(X^s; \boldsymbol{k}, K^n) \\ & + \frac{1}{n^{1/2}} \sum_{\nu=1}^{n} \frac{\mathrm{e}^{-\mathrm{i}\boldsymbol{k}_\nu.\boldsymbol{x}_\sigma}}{(2\omega(\boldsymbol{k}_\nu))^{1/2}} \alpha(X^s; K^n \backslash \boldsymbol{k}_\nu)\Big).\end{aligned} \tag{20}$$

The sums over σ and ν are to be understood as zero for $s = 0$ and $n = 0$, respectively. The usual zero-point energy has been omitted.

Equation (20) shows explicitly that the sectors $\mathscr{H}^s$ of $\mathscr{H}$ are invariant under H. So we can indeed write H in the form (9*a*) with H^s now *defined* by the right-hand side of (20), i.e. by $(H^s\alpha)(X^s; K^n) = (H\alpha)(X^s; K^n)$ for any $\alpha \in \mathscr{H}^s$. We note further that if $\tilde{j}(\boldsymbol{k})/(2\omega(\boldsymbol{k}))^{1/2}$ is integrable on $\mathbb{R}^3$, a condition which is satisfied in practically any case of interest, then $(H^s\alpha)(X^s; K^n)$ is an AE defined function of X^s, K^n for a dense set of $\alpha \in \mathscr{H}^s$. So we have $H^s\alpha \in \mathscr{V}$, but $H^s\alpha \notin \mathscr{H}^s$ for any $\alpha \in \mathscr{H}^s$, $\alpha \neq 0$. This is the origin of the divergence problems of the present field theory. Writing H in the form (20) does of course not solve these problems, but it allows more insight into their nature and thus permits 'physically motivated attacks' upon them.

3. Transition from 'external charges' to 'external fields'

For an appreciable part of this work it will be convenient to argue on the conceptual level of external fields though finally we must return to the 'true' level of external charges. We now discuss the relations between these conceptual levels.

For this we note that the operator H_j^s defined by the first and the third terms on the right-hand side of (20), can be written in the form

$$H_j^s = \int \mathrm{d}^3k\Big(\omega(\boldsymbol{k})a^+(\boldsymbol{k})a(\boldsymbol{k}) + \frac{Ze\tilde{j}(\boldsymbol{k})^*}{(2\omega(\boldsymbol{k}))^{1/2}}a(\boldsymbol{k}) + \frac{Ze\tilde{j}(\boldsymbol{k})}{(2\omega(\boldsymbol{k}))^{1/2}}a^+(\boldsymbol{k})\Big). \tag{21a}$$

Here the a's are understood to be defined by (17) for fixed s, i.e. on $\mathscr{H}^s$ only. The first term H_{p}^s alone defines a self-adjoint operator on $\mathscr{H}^s$. Considered alone the last two terms define a self-adjoint operator on $\mathscr{H}^s$ if and only if $\tilde{j}(\boldsymbol{k})/(2\omega(\boldsymbol{k}))^{1/2}$ is square integrable. The proof of this is a verbal repetition of the proof of Cook (1961) where H_j^s is considered on a Fock space. If H_j^s itself is to be self-adjoint, $\tilde{j}(\boldsymbol{k})$ must satisfy further conditions. It is suggestive to write it in the form

$$H_j^s = \int \mathrm{d}^3k\omega(\boldsymbol{k})(a^+(\boldsymbol{k}) + f(\boldsymbol{k})^*)(a(\boldsymbol{k}) + f(\boldsymbol{k})) - E_j^{\mathrm{B}} \tag{21b}$$

with the abbreviations

$$f(\boldsymbol{k}) := Ze\tilde{j}(\boldsymbol{k})/(2\omega(\boldsymbol{k})^{3/2}, \tag{22}$$

$$E_j^{\mathrm{B}} := Z^2e^2\int \mathrm{d}^3k|\tilde{j}(\boldsymbol{k})|^2/2\omega(\boldsymbol{k})^2. \tag{23}$$

The 'completion of the square' is legitimate (Cook 1961) if E_j^{B} is finite and $f(\boldsymbol{k})$ square integrable. In the latter case the unitary Weyl operator

$$\mathrm{W}^s\{\mathrm{f}(\mathbf{k})\} := \exp\Big(\int \mathrm{d}^3k(f(\boldsymbol{k})a^+(\boldsymbol{k}) - f(\boldsymbol{k})^*a(\boldsymbol{k}))\Big) \tag{24}$$

exists on $\mathscr{H}^s$ and satisfies on $\mathscr{H}^s$ the relations

$$\begin{aligned} a(\boldsymbol{k})W^s\{f(\boldsymbol{k})\} &= W^s\{f(\boldsymbol{k})\}(a(\boldsymbol{k}) + f(\boldsymbol{k})), \\ a^+(\boldsymbol{k})W^s\{f(\boldsymbol{k})\} &= W^s\{f(\boldsymbol{k})\}(a^+(\boldsymbol{k}) + f(\boldsymbol{k})^*). \end{aligned} \tag{25}$$

In terms of the quantities introduced we can write

$$H_j^s = W^s\{-f(\boldsymbol{k})\}(-E_j^{\mathrm{B}} + H_{\mathrm{p}}^s)W^s\{f(\boldsymbol{k})\}. \tag{21c}$$

We learn that H_j^s is self-adjoint if $W\{f(\boldsymbol{k})\}$ is unitary, i.e. $f(\boldsymbol{k})$ square integrable, and E_j^{B} finite.

It appears natural to extend the form (21c) of H_j^s to the total Hamiltonian H^s on $\mathscr{H}^s$, i.e. to introduce another Hamiltonian $\tilde{H}^s$ so that

$$H^s = W^s\{-f(\boldsymbol{k})\}\tilde{H}^sW^s\{f(\boldsymbol{k})\}. \tag{26}$$

If $f(\boldsymbol{k})$ is square integrable the operator

$$W\{f(\boldsymbol{k})\} := \bigoplus_{s=0}^{\infty} W^s\{f(\boldsymbol{k})\} \tag{27}$$

is unitary on $\mathscr{H}$ and we can extend (26) even to $\mathscr{H}$ by introducing the auxiliary operator

$$\bar{H} = W\{f(\boldsymbol{k})\}HW\{-f(\boldsymbol{k})\} = \bigoplus_{s=0}^{\infty} \bar{H}^s. \tag{28}$$

Applying this to (3) and using essentially only (25) we find

$$\begin{aligned}\bar{H} = &\int \mathrm{d}^3x\psi^\dagger(\boldsymbol{x})\Big(-\frac{\Delta}{2M}\Big)\psi(\boldsymbol{x})\\ &+\tfrac{1}{2}\int \mathrm{d}^3x(E(\boldsymbol{x})+E'(\boldsymbol{x}))^2+(\nabla A(\boldsymbol{x})+\nabla A'(\boldsymbol{x}))^2+\mu^2(A(\boldsymbol{x})+A'(\boldsymbol{x}))^2\\ &+e\int \mathrm{d}^3x(Zj(\boldsymbol{x})-\psi^\dagger(\boldsymbol{x})\psi(\boldsymbol{x}))(A(\boldsymbol{x})+A'(\boldsymbol{x})).\end{aligned} \tag{29a}$$

$E'(\boldsymbol{x})$, $A'(\boldsymbol{x})$ are the c-number functions obtained by replacing in (18) the operators $a(\boldsymbol{k})$ by $-f(\boldsymbol{k})$ and $a^\dagger(\boldsymbol{k})$ by $-f(\boldsymbol{k})^*$. We show in § 6 that this means $A'(\boldsymbol{x}) = V(\boldsymbol{x})$ (cf (8)). We further find the identities

$$\int \mathrm{d}^3x[E'(\boldsymbol{x})E(\boldsymbol{x})+(\nabla A'(\boldsymbol{x}))(\nabla A(\boldsymbol{x}))+\mu^2A'(\boldsymbol{x})A(\boldsymbol{x})] = -Ze\int \mathrm{d}^3xA(\boldsymbol{x})j(\boldsymbol{x}), \tag{30a}$$

$$\tfrac{1}{2}\int \mathrm{d}^3x[E'(\boldsymbol{x})^2+(\nabla A'(\boldsymbol{x}))^2+\mu^2A'(\boldsymbol{x})^2] = \int \mathrm{d}^3k\omega(\boldsymbol{k})|f(\boldsymbol{k})|^2 = E_j^{\mathrm{B}}, \tag{30b}$$

$$Ze\int \mathrm{d}^3xj(\boldsymbol{x})A'(\boldsymbol{x}) = -2E_j^{\mathrm{B}}. \tag{30c}$$

Inserting this into (29a) we get

$$\begin{aligned}\bar{H} = &\int \mathrm{d}^3x\psi^\dagger(\boldsymbol{x})\Big(-\frac{\Delta}{2M}-eV(\boldsymbol{x})\Big)\psi(\boldsymbol{x})-E_j^{\mathrm{B}}\\ &+\tfrac{1}{2}\int \mathrm{d}^3x[E(\boldsymbol{x})^2+(\nabla A(\boldsymbol{x}))^2+\mu^2A(\boldsymbol{x}^2)]-e\int \mathrm{d}^3x\psi^\dagger(\boldsymbol{x})A(\boldsymbol{x})\psi(\boldsymbol{x}).\end{aligned} \tag{29b}$$

The external charge $Zej(\boldsymbol{x})$ has disappeared. Instead of it we now have the external potential $V(\boldsymbol{x})$ and the irrelevant constant $-E_j^{\mathrm{B}}$.

For the remainder it will be convenient also to write $\bar{H}$ as a direct sum of operators $\bar{H}^s$ acting on the sectors $\mathscr{H}^s$ (cf (28)). Using the same methods as in the derivation of (20) we find

$$\begin{aligned}&(\bar{H}^s\alpha)(X^s;K^n)\\ &\quad=(\omega(\boldsymbol{k}_1)+\ldots+\omega(\boldsymbol{k}_n)-E_j^{\mathrm{B}})\alpha(X^s;K^n)\\ &\quad+\Big[\Big(-\frac{\Delta_1}{2M}-eV(\boldsymbol{x}_1)\Big)+\ldots+\Big(-\frac{\Delta_s}{2M}-eV(\boldsymbol{x}_s)\Big)\Big]\alpha(X^s;K^n)\\ &\quad-\frac{e}{(2\pi)^{3/2}}\sum_{\sigma=1}^{s}\Big((n+1)^{1/2}\int \mathrm{d}^3k\frac{\mathrm{e}^{\mathrm{i}\boldsymbol{k}.\boldsymbol{x}_\sigma}}{(2\omega(\boldsymbol{k}))^{1/2}}\alpha(X^s;\boldsymbol{k},K^n)\\ &\quad+\frac{1}{n^{1/2}}\sum_{\nu=1}^{n}\frac{\mathrm{e}^{-\mathrm{i}\boldsymbol{k}_\nu.\boldsymbol{x}_\sigma}}{(2\omega(\boldsymbol{k}_\nu))^{1/2}}\alpha(X^s;K^n\backslash\boldsymbol{k}_\nu)\Big).\end{aligned} \tag{31}$$

The same is obtained by applying (26) immediately to (20). In particular, we have omitted the same zero-point energy.

4. The fine grain Weisskopf–Wigner expansion

In § 3 we have verified the form $W^s(\bar{H}_0^s + \bar{H}_w^s)(W^s)^\dagger$ of H^s as announced in (10), $\bar{H}_0^s$ being defined by the first and second terms, $\bar{H}_w^s$ by the last term on the right-hand side of (31). In comparison with the familiar forms (29*b*) or (3) of $\bar{H}$ or H, the respective expressions (31) or (20) may appear clumsy and complicated. But they exhibit more mathematical structure and thus allow the use of methods of functional analysis which are now employed to verify our statements on the 'fine grain' Weisskopf–Wigner expansion (11), the mathematical core of this work.

For this it will be convenient to introduce other representatives of the states of the system (S, R, $Zj(\boldsymbol{x})$) than used up to now. Consider the stationary Schrödinger equation

$$\left(-\frac{\Delta}{2M} - eV(\boldsymbol{x})\right)u_a(\boldsymbol{x}) = E_a u_a(\boldsymbol{x}) \tag{32}$$

of an electron in the external potential $V(\boldsymbol{x})$. The index a comprises all atomic quantum numbers which completely specify an eigenstate $u_a(\boldsymbol{x})$ corresponding to an eigenvalue E_a. If eigenstates exist we assume them orthonormal, but in general not complete in the Hilbert space $\mathscr{H}_S^1 = \mathscr{L}_2(\mathbb{R}^3)$ of the theory defined by (32). But we can always complement them to an orthonormal base $\mathscr{B}_S^1$ of $\mathscr{H}_S^1$ by introducing further elements $u_a(\boldsymbol{x})$ where a of course no longer comprises atomic quantum numbers. Denote by $\{a\}$ the set of the indices a of all elements $u_a(\boldsymbol{x})$ of $\mathscr{B}_S^1$.

Consider now any set $A^s := (a_1, \ldots, a_s)$ of s different elements $a \in \{a\}$ and denote by $[A^s]$ their 'class', i.e. the set of the sets A^s obtained from a given A^s by permuting only the elements a_σ of this A^s. In each class we elect one arbitrary 'class representative' A^s and define for it the function

$$U(A^s; X^s) := \frac{1}{(s!)^{1/2}} \det u_{a_\rho}(\boldsymbol{x}_\tau), \qquad \rho, \tau = 1, \ldots, s. \tag{33}$$

The set of all these determinants, one for every class $[A^s]$, forms an orthonormal base $\mathscr{B}_S^s$ of $\mathscr{H}_S^s$. So any element $f(X^s)$ of $\mathscr{H}_S^s$ can be expanded in the form

$$f(X^s) = \sum_{[A^s]} F(A^s) U(A^s; X^s). \tag{34}$$

By definition the sum contains one term for any class. The expansion coefficients are given by

$$F(A^s) := \int \mathrm{d}X^s U(A^s; X^s)^* f(X^s) \tag{35}$$

with $\int \mathrm{d}X^s \ldots := \int \mathrm{d}^3x_1 \ldots \int \mathrm{d}^3x_s \ldots$. We note that $U(A^s; X^s)$ as well as $F(A^s)$ are antisymmetric in the a_σ. A common permutation of the a_σ in both factors in (34) therefore changes nothing. The sum over all classes can therefore be written in the form of a conventional multiple sum

$$\sum_{[A^s]} \ldots = \frac{1}{s!} \sum_{a_1 \in \{a\}} \cdots \sum_{a_s \in \{a\}} \ldots \tag{36}$$

The $F(A^s)$ are the components of another representation of the abstract Hilbert space of s electrons. Similarly we can represent a state $\alpha \in \mathcal{H}^s$ by components $\alpha(A^s; K^n)$ instead of the $\alpha(X^s; K^n)$ introduced in (12). In this representation the operator $\bar{H}^s$ is given in terms of the elements

$$(\bar{H}^s\alpha)(A^s; K^n) := \int \mathrm{d}X^s U(A^s; X^s)^*(\bar{H}^s\alpha)(X^s; K^n), \tag{37}$$

the $\alpha(X^s; K^n)$ occurring in $\bar{H}^s\alpha$ being expressed by (34) in terms of their $\alpha(A^s; K^n)$.

Starting with the first and second terms in (31) and proceeding along these lines we find, for $\bar{H}^s_0$, with the abbreviation

$$T(a, b) := \int \mathrm{d}^3x u_a^*(\boldsymbol{x})\Big(-\frac{\Delta}{2M} - eV(\boldsymbol{x})\Big)u_b(\boldsymbol{x}), \tag{38}$$

the final form

$$\begin{aligned}(\bar{H}^s_0\alpha)&(A^s; K^n)\\ &= (\omega(\boldsymbol{k}_1)+\ldots+\omega(\boldsymbol{k}_n)-E_j^{\mathrm{B}})\alpha(A^s; K^n)\\ &\quad + \sum_{a\in\{a\}}\sum_{\sigma=1}^{s} T(a, a_\sigma)\alpha(A^s: a_\sigma \to a; K^n).\end{aligned} \tag{39}$$

$(A^s: a_\sigma \to a)$ stands for $(a_1, \ldots, a_{\sigma-1}, a, a_{\sigma+1}, \ldots, a_s)$. Computing $\bar{H}^s_{\mathrm{w}}$ similarly we find

$$\begin{aligned}(\bar{H}^s_{\mathrm{w}}\alpha)&(A^s; K^n)\\ &= \sum_{a\in\{a\}}\sum_{\sigma=1}^{s}\Big((n+1)^{1/2}\int \mathrm{d}^3k M(a_\sigma, a; \boldsymbol{k})\alpha(A^s: a_\sigma \to a; \boldsymbol{k}, K^n)\\ &\quad + \frac{1}{n^{1/2}}\sum_{\nu=1}^{n} M(a, a_\sigma; \boldsymbol{k}_\nu)^*\alpha(A^s: a_\sigma \to a; K^n\backslash\boldsymbol{k}_\nu)\Big)\end{aligned} \tag{40}$$

with the abbreviation

$$M(a, b; \boldsymbol{k})^* := -\frac{e}{(2\omega(\boldsymbol{k})(2\pi)^3)^{1/2}}\int \mathrm{d}^3x u_a(\boldsymbol{x})^*\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}.\boldsymbol{x}}u_b(\boldsymbol{x}). \tag{41}$$

Equations (39) and (40) are the starting points of our considerations. Therefore we note their relevant properties.

(i) The first term in (39) defines the Hamiltonian of free photons. It is self-adjoint for $E_j^{\mathrm{B}} < \infty$. The second term is the Hamiltonian of s electrons without mutual interaction, but in the external potential $V(\boldsymbol{x})$ (cf (31)). It can also be considered as self-adjoint in any case of interest. As these operators act effectively only on the factors $\mathcal{F}_{\mathrm{R}}$ and $\mathcal{H}^s_{\mathrm{S}}$ of $\mathcal{H}^s$, their sum $\bar{H}^s_0$ is self-adjoint again.

(ii) If at least one of the two states $u_a(\boldsymbol{x})$, $u_b(\boldsymbol{x})$ in (38) is an eigenstate of (32) we get $T(a, b) = E_a\delta_{ab}$ and the corresponding sum over a in (39) can be carried out readily. If all a_σ in A^s refer to eigenstates of (32) the second term of (39) yields simply $(E_{a_1}+\ldots+E_{a_s})\alpha(A^s; K^n)$.

(iii) *We shall assume that the eigenstates $u_a(\boldsymbol{x})$ of* (32) *as well as all other elements of $\mathcal{B}^1_{\mathrm{S}}$ are such that $M(a, b; \boldsymbol{k})$ is square integrable in $\boldsymbol{k}$ for any $a, b \in \{a\}, \{a\}$.* This is decisive (cf Grimm and Ernst 1974, 1977) for all that follows. Grimm and Ernst (1974) have *proven* the square integrability of the quantities which in the case of the

Dirac atom correspond to our $M(a, b; \boldsymbol{k})$. Orthonormal bases $\mathcal{B}_S^1$ in $\mathcal{H}_S^1 = \mathcal{L}_2(\mathbb{R}^3)$ leading to square integrable $M(a, b; \boldsymbol{k})$ can be found easily. It is not easy, however, to find a reasonable $V(\boldsymbol{x})$ such that the eigenstates of (32) do not lead to square integrable M's.

(iv) As the summation index a in (40) runs over the elements a of the A^s named on the left-hand side, only the term $a = a_\sigma$ yields a contribution because of the antisymmetry of $\alpha(A^s; K^n)$. This consequence of the Pauli principle is one of the keys to the specific results on the self-energy of our electrons (cf §§ 7–10).

We are ready now to show that $\bar{H}_w^s$ can really be expanded in the form (11). For this we use the fact that $\mathcal{H}^s$ can be decomposed as

$$\mathcal{H}^s = \mathcal{H}_S^s \otimes \mathcal{F}_R = \Big(\bigoplus_{[A^s]} \mathcal{U}(A^s)\Big) \otimes \Big(\bigoplus_{n=0}^{\infty} \mathcal{H}_R^n\Big) = \bigoplus_{[A^s]} \bigoplus_{n=0}^{\infty} \mathcal{U}(A^s) \otimes \mathcal{H}_R^n = \bigoplus_{[A^s]} \bigoplus_{n=0}^{\infty} \mathcal{H}(A^s, n). \tag{42}$$

$\mathcal{U}(A^s)$ denotes the subspace of $\mathcal{H}_S^s$ which is spanned by the one element $U(A^s; X^s)$ defined in (33). $\mathcal{H}(A^s, n)$ therefore is the Hilbert space of all states of n photons under the condition that S is in the s-electron state $U(A^s; X^s)$, i.e. that each of the states $u_{a_1}(\boldsymbol{x}), \ldots, u_{a_s}(\boldsymbol{x})$ is 'occupied by one electron'. Further, let $p(A^s, n)$ be the projector which maps any element $|\alpha\rangle \in \mathcal{H}^s$ onto its component $\alpha(A^s; K^n)$ in $\mathcal{H}(A^s; n)$, i.e. $p(A^s, n)|\alpha\rangle = \alpha(A^s; K^n)$. Define $i(A^s; n)$ as that operator which identifies an element $\alpha(A^s; K^n) \in \mathcal{H}(A^s, n)$ with that vector of $\mathcal{H}^s$ which has the component $\alpha(A^s; K^n)$ in $\mathcal{H}(A^s, n)$, and zero components in all other subspaces $\mathcal{H}(A'^s, n')$. The product $p(A^s, n) i(A'^s, n')$ is 1 for $n = n'$ *and* $A^s = A'^s$, and zero in any other case.

Consider now the map $T^*(a_\sigma \leftarrow a; n \leftarrow n+1)$ of $\mathcal{H}(A^s: a_\sigma \to a; n+1)$ onto $\mathcal{H}(A^s; n)$ as defined by

$$\alpha(A^s: a_\sigma \to a; K^{n+1}) \mapsto \alpha(A^s; K^n) := (n+1)^{1/2} \int \mathrm{d}^3k M(a_\sigma, a; \boldsymbol{k}) \alpha(A^s: a_\sigma \to a; \boldsymbol{k}, K^n). \tag{43a}$$

This map is defined everywhere on $\mathcal{H}(A^s: a_\sigma \to a; n+1)$ if $M(a_\sigma, a; \boldsymbol{k})$ is square integrable, as assumed. Consider further the map $T(a \leftarrow a_\sigma; n+1 \leftarrow n)$ of $\mathcal{H}(A^s, n)$ onto $\mathcal{H}(A^s: a_\sigma \to a; n+1)$ as defined by

$$\alpha(A^s; K^n) \mapsto \alpha(A^s: a_\sigma \to a; K^{n+1}) := \frac{1}{(n+1)^{1/2}} \sum_{\nu=1}^{n+1} M(a_\sigma, a; \boldsymbol{k}_\nu) \alpha(A^s; K^{n+1} \backslash \boldsymbol{k}_\nu). \tag{43b}$$

If $M(a_\sigma, a; \boldsymbol{k})$ is square integrable, as assumed, this map is again defined everywhere on $\mathcal{H}(A^s; n)$. Consider finally on $\mathcal{H}^s$, for given $\sigma \leqslant s$, and given $n \geqslant 0$, the operator

$$\begin{aligned} L^s[(A^s; n) \rightleftarrows (A^s: a_\sigma \to a; n+1)] \\ := i(A^s, n) T^*(a_\sigma \leftarrow a; n \leftarrow n+1) p(A^s: a_\sigma \to a; n+1) \\ + i(A^s: a_\sigma \to a; n) T(a \leftarrow a_\sigma; n+1 \leftarrow n) p(A^s; n). \end{aligned} \tag{44}$$

It is *defined everywhere* on $\mathcal{H}^s$ with range in $\mathcal{H}^s$ if $M(a_\sigma, a; \boldsymbol{k})$ is square integrable. Furthermore it is *symmetric* on $\mathcal{H}^s$ because $\langle \alpha | L^s[(A^s; n) \rightleftarrows (A^s: a_\sigma \to a; n+1)] | \alpha \rangle$ is real for any $|\alpha\rangle \in \mathcal{H}^s$ as verified easily by using the above definitions. So it is *self-adjoint and bounded* on $\mathcal{H}^s$, by a well known theorem of functional analysis (e.g. Yosida 1968).

Now *define* the operator $\bar{H}^s_w$ by

$$\bar{H}^s_w = \sum_{[A^s]} \sum_{a\in\{a\}} \sum_{n=0}^{\infty} \sum_{\sigma=1}^{s} L^s[(A^s; n) \rightleftarrows (A^s : a_\sigma \to a; n+1)]. \tag{45}$$

Using the above definitions it poses no problems to verify that $p(a; n)\bar{H}^s_w|\alpha\rangle$ equals 'term by term' the right-hand side of (40). In this sense the operator $\bar{H}^s_w$ defined by (40) equals $\bar{H}^s_w$ defined by (45). As the right-hand side of (45) contains a *countable* number of terms we can number them through in some sense and obtain in this way the operators L^s_ρ in (11) with all stated properties.

5. The coarse grain Weisskopf–Wigner expansion

The fine grain expansion (45) of $\bar{H}^s_w$ exhibits perhaps more of the 'fine structure' of the theory than we are interested in. So it is natural to seek 'coarser' structures, e.g. in the form of *useful partial sums* Σ^s of (45) with an *infinite* number of terms. The criterion for 'useful' will be that the theory defined by Σ^s 'describes' a characteristic class of physical phenomena which are well distinguished from the phenomena described by other Σ^s, and that the theory defined by Σ^s is equipped with a *self-adjoint* Hamilton operator. We now define such Σ^s and show that the Hamiltonians defined by them are self-adjoint at least for $\mu > 0$. Their physical utility is considered in §§ 7–10.

Consider some *finite* subset I of the index set $\{a\}$ introduced in § 4 with a number $i \geqslant s$ of elements a, and consider for any s the partial sum Σ^s_I obtained from (45) by restricting the sum over a to the sum over all $a \in I$ and the sum over all classes A^s to the $\binom{i}{s}$ classes A^s which contain only elements $a_\sigma \in I$. We note that Σ^s_I has its *range* in the subspace $\mathcal{H}^s_I \subset \mathcal{H}^s$,

$$\mathcal{H}^s_I := \bigoplus_{n=0}^{\infty} \bigoplus_{A^s\in I} \mathcal{H}(A^s; n) = \bigoplus_{A^s\in I} \mathcal{U}(A^s) \otimes \mathcal{F}_R, \tag{46}$$

provided the infinite sum over n in Σ^s_I converges at all. The sum over A^s covers all classes with elements from I only. Due to the projectors $p(A^s; n)$ in the L^s we lose nothing if the domain of Σ^s_I is restricted to $\mathcal{H}^s_I \subset \mathcal{H}^s$. We note further that the first term in (39) can be written in the form ${}^1H^s_{0I} \oplus {}^1H^s_{0C}$ with a self-adjoint operator ${}^1H^s_{0I}$ acting on $\mathcal{H}^s_I$ and a self-adjoint operator ${}^1H^s_{0C}$ acting on the complement space $\mathcal{H}^s \ominus \mathcal{H}^s_I$. Consider finally the second term of (39) and write the sum over a as (sum over $a \in I$) + (sum over $a \in (\{a\} \backslash I)$). If restricted to $\mathcal{H}^s_I$ the first sum defines on $\mathcal{H}^s_I$ a self-adjoint and bounded operator ${}^2H^s_{0I}$. The range of the second sum is in any case outside $\mathcal{H}^s_I$, i.e. in $\mathcal{H}^s \ominus \mathcal{H}^s_I$. Consider now the operator

$$\bar{H}^s_I := {}^1\bar{H}^s_{0I} + {}^2\bar{H}^s_{0I} + \Sigma^s_I \tag{47}$$

consisting of parts of (39) and (40). We show below that it is *self-adjoint on* $\mathcal{H}^s_I$ if $\mu > 0$. So it defines on $\mathcal{H}^s_I$ a certain quantum theory if it is considered as the 'total Hamiltonian' of that theory. The 'coarse grain hierarchy of Weisskopf–Wigner theories' is *defined* by the sequence of Hamiltonians $\bar{H}^s_{I_1}, \bar{H}^s_{I_2}, \ldots$ which correspond to a sequence $I_1 \subset I_2 \subset I_3 \subset \ldots$ which finally 'tends' to $I_\infty = \{a\}$. Note that the Hamiltonians $\bar{H}^s_I$ contain more and more terms of the 'exact' $\bar{H}^s$ as I tends to $\{a\}$, and that no terms of $\bar{H}^s$ are left out.

We prove now the self-adjointness of $\bar{H}_I^s$ for any finite I and any $\mu > 0$. For this we show that Σ_I^s is *bounded relative* to ${}^1\bar{H}_{0I}^s + E_j^B =: \bar{H}_{tI}^s$ with bound smaller than 1. $\bar{H}_{tI}^s$ is self-adjoint, but not bounded. So $\bar{H}_{tI}^s + \Sigma_I^s$ is self-adjoint (Kato 1966, p 287). Adding to this any bounded and self-adjoint operator we get a self-adjoint operator again. In our case we add $-E_j^B + {}^2H_{0I}^s$ to obtain $\bar{H}_I^s$ together with its self-adjointness.

To show that Σ_I^s is bounded relative to $\bar{H}_{tI}^s$ we note that $\bar{H}_{tI}^s$ is defined by $\alpha(A^s; K^n) \to (\omega(\boldsymbol{k}_1) + \ldots + \omega(\boldsymbol{k}_n))\alpha(A^s; K^n)$ so that because of $\omega(\boldsymbol{k}_1) + \ldots + \omega(\boldsymbol{k}_n) \geq n\mu$ it satisfies for any $|\beta\rangle \in \mathcal{D}(H_{tI}^s)$ the inequality

$$\|H_{tI}^s|\beta\rangle\| \geq \mu \|N_I^s|\beta\rangle\|, \qquad \text{i.e.} \qquad \mathcal{D}(H_{tI}^s) \subseteq \mathcal{D}(N_I^s) \tag{48}$$

with $\|\ldots\|$ denoting the norm on $\mathcal{H}_I^s$ and N_I^s the operator $\alpha(A^s; K^n) \to n\alpha(A^s; K^n)$. As in Nelson (1964) and Grimm and Ernst (1974) we can find for any $\epsilon > 0$ a $b_\epsilon > 0$ so that for any $|\beta\rangle \in \mathcal{D}(N_I^s)$ we get

$$\|(N_I^s + 1)^{1/2}|\beta\rangle\| \leq \epsilon \|N_I^s|\beta\rangle\| + b_\epsilon \||\beta\rangle\| \tag{49}$$

for the operator $(N_I^s + 1)^{1/2}$ defined by $\alpha(A^s; K^n) \mapsto (n+1)^{1/2}\alpha(A^s; K^n)$. Combining (48) and (49) we can find for any $\epsilon > 0$ a number $b_\epsilon > 0$ so that

$$\|(N_I^s + 1)^{1/2}|\beta\rangle\| \leq \frac{\epsilon}{\mu} \|H_{tI}^s|\beta\rangle\| + b_\epsilon \||\beta\rangle\| \tag{50}$$

for any $|\beta\rangle \in \mathcal{D}(H_{tI}^s)$. We show below that Σ_I^s satisfies for any $|\beta\rangle \in \mathcal{D}((N_I^s + 1)^{1/2})$ an inequality

$$\|\Sigma_I^s|\beta\rangle\| \leq C\|(N_I^s + 1)^{1/2}|\beta\rangle\| \tag{51}$$

with a finite constant C. This means that Σ_I^s is defined at least on the *dense* domain $\mathcal{D}((N_I^s + 1)^{1/2})$. So we get with the above $\mathcal{D}(\Sigma_I^s) \supseteq \mathcal{D}((N_I^s + 1)^{1/2} \supseteq \mathcal{D}(N_I^s + 1) = \mathcal{D}(N_I^s) \supseteq \mathcal{D}(H_{tI}^s)$, i.e. we satisfy the first condition $\mathcal{D}(\Sigma_I^s) \supseteq \mathcal{D}(H_{tI}^s)$ for Σ_I^s being bounded relative to H_{tI}^s. It poses no problem to verify that Σ_I^s is real whenever it is finite. Since Σ_I^s has a *dense* domain $\mathcal{D}(\Sigma_I^s)$, as shown above, it is *symmetric* on $\mathcal{H}_I^s$. So it meets the second condition for relative boundedness. Combining (51) with (50) we get

$$\|\Sigma_I^s|\beta\rangle\| \leq C\frac{\epsilon}{\mu} \|H_{tI}^s|\beta\rangle\| + Cb_\epsilon \||\beta\rangle\|. \tag{52}$$

Choosing now ϵ smaller than μ/C we satisfy the third and last condition (cf Kato 1966, p 287) for $\bar{H}_{tI}^s + \Sigma_I^s$ to be self-adjoint. This proof cannot be extended to the case $\mu = 0$, and it seems that $\bar{H}_I^s$ is indeed not self-adjoint in this case.

Finally we verify (51). We have by definition

$$\|\Sigma_I^s|\beta\rangle\|^2 = \sum_{A^s \in I} \sum_{n=0}^{\infty} \int \mathrm{d}K^n \Big| (n+1)^{1/2} \sum_{\sigma=1}^{s} \sum_{a \in I} \int \mathrm{d}^3k M(a_\sigma, a; \boldsymbol{k})^* \beta(A^s : a_\sigma \to a; \boldsymbol{k}, K^n)$$

$$+ \frac{1}{n^{1/2}} \sum_{\sigma=1}^{s} \sum_{a \in I} \sum_{\nu=1}^{n} M(a, a_\sigma; \boldsymbol{k}_\nu)\beta(A^s : a_\sigma \to a; K^n \backslash \boldsymbol{k}_\nu) \Big|^2. \tag{53}$$

For given A^s and n the integral $\int \mathrm{d}K^n |\ldots|^2 = \int \mathrm{d}^3k_1 \ldots \int \mathrm{d}^3k_n |\ldots|^2$ defines the square of the norm $\||V\rangle\|_n$ of a vector $|V\rangle$ of the Hilbert space $\mathcal{H}(A^s; n)$. In our case $|V\rangle$ is a finite sum $\Sigma(|V_i\rangle + |V_i'\rangle)$ of other such vectors, namely the summands of the sums over σ and a. So we can use the triangle relation $\|\Sigma(|V_i\rangle + |V_i'\rangle)\|_n^2 \leq$

$[\Sigma(\|\,|V_i\rangle\|_n + \|\,|V_i'\rangle\|_n)]^2$ with respect to the sum over σ and a. This yields

$$\|\Sigma_I^s|\beta\rangle\|^2 \leqslant \sum_{A^s \in I} \sum_{n=0}^{\infty} \Big[\sum_{a \in I} \sum_{\sigma=1}^{s} \Big(\Big\| (n+1)^{1/2} \int d^3k M(a_\sigma, a; k)^* \beta(A^s : a_\sigma \to a; \boldsymbol{k}, K^n) \Big\|_n$$

$$+ \|n^{1/2} M(a, a_\sigma; \boldsymbol{k}_1) \beta(A^s : a_\sigma \to a; K^n \backslash \boldsymbol{k}_1)\|_n \Big) \Big]^2. \tag{54}$$

The K^n are now the integration variables relative to the norm $\|\ldots\|_n$. In the last term we have taken into account that after the use of the triangle relation the sum over ν yields only a factor n. Now let the finite $\mathscr{L}_2(\mathbb{R}^3)$ norm of $M(a, a_\sigma; k)$ be denoted by $m(a, a_\sigma)$. Applying the Schwarz inequality to the integration over $\boldsymbol{k}$ in the first term, and using $m(a, b) = m(b, a)$ and the fact that $m(a, a_\sigma)$ factors out in the second term we find that the large round bracket is bounded by

$$m(a, a)[\|(n+1)^{1/2} \beta(A^s : a_\sigma \to a; K^{n+1})\|_{n+1} + \|n^{1/2} \beta(A^s : a_\sigma \to a; K^{n-1})\|_{n-1}].$$

Inserting this into (54), carrying out the simple substitutions $n+1 \to n$, $n-1 \to n$, and using $\|n^{1/2} \ldots\| \leqslant \|(n+1)^{1/2} \ldots\|$ we get

$$\|\Sigma_I^s|\beta\rangle\|^2 \leqslant 4 \sum_{A^s \in I} \sum_{n=0}^{\infty} \Big(\sum_{a \in I} \sum_{\sigma=1}^{s} m(a, a_\sigma)(n+1)^{1/2} \|\beta(A^s : a_\sigma \to a; K^n)\|_n \Big)^2. \tag{55}$$

Using now $|\Sigma\, c_i d_i| \leqslant (\Sigma\, |c_i|^2)^{1/2} (\Sigma\, |d_i|^2)^{1/2}$ with respect to the sum over a and σ, we get

$$\|\Sigma_I^s|\beta\rangle\|^2 \leqslant 4 \sum_{A^s \in I} \sum_{n=0}^{\infty} \Big(\sum_{a \in I} \sum_{\sigma=1}^{s} m(a, a_\sigma)^2 \Big) \Big(\sum_{a \in I} \sum_{\sigma=1}^{s} (n+1) \|\beta(A^s : a_\sigma \to a; K^n)\|_n^2 \Big). \tag{56}$$

The first sum over σ and a is finite, we denote it by m. In the second sum the sum over σ yields a factor s. So we get

$$\|\Sigma_I^s|\beta\rangle\|^2 \leqslant 4ms \sum_{A^s \in I} \sum_{n=0} \sum_{a \in I} (n+1) \|\beta(A^s : a_1 \to a; K^n)\|_n^2. \tag{57}$$

We remember now that the sum over all A^s can be written as an s-fold sum over $a_\sigma \in I$, $\sigma = 1, \ldots, s$, (cf (36)). As the summand does not depend on a_1 the sum over a_1 yields a factor i, the number of elements in I. Substituting now $a \to a_1$ we obtain the sum over A^s. Putting finally $C^2 = 4msi$ we get

$$\|\Sigma_I^s|\beta\rangle\|^2 \leqslant C^2 \sum_{A^s \in I} \sum_{n=0} (n+1) \|\beta(A^s; K^n)\|_n^2 = C^2 \|(N_I^s + 1)|\beta\rangle\|^2, \tag{58}$$

as stated in (51).

It should be noted that the corresponding results of Grimm and Ernst (1974) have not only been extended from $s = 1$ to any s, but also to cases where the Schrödinger equation of one electron in an external field has a mixed spectrum or no eigenstates at all, as is frequently the case. This was necessary to show that the idea of the Weisskopf–Wigner approximation is indeed applicable to interacting fields. The above estimates of $\Sigma_I^s|\beta\rangle$ have a remarkable parallel in the interaction of many atoms with photons (Stelzer *et al* 1977) though the physical situation is quite different.

For the reasons given or referred to in § 1 we shall not further analyse the mathematical aspects of the operator expansions (11) or (45), but show that they are physically interesting because certain Σ_I^s 'describe' autonomous classes of physical phenomena.

6. The concept of bound photons

For this purpose we must first consider the physical aspects of the transition between the conceptual levels of 'external charges' and 'external fields'. So we must discuss once more the Hamiltonian H_j^s defined by (21*a*). This will lead us to a concept of 'photons *bound* to the external charge' which in § 7 will be extended to 'photons bound to *electrons*' and in § 8 to 'photons bound to the external charge as well as to electrons'.

We saw in § 3 that the conditions for a 'legal' transition between the above 'levels' are the square integrability of $f(\boldsymbol{k})$ and thus the unitarity of $W\{-f(\boldsymbol{k})\}$ as defined in (27), and the finiteness of E_j^B as given in (22). So we come to consider the relations

$$n_j^B := \int \mathrm{d}^3k\,|f(\boldsymbol{k})|^2 = Z^2e^2 \int \mathrm{d}^3k\,|\tilde{j}(\boldsymbol{k})|^2/2\omega(\boldsymbol{k})^3 < \infty, \tag{59a}$$

$$E_j^B := \int \mathrm{d}^3k\omega(\boldsymbol{k})|f(\boldsymbol{k})|^2 = Z^2e^2 \int \mathrm{d}^3k\,|\tilde{j}(\boldsymbol{k})|^2/2\omega(\boldsymbol{k})^2 < \infty, \tag{59b}$$

$$\int \mathrm{d}^3k\omega(\boldsymbol{k})^2|f(\boldsymbol{k})|^2 = Z^2e^2 \int \mathrm{d}^3k\,|\tilde{j}(\boldsymbol{k})|^2/2\omega(\boldsymbol{k}) < \infty, \tag{59c}$$

$$\int \mathrm{d}^3k\omega(\boldsymbol{k})^3|f(\boldsymbol{k})|^2 = Z^2e^2 \int \mathrm{d}^3k\,|\tilde{j}(\boldsymbol{k})|^2/2 < \infty. \tag{59d}$$

Conditions (*a*) and (*b*) are sufficient for H_j^s to be self-adjoint on $\mathscr{H}^s$ (cf (21*c*)). Condition (*c*) is necessary and sufficient for the last two terms in (21*a*) to define a self-adjoint operator. For $\mu = 0$ the auxiliary condition (*d*) is *sufficient* for (*a*), (*b*) and (*c*). For $\mu = 0$, (*b*) and (*c*) follow only from (*a*) and (*d*). This is another peculiarity of the infrared problem (cf (49)).

Let us consider (59) from the physical point of view. From (19) and (23) we get

$$\begin{aligned} E_j^B &= \frac{Z^2e^2}{2(2\pi)^3} \int \mathrm{d}^3k \frac{1}{\omega(\boldsymbol{k})^2} \int \mathrm{d}^3x' j(\boldsymbol{x}')\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}'} \int \mathrm{d}^3x'' j(\boldsymbol{x}'')\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}''} \\ &= \frac{Z^2e^2}{2} \int \mathrm{d}^3x' \int \mathrm{d}^3x'' \frac{j(\boldsymbol{x}')j(\boldsymbol{x}'')}{4\pi|\boldsymbol{x}'-\boldsymbol{x}''|} \exp(-\mu|\boldsymbol{x}'-\boldsymbol{x}''|). \end{aligned} \tag{60}$$

This is the 'static field energy' of the Coulomb or Yukawa field of force which surrounds the charge $Zej(\boldsymbol{x})$ (cf (8)). Condition (*b*) therefore has a very reasonable, classical meaning.

Condition (*a*) has an equally reasonable, but quantum mechanical meaning. From (21*c*) we see namely that $-E_j^B$ is the *eigenvalue* of H_j^s corresponding to the *eigenspace* $\mathscr{B}_j^s := W^s\{-f(\boldsymbol{k})\}(\mathscr{H}_S^s \otimes |v\rangle)$ where $|v\rangle := (1, 0, 0, \ldots)$ is the vacuum state in $\mathscr{F}_R$. $W_R\{-f(\boldsymbol{k})\}|v\rangle$ is a 'modified vacuum state' (Friedrichs 1953) or a 'fully coherent state' (Glauber 1963a, b) in $\mathscr{F}_R$ if $W_R\{f(\boldsymbol{k})\}$ is defined on $\mathscr{F}_R$ by (24). Using (25) we find that E_j^B is equal to the expectation value $\langle b_j^s|H_p^s|b_j^s\rangle$ of the operator H_p^s of the 'energy of the photons' (cf (21*a*)) in any eigenstate $|b_j^s\rangle$ of H_j^s. If H_j^s is the 'governing total Hamiltonian' of a physical system this system cannot make any 'transitions' between the eigenstates of H_j^s. The photons in these states thus cannot take part in any 'dynamical process' which is governed by H_j^s alone. So they are 'fixed', 'bound' (Cook 1961, Grimm and Ernst 1974, 1975, 1977, Ernst 1976) to the external charge $Zej(\boldsymbol{x})$, and cannot be removed from it within a theory which is governed by H_j^s alone. Their

energy E_j^{B} can obviously be looked upon as some sort of *binding energy*, hence the index B. As this binding energy is not available for the dynamical processes governed by H_j^s the spectrum of H_j^s should be shifted against the spectrum H_{p}^s of 'free' photons by the amount $-E_j^{\mathrm{B}}$. This is the meaning of (21*c*). The 'mean number of photons bound to $Zej(\boldsymbol{x})$' should obviously be defined as the expectation value $\langle b_j^s|N^s|b_j^s\rangle$ of the photon number operator N^s in any eigenstate $|b_j^s\rangle$ of H_j^s. N^s is defined on $\mathscr{H}^s$ by

$$N^s := \int \mathrm{d}^3k a^+(\boldsymbol{k})a(\boldsymbol{k}) = \bigoplus_{n=0}^{\infty} n, \tag{61}$$

(cf (21*a*)). Using (25) and (*a*) we find $\langle b_j^s|N^s|b_j^s\rangle = n_j^{\mathrm{B}}$. Condition (*a*) means therefore that a finite mean number of photons is being bound to $Zej(\boldsymbol{x})$.

These bound photons 'build up' the Coulomb–Yukawa field of force that surrounds the external charge. To show this we compute the expectation value of the operator $A(\boldsymbol{x})$ of the 'potential amplitude of R' in any eigenstate $|b_j^s\rangle \in \mathscr{B}_j^s$. Using (25), (22), (19) and (8) we get

$$\begin{aligned}
\langle b_j^s|A(\boldsymbol{x})|b_j^s\rangle &= \langle v|W_{\mathrm{R}}\{f(\boldsymbol{k})\}A_{\mathrm{R}}(\boldsymbol{x})W_{\mathrm{R}}\{-f(\boldsymbol{k})\}|v\rangle \\
&= -\frac{1}{(2\pi)^{3/2}}\int \mathrm{d}^3k(\mathrm{e}^{\mathrm{i}\boldsymbol{k}.\boldsymbol{x}}f(\boldsymbol{k})+\mathrm{cc})/(2\omega(\boldsymbol{k}))^{1/2} = A'(\boldsymbol{x}) \\
&= -\frac{Ze}{(2\pi)^{3/2}}\int \mathrm{d}^3k(\mathrm{e}^{\mathrm{i}\boldsymbol{k}.\boldsymbol{x}}\tilde{j}(\boldsymbol{k})+\mathrm{cc})/2\omega(\boldsymbol{k})^2 \\
&= -\frac{Ze}{2}\int \mathrm{d}^3x' j(\boldsymbol{x}')\frac{1}{(2\pi)^3}\int \mathrm{d}^3k\int \mathrm{d}^3k\left(\frac{\mathrm{e}^{\mathrm{i}\boldsymbol{k}.(\boldsymbol{x}-\boldsymbol{x}')}}{\omega(\boldsymbol{k})^2}+\mathrm{cc}\right) \\
&= -Ze\int \mathrm{d}^3x' j(\boldsymbol{x}')\frac{\exp(-\mu|\boldsymbol{x}-\boldsymbol{x}'|)}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|} = V(\boldsymbol{x}).
\end{aligned} \tag{62}$$

$A_{\mathrm{R}}(\boldsymbol{x})$ is defined on $\mathscr{F}_{\mathrm{R}}$ by (18*b*). It is clear that the potential $V(\boldsymbol{x})$ and the field of force it represents must be considered as being built up by the photons bound to $Zej(\boldsymbol{x})$. The energy of this field is given by the right-hand side of (60) and therefore equals the binding energy of the photons which build it up.

We note without proof: the 'full coherence' of $|b_j^s\rangle$ guarantees for the expectation value (62) the smallest quantum mechanical variance that is possible at all. There are of course infinitely many other states in $\mathscr{H}^s$ which have the same $V(\boldsymbol{x})$ as expectation value of $A(\boldsymbol{x})$, but the variance of this expectation value is always greater than the variance of $V(\boldsymbol{x})$ as defined by (62). The 'quantum mechanical fluctuations' of this 'field' are therefore the weakest field fluctuations which are possible at all. Formally, the latter are of course infinite, but for any proper 'spatial average' of $A(\boldsymbol{x})$ they are finite and still minimal. In this sense the bound photons build up the *best* 'classical fields' like $V(\boldsymbol{x})$ that are possible in a quantum theory.

Let us consider in more detail the mean number of bound photons. Inserting (19) into (59*a*) we get

$$\begin{aligned}
n_j^{\mathrm{B}} &= \frac{Z^2e^2}{2}\int \mathrm{d}^3x\int \mathrm{d}^3x' j(\boldsymbol{x})j(\boldsymbol{x}')\frac{1}{(2\pi)^3}\int \mathrm{d}^3k\frac{\mathrm{e}^{-\mathrm{i}\boldsymbol{k}.(\boldsymbol{x}-\boldsymbol{x}')}}{\omega(\boldsymbol{k})^3} \\
&= \frac{Z^2e^2}{2}\int \mathrm{d}^3x\int \mathrm{d}^3x' j(\boldsymbol{x})j(\boldsymbol{x}')K_0(\mu|\boldsymbol{x}-\boldsymbol{x}'|)/2\pi^2.
\end{aligned} \tag{63}$$

$K_0(z)$ is the modified Hankel function as tabulated and plotted, for example, in Jahnke, Emde and Lösch (1960). For real $z>0$ it is positive and monotonically decreasing, for $z\to 0$ it behaves like $\ln(2/\gamma z)$ with Euler's constant $\gamma = 1{\cdot}781\ldots$, for $z\to\infty$ like $e^{-z}(\pi/2z)^{1/2}$.

We see that n_j^B increases logarithmically if the charge is gradually concentrated into one point, say $j(\boldsymbol{x})\to\delta(\boldsymbol{x})$. This is an 'ultraviolet divergence' because for $j(\boldsymbol{x})\to\delta(\boldsymbol{x})$ we get $\tilde{j}(\boldsymbol{k})\to 1/(2\pi)^{3/2}$ and the integral (59*a*) for n_j^B diverges from the contributions of large photon momenta. As an infinite number of bound massive photons is clearly absurd, we must exclude the case of external point charges for good physical reasons as well as by the requirements of a 'legal' transition between the 'levels' of external charges and fields. For $\mu = 0$ this argument is clearly not so stringent relative to n_j^B, but the ultraviolet divergence of E_j^B is as serious as before. This implies obviously the abandonment of the notion of the classical Coulomb or Yukawa force between finite *point* charges. However, we do retain the Coulomb–Yukawa force as an 'infinitesimal force element' acting between the infinitesimal charge elements of a *square integrable charge distribution.* This is indeed the 'basic interaction ingredient' of our general Hamiltonian H, as shown by (20) for $\tilde{j}(\boldsymbol{k}) = 1/(2\pi)^{3/2}$. If $j(\boldsymbol{x})$ is understood as an 'approximate representative' of a quantum mechanical system (see the appendix) its square integrability is very natural, so we adopt it for the remainder of this work. But for obvious physical reasons we also require the existence of a finite total charge $Q = Ze\int d^3x j(\boldsymbol{x})$, this integral being understood in the Lebesgue sense so that also $\int d^3x|j(\boldsymbol{x})|<\infty$ and $\tilde{j}(\boldsymbol{k})$ is continuous at $\boldsymbol{k}=0$.

For $\mu = 0$ this guarantees only the absence of ultraviolet divergences. Equation (63) still shows a logarithmical infrared divergence which disappears only for $Q = 0$. As the binding energy of the infinitely many bound photons remains finite we shall not restrict the discussion to the harmless case $Q = 0$. Our calculations are therefore 'formal' and take place outside the Hilbert space $\mathcal{H}$, but they remain well defined and unique in the greater vector space $\mathcal{V}$ introduced for this reason in § 2. The 'detour through $\mathcal{V}$' will lead us back into $\mathcal{H}$ in some special, but very important cases. Of course, we may also consider μ as a renormalisation constant and go back to the limit $\mu\to 0$ only in the final results. Both 'methods' yield the same result.

7. A quantum theory of the self-energy of the electron

We return first to the auxiliary conceptual level of external fields and consider in detail the lowest coarse grain Weisskopf–Wigner theory defined in § 5 by $i = s$ and hence $I = A^s$. For $s = 1$ this corresponds to a known theory (example 3 of Grimm and Ernst 1974, figure 5 of Grimm and Ernst 1977) which shows phenomena of photon binding. So we can certainly expect such phenomena in our theory. It is surprising, however, that the simple assumption $i = s$ leads to a satisfactory and complete theory of the self-interaction effects of our electrons as well as of their mutual interaction, the latter of course only for $s>1$. This proves that the 'expansions' of § 4 and § 5 employ and reveal 'natural structures' of our interacting fields.

The condition $i = s$ implies the assumption that s electrons are considered in some *given* state $U(A^s; X^s)\in\mathcal{H}_S^s$ which is 'prescribed' by the choice of $I = A^s = (a_1,\ldots,a_s)$. This is the state obtained by occupying the one-electron states $u_{a_1}(\boldsymbol{x}),\ldots,u_{a_s}(\boldsymbol{x})$ with one electron each. But these electrons are still allowed to interact with the photons. The Hamiltonian of this interaction is determined by the

choice of I and reads for the present case $I = A^s$ to

$$(\tilde{H}^s_I\alpha)(A^s; K^n)$$
$$= (\omega(\boldsymbol{k}_1)+\ldots+\omega(\boldsymbol{k}_n)+T(A^s))\alpha(A^s; K^n)$$
$$+(n+1)^{1/2}\int \mathrm{d}^3k M^*(A^s; \boldsymbol{k})\alpha(A^s; \boldsymbol{k}, K^n)$$
$$+\frac{1}{n^{1/2}}\sum_{\nu=1}^{n} M(A^s; \boldsymbol{k}_\nu)\alpha(A^s; K^n\backslash\boldsymbol{k}_\nu). \tag{64}$$

We have introduced the abbreviations (cf (38) and (41))

$$M_I(\boldsymbol{k}) := M(A^s; \boldsymbol{k}) := M(a_1, a_1; \boldsymbol{k})+\ldots+M(a_s, a_s; \boldsymbol{k}), \tag{65a}$$

$$T_I := T(A^s) := T(a_1, a_1)+\ldots+T(a_s, a_s)-E^{\mathrm{B}}_j. \tag{65b}$$

The point of the condition $i = s$ is that the sums over a in (39) and (40) are restricted to $a \in I = A^s$ so that as a consequence of the Pauli principle only the terms $a = a_\sigma$ are different from zero (see remark (iv) following (41)). The remaining sum over σ is contained in the sums in (65). In terms of (45) the interaction part of (64) is given by the term $A^s = I$, and by restricting the sum over all a to the sum over $a \in I$.

In analogy with (21a) the Hamiltonian defined by (64) can be written in the form

$$\tilde{H}^s_I = T_I + \int \mathrm{d}^3k\omega(\boldsymbol{k})a^+(\boldsymbol{k})a(\boldsymbol{k})+\int \mathrm{d}^3k(M^*_I(\boldsymbol{k})a(\boldsymbol{k})+M_I(\boldsymbol{k})a^+(\boldsymbol{k})) \tag{66}$$

with photon creation and annihilation operators restricted to $\mathscr{H}^s_I := \mathscr{U}(A^s)\otimes\mathscr{F}_{\mathrm{R}}$, $A^s = I$. As in § 3 we 'complete the square' by writing

$$\tilde{H}^s_I = E^s_I+\int \mathrm{d}^3k\omega(\boldsymbol{k})(a^+(\boldsymbol{k})+M^*_I(\boldsymbol{k})/\omega(\boldsymbol{k}))(a(\boldsymbol{k})+M_I(\boldsymbol{k})/\omega(\boldsymbol{k})) \tag{67}$$

with the definitions

$$E^s_I := T_I - E^{\mathrm{B}}_I, \qquad E^{\mathrm{B}}_I := \int \mathrm{d}^3k|M_I(\boldsymbol{k})|^2/\omega(\boldsymbol{k}). \tag{68}$$

As in § 3 the completion of the square is legitimate if $M_I(\boldsymbol{k})/\omega(\boldsymbol{k})$ is square integrable and $E^{\mathrm{B}}_I < \infty$. In this case the Weyl operator $W^s_I\{M_I(\boldsymbol{k})/\omega(\boldsymbol{k})\}$ exists and is defined on $\mathscr{H}^s_I$ in analogy to (24) and we can write

$$\tilde{H}^s_I = W^s_I\{-M_I(\boldsymbol{k})/\omega(\boldsymbol{k})\}\Big(E^s_I+\int \mathrm{d}^3k\omega(\boldsymbol{k})a^+(\boldsymbol{k})a(\boldsymbol{k})\Big)W^s_I\{M_I(\boldsymbol{k})/\omega(\boldsymbol{k})\}. \tag{69}$$

We see that $\tilde{H}^s_I$ assumes an *eigenstate*

$$|\tilde{b}^s_I\rangle := U(A^s; X^s)\otimes W_{\mathrm{R}}\{-M_I(\boldsymbol{k})/\omega(\boldsymbol{k})\}|v\rangle, \qquad U(A^s; X^s) = U(I; X^s), \tag{70}$$

to the *eigenvalue* E^s_I. In contrast to § 6 this eigenvalue is not degenerate. The existence of these eigenstates and eigenvalues, one in each $\mathscr{H}^s_I$ with arbitrary s and arbitrary I with $i = s$, is the main result of this work which requires careful discussion.

For this we assume first that the indices $a_1, \ldots, a_s$ contained in I refer to eigenstates of the Schrödinger equation (32). So we consider an s-electron 'atom' in the state $U(A^s; X^s)$ in which the levels $u_{a_1}(\boldsymbol{x}), \ldots, u_{a_s}(\boldsymbol{x})$ of the one-electron Schrödinger atom are occupied with one electron each. The eigenvalue of $\tilde{H}^s_I$ is then given by

$$E^s_I := E_{a_1}+\ldots+E_{a_s}-E^{\mathrm{B}}_I-E^{\mathrm{B}}_I, \tag{71}$$

as seen from remark (ii) following (41). E_I^{B} has been discussed in § 6, it is independent of I. $E_{a_1}+\ldots+E_{a_s}$ is the eigenvalue of the s-electron atom in the state $U(A^s;X^s)$ in the case of no interaction of the electrons with themselves and with each other. $-E_I^{\mathrm{B}}$ is the 'correction' of this eigenvalue due to the self- and mutual interaction of the electrons as far as is achieved in the present Weisskopf–Wigner approximation.

We consider this correction first for $s=1$, the case of a one-electron atom with the external potential $V(\boldsymbol{x})$. I coincides in this case with the index a of some chosen eigenstate $u_a(\boldsymbol{x})$. Inserting (41) into (65a) and this into (68) we get $E_I^1 = E_a^{\mathrm{B}}$ with

$$E_a^{\mathrm{B}} := \frac{e^2}{2(2\pi)^3}\int \mathrm{d}^3k \left|\int \mathrm{d}^3x u_a^*(\boldsymbol{x})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}u_a(\boldsymbol{x})\right|^2 \omega(\boldsymbol{k})^{-2}$$

$$= \tfrac{1}{2}\int \mathrm{d}^3x \int \mathrm{d}^3x'(-e|u_a(\boldsymbol{x})|^2)(-e|u_a(\boldsymbol{x}')|^2)\frac{\exp(-\mu|\boldsymbol{x}-\boldsymbol{x}'|)}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|}. \tag{72}$$

We refer to E_a^{B} as the self-energy of a single electron in the state $u_a(\boldsymbol{x})$. It is computed like the energy of the classical Coulomb–Yukawa field of force that surrounds a classical charge density $-e|u_a(\boldsymbol{x})|^2$, (cf (60)). So it is the self-energy of a 'smeared' electron in the sense of Schrödinger's (1926) pre-statistical interpretation of quantum mechanics, the term self-energy being used in its classical sense (cf § 10). It is easily verified that E_a^{B} is also the expectation value of the operator of the energy of the photons in the eigenstate $|\bar{b}_I^1\rangle = |\bar{b}_a^1\rangle$ of the Hamiltonian $\bar{H}_I^1 = \bar{H}_a^1$. So it can be considered as the *binding energy of photons bound to the bound electron.* Equation (71) tells us that the eigenvalue $E_a - E_I^{\mathrm{B}}$ of the eigenstate $u_a(\boldsymbol{x})$ of this electron is *shifted* by the self-energy of the electron due to photons bound to it. This shift is *finite* because the pre-statistical Schrödinger electron is smeared out and so has lost its 'point-likeness'. The number of photons bound to the bound electron is (cf § 6)

$$\bar{n}_a^{\mathrm{B}} := \langle \bar{b}_a^1|N_a^1|\bar{b}_a^1\rangle$$

$$= \int \mathrm{d}^3k|M(a,a;\boldsymbol{k})|^2/\omega(\boldsymbol{k})^2$$

$$= \tfrac{1}{2}\int \mathrm{d}^3x \int \mathrm{d}^3x'(-e|u_a(\boldsymbol{x})|^2)(-e|u_a(\boldsymbol{x}')|^2)K_0(\mu|\boldsymbol{x}-\boldsymbol{x}'|)/2\pi^2. \tag{73}$$

N_I^s is defined on the Hilbert space $\mathscr{H}_I^s$ in analogy with (61). The last expression has been obtained by inserting (41) into $M(a,a;\boldsymbol{k})$ and then proceeding as in (63). The photons bound to the bound electron build up an 'eigenpotential of the electron', $V_a^1(\boldsymbol{x})$, in the sense of an expectation value of the potential operator $A(\boldsymbol{x}) = A_a^1(\boldsymbol{x})$ on $\mathscr{H}_a^1$ in the state $|\bar{b}_a^1\rangle$ of the bound photons:

$$V_a^1(\boldsymbol{x}) := \langle \bar{b}_a^1|A_a^1(\boldsymbol{x})|\bar{b}_a^1\rangle = \langle v|W_{\mathrm{R}}\{M(a,a;\boldsymbol{k})/\omega(\boldsymbol{k})\}A_{\mathrm{R}}(\boldsymbol{x})W_{\mathrm{R}}\{-M(a,a;\boldsymbol{k})/\omega(\boldsymbol{k})\}|v\rangle$$

$$= -\frac{-e}{4\pi}\int \mathrm{d}^3x'|u_a(\boldsymbol{x}')|^2\frac{\exp(-\mu|\boldsymbol{x}-\boldsymbol{x}'|)}{|\boldsymbol{x}-\boldsymbol{x}'|}, \tag{74}$$

(cf (8)). This is clearly the potential we would ascribe to a smeared, pre-statistical Schrödinger electron. *But as a quantum mechanical expectation value it is compatible with a statistical interpretation as well.* A classical potential $V_a^1(\boldsymbol{x})$ is clearly not compatible with a statistical charge density $-e|u_a(\boldsymbol{x})|^2$. Note that the energy of the 'field' $V_a^1(\boldsymbol{x})$ is again the binding energy of photons building it up.

Comparing (73) and (74) with § 6 we see that $-e|u_a(\boldsymbol{x})|^2$ has taken over the role of a charge density which binds photons. The square integrability of $u_a(\boldsymbol{x})$, i.e. the linear integrability of $|u_a(\boldsymbol{x})|^2$, does not yet guarantee $\bar{n}_a^{\mathrm{B}} < \infty$, i.e. the absence of ultraviolet divergences. However, as $|u_a(\boldsymbol{x})|^4$ is linearly integrable for practically any reasonable external potential $V(\boldsymbol{x})$, the absence of ultraviolet divergences is guaranteed in practically any case of interest though in principle we must postulate it in the form of additional conditions on $j(\boldsymbol{x})$. As $u_a(\boldsymbol{x})$ is normalised to 1 the infrared problem cannot be postulated away so easily. *The number of massless photons bound to a bound electron is always infinite.* However, on the 'correct' level of external charges the infrared problem will disappear at least in the case of a neutral atom, as we shall see.

We want to emphasise that we do not advocate the pre-statistical interpretation of Schrödinger. On the contrary, our results are compatible with the Born interpretation and extend the latter to the notion of 'forces' and 'Coulomb fields'.

We consider now the case $s > 1$, $I = (a_1, \ldots, a_s)$. The correction E_I^{B} of the energy $E_{a_1} + \ldots + E_{a_s}$ of the eigenstate $U(A^s; X^s)$ of s electrons without self- and mutual interaction is given in (68). Inserting (65a) we find

$$E_I^{\mathrm{B}} = \frac{1}{2} \sum_{\sigma=1}^{s} \sum_{\tau=1}^{s} \int \mathrm{d}^3x \int \mathrm{d}^3x' (-e|u_{a_\sigma}(\boldsymbol{x})|^2)(-e|u_{a_\tau}(\boldsymbol{x})|^2) \frac{\exp(-\mu|\boldsymbol{x}-\boldsymbol{x}'|)}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|}$$

$$= \sum_{\sigma=1}^{s} E_{a_\sigma}^{\mathrm{B}} + \sum_{\sigma=1}^{s} \sum_{\tau<\sigma} E_{\sigma\tau}^{\mathrm{B}}. \tag{75}$$

$E_{\sigma\tau}^{\mathrm{B}} \geqslant 0$ is short for the double integral in the case $\sigma \neq \tau$. It can obviously be understood as the static Coulomb–Yukawa interaction energy of the infinitesimal charge elements belonging to Schrödinger electrons in *different* states $u_{a_\sigma}(\boldsymbol{x})$, $u_{a_\tau}(\boldsymbol{x})$, i.e. to 'different electrons'. We learn that the energy correction E_I^{B} of the s-electron state $U(A^s; X^s)$ is the sum of the self-energies of the single electrons plus the mutual interaction energies of all pairs of electrons, each pair being counted once. Whatever the nature of this interaction, it is in any case a 'two-body interaction'. Its close relation to the Coulomb–Yukawa force will become clear in § 9.

As E_I^{B} is again the expectation value of the operator of the energy of photons in the eigenstate $|\bar{b}_I^s\rangle$ of $\bar{H}_I^s$ it can again be considered as the binding energy of photons bound to the s electrons in the state $U(A^s; X^s)$ with $A^s = I$. Equation (75) tells us that this binding energy is greater than the sum of the binding energies of photons bound to 'isolated' electrons in the corresponding states. This excess causes the interaction *between* the electrons.

The number of photons bound to s electrons in the state $U(A^s; X^s)$ shows a similar excess. We find that

$$\bar{n}_I^{\mathrm{B}s} := \langle \bar{b}_I^s | N_I^s | \bar{b}_I^s \rangle$$

$$= \int \mathrm{d}^3k |M_I(\boldsymbol{k})/\omega(\boldsymbol{k})|^2$$

$$= \frac{e^2}{2} \sum_{\sigma=1}^{s} \sum_{\tau=1}^{s} \int \mathrm{d}^3x \int \mathrm{d}^3x' |u_{a_\sigma}(\boldsymbol{x})|^2 |u_{a_\tau}(\boldsymbol{x}')|^2 K_0(\mu|\boldsymbol{x}-\boldsymbol{x}'|)/2\pi^2. \tag{76}$$

As $K_0(z) \geqslant 0$, all terms in the double sum are non-negative. The terms $\tau = \sigma$ yield the sum of the numbers of photons bound to 'isolated' electrons. The other terms account

for photons bound in addition which obviously cause the excess of binding energy mentioned above.

The potential built up by these bound photons is

$$V_I^s(\boldsymbol{x}) := \langle \bar{b}_I^s | A_I^s(\boldsymbol{x}) | \bar{b}_I^s \rangle$$

$$= -\frac{1}{(2\pi)^{3/2}} \int \mathrm{d}^3k [\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} M_I(\boldsymbol{k})/(2\omega(\boldsymbol{k}))^{1/2} + \mathrm{cc}]$$

$$= V_{a_1}^1(\boldsymbol{x}) + \ldots + V_{a_s}^1(\boldsymbol{x}). \tag{77}$$

The additional photons do not explicitly contribute to $V_I^s(\boldsymbol{x})$, but their energy is contained in the field energy of $V_I^s(\boldsymbol{x})$ which is greater than the sum of the field energies of the single terms in (77).

8. A quantum theory of the screening of an external charge by bound electrons

So far we have emphasised that bound electrons themselves 'bind' photons which leads to the various self-energy effects discussed so far. These energy corrections indicated already that this binding of photons must also have some other consequences. First we consider the screening of the external charge by the electrons bound to it.

It is clear that $V(\boldsymbol{x}) + V_I^s(\boldsymbol{x})$ is the first candidate for the 'total potential of an s-electron atom in the state $U(A^s; X^s)$'. But on the conceptual level of external fields $V(\boldsymbol{x})$ is a *classical field* which in principle is free of quantum fluctuations whereas $V_I^s(\boldsymbol{x})$ is a *quantum mechanical expectation value* which in principle is equipped with quantum mechanical variances. In our case the corresponding quantum field fluctuations are even infinitely strong. The sum $V(\boldsymbol{x}) + V_I^s(\boldsymbol{x})$ therefore makes no sense.

We remember now, however, that $\bar{H}_I^s$ is a part of the *auxiliary* Hamiltonian $\bar{H}^s$ which was introduced in (31) for convenience. The part H_I^s of the true H^s which corresponds to $\bar{H}_I^s$ is obviously given by

$$H_I^s = W^s\{-f(\boldsymbol{k})\} \bar{H}_I^s W\{f(\boldsymbol{k})\}, \tag{78}$$

(cf (26)). Noting that each minimal $I = A^s$ defines a base vector $U(A^s; X^s)$ of $\mathscr{H}_S^s$ the operator $W^s\{-f(\boldsymbol{k})\}$ can be considered as the *direct* sum of the $W_I^s\{-f(\boldsymbol{k})\}$ defined by (25) on the Hilbert spaces $\mathscr{U}(A^s) \otimes \mathscr{F}_R$. So in (78) we may replace W^s by W_I^s. Using the relation

$$W_R\{f(\boldsymbol{k}) + g(\boldsymbol{k})\} = W_R\{f(\boldsymbol{k})\} W_R\{g(\boldsymbol{k})\} \exp\left(\mathrm{i}\,\mathrm{Im} \int \mathrm{d}^3k f^*(\boldsymbol{k}) g(\boldsymbol{k})\right) \tag{79}$$

we get by inserting (69) into (78)

$$H_I^s = W_I^s\{-f_I(\boldsymbol{k})\} \left(E_I^s + \int \mathrm{d}^3k \omega(\boldsymbol{k}) a^+(\boldsymbol{k}) a(\boldsymbol{k})\right) W_I^s\{f_I(\boldsymbol{k})\} \tag{80}$$

with the definition

$$f_I(\boldsymbol{k}) = f(\boldsymbol{k}) + M_I(\boldsymbol{k})/\omega(\boldsymbol{k}). \tag{81}$$

H_I^s assumes an *eigenstate*

$$|b_I^s\rangle := U(A^s; X^s) \otimes W_R\{-f_I(\boldsymbol{k})\} |v\rangle \tag{82}$$

to the same eigenvalue E_I^s as the auxiliary $\tilde{H}_I^s$. The physical structure and explanation of the *eigenvalue* can be taken over from § 7. But the *true eigenstate* $|b_I^s\rangle$ is different from the auxiliary $|\tilde{b}_I^s\rangle$, and this difference is of decisive importance as we shall see now.

We note first that the screening of the external charge $Zej(\boldsymbol{x})$ by the electrons bound to it is achieved *automatically* on the correct conceptual level of external charges. As 'total potential of the s-electron atom in the state $U(A^s; X^s)$' we must obviously take the expectation value of the potential operator $A_I^s(\boldsymbol{x})$ in the true eigenstate $|b_I^s\rangle$ of H_I^s. *By means of* (81) we get for this $V(\boldsymbol{x})+V_I(\boldsymbol{x})$. This sum is now acceptable because both summands are quantum mechanical expectation values of the same kind with (infinite) variances of the same kind. A glance at (8), (74), and (77) shows that $V(\boldsymbol{x})$ and $V_I^s(\boldsymbol{x})$ have opposite signs if $Zej(\boldsymbol{x})>0$, as it is natural, for example, if $Zej(\boldsymbol{x})$ 'describes' a nucleus with Z proton charges. For $s=Z$ the long-range tails of $V(\boldsymbol{x})$ and $V_I^s(\boldsymbol{x})$ cancel so that $V(\boldsymbol{x})+V_I^s(\boldsymbol{x})$ falls off at large $|\boldsymbol{x}|$ like $|\boldsymbol{x}|^{-2}$. Therefore, if the 'atom' is considered from the outside it appears as 'neutral' because the nuclear charge is completely screened by the electrons.

As $|b_I^s\rangle$ is again an eigenstate of the 'governing Hamiltonian' H_I^s the total potential $V(\boldsymbol{x})+V_I^s(\boldsymbol{x})$ is again 'built up' by photons which are now *simultaneously bound* to the electrons and the external charge. The mean number of these photons is

$$
\begin{aligned}
n_I^{Bs} &:= \langle b_I^s|N_I^s|b_I^s\rangle \\
&= \int \mathrm{d}^3k\,|f(\boldsymbol{k})+M_I(\boldsymbol{k})/\omega(\boldsymbol{k})|^2 \\
&= \frac{e^2}{2}\int \mathrm{d}^3k\frac{1}{\omega(\boldsymbol{k})^3(2\pi)^3}\left|\int \mathrm{d}^3x\ \mathrm{e}^{\mathrm{i}\boldsymbol{k}.\boldsymbol{x}}\Big(Zj(\boldsymbol{x})-\sum_{\sigma=1}^{s}|u_a(\boldsymbol{x})|^2\Big)\right|^2 \\
&= \bar{n}_j^{B}+\bar{n}_I^{Bs}-Ze\sum_{\sigma=1}^{s}\int \mathrm{d}^3x\int \mathrm{d}^3x' j(\boldsymbol{x})|u_a(\boldsymbol{x}')|^2K_0(\mu|\boldsymbol{x}-\boldsymbol{x}'|)/2\pi^2. \qquad (83)
\end{aligned}
$$

For $j(\boldsymbol{x})\geqslant 0$ this is smaller than the sum $n_j^{B}+\bar{n}_I^{Bs}$ of the numbers of photons bound *separately* to the 'nuclear' charge and to s electrons. The second integral over $\boldsymbol{k}$ shows further that n_I^{Bs} remains finite in the case $Z=s$ of a neutral atom even for massless photons. The integral over $\boldsymbol{x}$ defines a continuous function of $\boldsymbol{k}$ which vanishes at $\boldsymbol{k}=0$ so that the integral over $\boldsymbol{k}$ exists. This means that the infrared problem does not show up in the case of a neutral atom.

Note that n_I^{Bs}, considered as a function of s, assumes a minimum roughly for $s=Z$. As $\omega(\boldsymbol{k})^{-3}$ has for any $\mu>0$ a maximum at $\boldsymbol{k}=0$, the main contributions to the integral over $\boldsymbol{k}$ come from the region about $\boldsymbol{k}=0$ where the integral over $\boldsymbol{x}$ assumes a minimum for $s=Z$. For $\mu=0$ this minimum is zero and compensates the infrared divergence of $|\boldsymbol{k}|^{-3}$ to such a degree that n_I^{Bs} remains finite.

The energy of the photons bound simultaneously to $Zej(\boldsymbol{x})$ and to the electrons in the state $U(A^s; X^s)$ is given by

$$
\begin{aligned}
E_{Ij}^{B} &:= \left\langle b_I^s\middle|\int \mathrm{d}^3k\omega(\boldsymbol{k})a^+(\boldsymbol{k})a(\boldsymbol{k})\middle|b_I^s\right\rangle \\
&= \int \mathrm{d}^3k\omega(\boldsymbol{k})|f(\boldsymbol{k})+M_I(\boldsymbol{k})/\omega(\boldsymbol{k})|^2
\end{aligned}
$$

$$= \frac{e^2}{2} \int \mathrm{d}^3k \frac{1}{\omega(\boldsymbol{k})^2 (2\pi)^3} \left| \int \mathrm{d}^3x \, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \left(Zj(\boldsymbol{x}) - \sum_{\sigma=1}^{s} |u_{a_\sigma}(\boldsymbol{x})|^2 \right) \right|^2$$

$$= E_j^{\mathrm{B}} + E_I^{\mathrm{B}} - Ze^2 \sum_{\sigma=1}^{s} \int \mathrm{d}^3x \int \mathrm{d}^3x' j(\boldsymbol{x}) |u_a(\boldsymbol{x}')|^2 \frac{\exp(-\mu|\boldsymbol{x}-\boldsymbol{x}'|)}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|}. \tag{84}$$

For $Zj(\boldsymbol{x}) \geqslant 0$ this is smaller than $E_j^{\mathrm{B}} + E_I^{\mathrm{B}}$, the sum of the binding energies of photons bound *separately* to the external charge and to the electrons. Considered as a function of s, E_{Ij}^{B} also has a minimum around $s = Z$, but it is less pronounced than the minimum of $n_{Ij}^{\mathrm{B}s}$, as seen by a comparison of the second integrals over $\boldsymbol{k}$ in (84) and (83).

If we assume that nature seeks to attain a minimum of the total binding energy, or, still more pronounced, a minimum of the number of bound photons, we can conclude that a state with $s < Z$ *attracts* further electrons whereas a state with $s > Z$ *repels* them. The idea of attractive or repulsive 'forces' can so be 'deduced' from an extremal principle related to bound photons. Note also that the binding of the electrons appears here as a consequence of the simultaneous binding of photons to the external charge and the electrons.

All photon binding phenomena occur also if some or all indices $a_1, \ldots, a_s$ in I do not refer to eigenstates of the Schrödinger equation (32). The difference will show up in higher-order corrections (greater I in the sense of § 5) where 'transitions' between the s-electron states $U(A^s; X^s)$ are allowed to occur. If $U(A^s; X^s)$ contains only eigenstates these transitions are governed only by the interaction Hamiltonian. In the general case the non-diagonal elements $T(a, b)$ of the Hamiltonian of the 'free' electrons (cf (39)) have also an influence on these transitions. The 'stability' of the eigenstates $|b_I^s\rangle$ can therefore be expected to be much weaker for 'free' than for 'bound' electrons, but practically all work on these transitions remains to be done.

9. Comparison of the 'force due to bound photons' with the conventional Coulomb–Yukawa force

The discussion of the binding energies E_I^{B} and E_{Ij}^{B} showed already that the bound photons act as a mediating agent between the electrons which resembles to some degree a repulsive Coulomb–Yukawa 'force'. To learn more about this mechanism we now compare it with the usual Coulomb–Yukawa force.

For this purpose we 'derive' first from the present theory the familiar non-relativistic field theory of Jordan and Wigner (1928) which comprises the usual quantum theories of $s = 1, 2, \ldots$ electrons with Coulomb–Yukawa interaction. Consider the Heisenberg equations

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\bar{\psi}(\boldsymbol{x}, t) = \left(-\frac{\Delta}{2M} - eV(\boldsymbol{x}) \right) \bar{\psi}(\boldsymbol{x}, t) - e\bar{A}(\boldsymbol{x}, t)\bar{\psi}(\boldsymbol{x}, t), \tag{85a}$$

$$\Box \bar{A}(\boldsymbol{x}, t) = -e\bar{\psi}^{\dagger}(\boldsymbol{x}, t)\bar{\psi}(\boldsymbol{x}, t) \tag{85b}$$

which correspond to the auxiliary Hamiltonian $\bar{H}$ given in (31). If $\{\psi^{\dagger}(\boldsymbol{x}, t), \psi(\boldsymbol{x}, t), E(\boldsymbol{x}, t), A(\boldsymbol{x}, t)\}$ is the 'correct' solution of (2), the correct solution of (85) is $\{\bar{\psi}^{\dagger}(\boldsymbol{x}, t) = W\{f(\boldsymbol{k})\}\psi(\boldsymbol{x}, t)W\{-f(\boldsymbol{k})\}, \ldots\}$, with $W\{f(\boldsymbol{k})\}$ defined in (25). The initial conditions for this solution read accordingly. We ignore now the correct initial conditions as well as the correct equal-time commutation relations and take as an

'approximate' solution of (85*b*) the Poisson–Yukawa integral

$$\bar{A}_1(\boldsymbol{x}, t) := e \int \mathrm{d}^3x' \bar{\psi}^\dagger(\boldsymbol{x}', t)\bar{\psi}(\boldsymbol{x}', t)\frac{\exp(-\mu|\boldsymbol{x}-\boldsymbol{x}'|)}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|}. \tag{86}$$

This is an 'approximation' in the same sense in which the Laplace operator Δ is an 'approximation' of the d'Alembert operator $\Box$. We replace, in particular, the 'retarded action' between S and R by an 'action at a distance'. If (86) is inserted into (85*a*) in the order as given we get a Heisenberg equation for the 'approximate' $\bar{\psi}_1(\boldsymbol{x}, t)$ corresponding to the 'approximate' $\bar{A}_1(\boldsymbol{x}, t)$. If the commutation relations (1*a*) are retained for the field operators $\bar{\psi}_1^\dagger(\boldsymbol{x}, t)$, $\bar{\psi}_1(\boldsymbol{x}, t)$, this Heisenberg equation follows from the Hamiltonian

$$\bar{H}_1 := \int \mathrm{d}^3x \bar{\psi}_1^\dagger(\boldsymbol{x})\Big(-\frac{\Delta}{2M} - eV(\boldsymbol{x})\Big)\bar{\psi}_1(\boldsymbol{x})$$
$$-\frac{e^2}{2}\int \mathrm{d}^3x \int \mathrm{d}^3x' \bar{\psi}_1^\dagger(\boldsymbol{x})\bar{\psi}_1^\dagger(\boldsymbol{x}')\bar{\psi}_1(\boldsymbol{x}')\bar{\psi}_1(\boldsymbol{x})\frac{\exp(-\mu|\boldsymbol{x}-\boldsymbol{x}'|)}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|}. \tag{87}$$

As the Schrödinger operators $\bar{\psi}_1^\dagger(\boldsymbol{x})$, $\bar{\psi}_1(\boldsymbol{x})$ must satisfy (4*a*) we may define them by (15), but only on $\mathscr{F}_\mathrm{S}$ which is the natural Hilbert space of S alone. $\bar{H}_1$ is the Hamiltonian of the non-relativistic field theory of Jordan and Wigner (1928) of 'electrons with Coulomb–Yukawa interaction' (with spins omitted). Its interaction part, the second term in (87), looks like a tremendous four-fermion interaction and has been discussed from this point of view by Wahl (1975) (with a special $V(\boldsymbol{x})$).

We look at $\bar{H}_1$ from another point of view. We note that it commutes with the electron number operator (16) so that it 'decays' necessarily into a direct sum of Hamiltonians $\bar{H}_1^s$ which act on the sectors $\mathscr{H}_\mathrm{S}^s$ of $\mathscr{F}_\mathrm{S}$. By a straightforward calculation we find $\bar{H}_1^0 = 0$ and

$$\bar{H}_1^s = \sum_{\sigma=1}^{s}\Big(-\frac{\Delta_\sigma}{2M} - eV(\boldsymbol{x}_\sigma)\Big) - \frac{e^2}{2}\sum_{\sigma=1}^{s}\sum_{\substack{\tau=1\\ \tau\neq\sigma}}^{s}\frac{\exp(-\mu|\boldsymbol{x}_\sigma-\boldsymbol{x}_\tau|)}{4\pi|\boldsymbol{x}_\sigma-\boldsymbol{x}_\tau|}. \tag{88}$$

This operator is understood as acting on an element $\varphi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_s)$ of $\mathscr{H}_\mathrm{S}^s$. So it is the conventional Hamiltonian of s electrons in the potential $V(\boldsymbol{x})$ which interact with the classical Coulomb–Yukawa force. Its 'derivation' from our $\bar{H}$ shows that our theory generalises the concept of the classical Coulomb–Yukawa force and thus in some sense 'contains' it.

The second term of (88), $-\bar{H}_\mathrm{CY}^s$, is obviously the operator of the Coulomb–Yukawa interaction of s electrons. It contains nothing that could be related with the self-energy of the electrons because the terms $\sigma = \tau$ do not occur. By comparing the expectation value $-E_\mathrm{CY}^s$ of $-\bar{H}_\mathrm{CY}^s$ in the state $U(A^s; X^s)$ of these electrons with the correction $-E_I^\mathrm{B}$ of their energy $E_{a_1} + \ldots + E_{a_s}$ due to bound photons we can learn something about the following problems. How much of the usual concept of the Coulomb–Yukawa force is still contained in the quantum field theory defined by (2), and how much of this is contained in the lowest order of the coarse grain expansion of § 5? The answers are obviously decisive for the 'replacement of the classical Coulomb–Yukawa interaction by an interaction mediated by bound photons', as well as for the quality of the approximation method developed in § 4 and § 5, and the interest it deserves.

We consider first some details. By definition we have

$$E^s_{\mathrm{CY}} := \frac{e^2}{4\pi} \int \mathrm{d}X^s U(A^s; X^s)^* \Big(\sum_{\sigma=1}^{s} \sum_{\tau<\sigma} \frac{\exp(-\mu|\boldsymbol{x}_\sigma - \boldsymbol{x}_\tau|)}{|\boldsymbol{x}_\sigma - \boldsymbol{x}_\tau|} \Big) U(A^s; X^s). \tag{89}$$

Using the expansion law of determinants and introducing

$$E^{\mathrm{th}}_{\sigma\tau} := \int \mathrm{d}^3k |M(a_\sigma, a_\tau; \boldsymbol{k})|^2/\omega(\boldsymbol{k}), \tag{90}$$

the shift of the line corresponding to the transition $u_{a_\sigma}(\boldsymbol{x}) \leftrightarrow u_{a_\tau}(\boldsymbol{x})$ of the one-electron atom (cf Källén 1958, Grimm and Ernst 1975) or, more precisely, the threshold energy (Grimm and Ernst 1975) of this transition, we find after some straightforward computation

$$E^s_{\mathrm{CY}} = \sum_{\sigma=1}^{s} \sum_{\tau<\sigma} (E^{\mathrm{B}}_{\sigma\tau} - E^{\mathrm{th}}_{\sigma\tau}). \tag{91}$$

Comparing this with (75) we get finally

$$E^{\mathrm{B}}_I = E^s_{\mathrm{CY}} + \sum_{\sigma=1}^{s} E^{\mathrm{B}}_{a_\sigma} + \sum_{\sigma=1}^{s} \sum_{\tau<\sigma} E^{\mathrm{th}}_{\sigma\tau}. \tag{92}$$

All terms are non-negative and finite. We recall now that the widely unsolved, classical problem of many-electron atomic physics is the computation of the eigenvalues of $\bar{H}^s_{\frac{1}{2}}$. If this problem is attacked by considering $-\bar{H}^s_{\mathrm{CY}}$ as a perturbation of the first term of (88), the first-order perturbation correction of the 'unperturbed' eigenvalue $E_{a_1} + \ldots + E_{a_s}$ is $-E^s_{\mathrm{CY}}$, as computed above. It follows therefore from (92) that the correction $-E^{\mathrm{B}}_I$ of this eigenvalue due to photons bound to the electrons is always larger in magnitude than the first-order correction $-E^s_{\mathrm{CY}}$ from the traditional Coulomb–Yukawa force. Equation (92) shows that the difference is due to typical quantum effects which are not contained in the traditional theories of electrons 'with classical Coulomb–Yukawa interaction'.

It is suggestive to assume that the eigenstates $|b^s_I\rangle$ of the H^s_I corresponding to the eigenvalues $E_{a_1} + \ldots + E_{a_s} - E^{\mathrm{B}}_I$ are the 'true' eigenstates of an s-electron atom. The main arguments in favour of this hypothesis are: (i) the expected 'stability' of these eigenstates under higher-order corrections; (ii) the perfect screening of the 'nuclear' charge $Zej(\boldsymbol{x})$ by the electrons bound to it by means of bound photons. This shows in particular that higher-order corrections should not lead to additional energy shifts because the latter are related to additional bound photons which in general should destroy the perfect screening already obtained. (iii) The 'true' eigenvalues lie always below the values obtained from the traditional Coulomb–Yukawa interaction in first-order perturbation theory. The hypothesis thus does not necessarily lead to contradictions of experience. (iv) A reason for wishing this hypothesis to be true is that even the 'true spectrum' of the iron atom could be computed numerically because the calculation of the terms in (92) is not difficult for an electronic computer.

At this point we must clearly remember that the present model is not yet realistic. But there are so many analogies to the covariant Gupta–Bleuler form of quantum electrodynamics that an extension of our methods appears to be highly prospective. We are well aware of the many problems ahead (state space 'with indefinite metric' instead of our $\mathscr{F}_{\mathrm{R}}$, charge conservation instead of our electron number conservation, to mention the severest only).

10. Comparison with the concepts of the self-energy of an electron in classical and quantum electrodynamics

We compare finally the concept of the self-energy of an electron as introduced in §§ 7–9 with the concepts used in classical and quantum electrodynamics.

Let us recall first that the classical self-energy of an electron at rest (cf Born and Infeld 1934, Sommerfeld 1961, Bopp and Lutzenberger 1974, and the literature cited there) is the electrostatic field energy $\frac{1}{2}\int d^3x \boldsymbol{E}(\boldsymbol{x})^2$ of the Coulomb field $E(\boldsymbol{x}) \sim |\boldsymbol{x}-\boldsymbol{X}_a|^{-2}$ surrounding an electron (='point charge') at $\boldsymbol{X}_a$. Electrons at different positions $\boldsymbol{X}_a$ have the same self-energy, and the self-energy of moving electrons is computed by means of Gallilei or Lorentz transformations. Considering an electron in its phase space ϕ we can therefore say that even classically its self-energy depends on its instantaneous 'state' $(\boldsymbol{P}_a, \boldsymbol{X}_a)$ in ϕ, although it may be degenerate with respect to the position $\boldsymbol{X}_a$.

As any 'quantisation' consists primarily of the replacement of the classical state space ϕ by the quantum mechanical state space, a Hilbert space (in our case: $\phi \to \mathscr{H}^1_S$), the closest analogue of the self-energy of an electron in some classical state $(\boldsymbol{P}_a, \boldsymbol{X}_a) \in \phi$ is the self-energy of an electron in some quantum mechanical state $u_a(\boldsymbol{x}) \in \mathscr{H}^1_S$. The results of §§ 7–9 suggest a very convincing definition of this self-energy, namely as the classical self-energy of a 'smeared electron' in the sense of Schrödinger's (1926) pre-statistical interpretation of quantum mechanics. The discussion of (72)–(74) showed that this allows a deep-lying, fully quantum mechanical interpretation as well, namely as binding energy of photons bound to the electron and building up the latter's 'eigen-Coulomb field' in the sense of a quantum mechanical expectation value. This self-energy is invariant under translations in the sense that the translated state $u_a(\boldsymbol{x}-\boldsymbol{X}_a)$ leads to the same self-energy as $u_a(\boldsymbol{x})$.

If $\boldsymbol{E}_1(\boldsymbol{x}), \ldots, \boldsymbol{E}_s(\boldsymbol{x})$ are the eigen-Coulomb fields of s electrons at rest, their common Coulomb field is $\boldsymbol{E}_1(\boldsymbol{x}) + \ldots + \boldsymbol{E}_s(\boldsymbol{x})$, and their common self-energy $\frac{1}{2}\int d^3x (\boldsymbol{E}_1(\boldsymbol{x}) + \ldots + \boldsymbol{E}_s(\boldsymbol{x}))^2$ is greater than the sum $\frac{1}{2}\int d^3x (\boldsymbol{E}_1(\boldsymbol{x})^2 + \ldots + \boldsymbol{E}_s(\boldsymbol{x})^2)$ of the individual self-energies. We saw in § 7 that the concept of bound photons leads to an exactly analogous situation.

The individual self-energy of a classical electron is infinite due to its 'point-likeness'. If quantisation, i.e. the replacement $\phi \to \mathscr{H}^1_S$, is taken seriously, this point-likeness disappears once and for all because all information on the electron is contained in $u_a(\boldsymbol{x})$ which is not related to some particular point $(\boldsymbol{P}_a, \boldsymbol{X}_a)$ of the classical phase space. In this sense the present approach has solved the problem of infinite self-energies. We are of course aware of the fact that this implies a certain *semantic* decision, but for the many good reasons discussed in §§ 7–9 this decision appears to be appropriate.

This implies, in particular, the decision that the self-energy of an electron in some proper state of the Hilbert space should be defined *before* one looks at singular cases like an electron localised in some point $\boldsymbol{X}_a$ of the position space or in some plane wave state. The former case could be described formally by $|u_a(\boldsymbol{x})|^2 = \delta(\boldsymbol{x}-\boldsymbol{X}_a)$ and leads to the classical divergence. However, there is no sequence of normalised Hilbert vectors whose squares converge in some reasonable sense against $\delta(\boldsymbol{x}-\boldsymbol{X}_a)$. The case of a plane wave is similarly not approachable within the unit sphere of the Hilbert space. In the sense of the usual box normalisation we might put $u_a(\boldsymbol{x}) = e^{i\boldsymbol{x}\cdot\boldsymbol{P}_a}/\Omega^{1/2}$ where Ω denotes the volume of the chosen box, and in view of later transitions to an infinite box we may restrict spatial integrations to one box. Evaluating (72) in this sense we

find $E_a^B = e^2/(2\mu^2\Omega)$. This allows no unambiguous limit for $\Omega \to \infty$ and $\mu \to 0$. In view of the long range of the Coulomb force it is further questionable whether the neglect of the 'other' boxes is justified even if they are at infinity.

In terms of Feynman graphs the self-energy of an electron is usually discussed in connection with the familiar self-energy graph corresponding to the element of the S-matrix for the transition from a state with one electron in some given plane wave state and no photons at $t = -\infty$ to the same state at $t = +\infty$. This implies the assumption that initially and finally the electron is 'bare of photons'. In our approach the self-energy problem is formulated differently. We ask for a state of *one electron* (maybe even a plane wave state) *and photons* such that the system evolves in time by a pure phase factor e^{-itE}. The initial state is therefore not specified by our *question*; it is to be determined by the *answer* we expect. So we get a typical eigenvalue problem. In this connection our present results mean the following. To any given Hilbert state of the electron one can indeed find a *partial* Hamiltonian so that a state of infinitely many photons can be constructed which, under the action of that partial Hamiltonian, evolves in time by a pure phase factor. In fact, an eigenstate of the total Hamiltonian is uninteresting because no transitions to and from it are possible at all. Since under the action of this partial Hamiltonian the electron remains in its initial state, only the four-momentum transfer $q = 0$ contributes to its self-energy in our sense. But as infinitely many photons exist already in the initial state, these contributions are sufficient to equip each electron with its own Coulomb field and to establish the Coulomb interaction between the electrons.

These comparisons show that the intriguing concept of the self-energy of an electron, as introduced here, cannot be expressed easily and in an unambiguous way in the terminology of Feynman graphs. We must emphasise again that the hierarchy of approximations described in § 5 and § 6 is self-reliant, autonomous, and independent of the hierarchy of perturbation theoretical approximations as expressed in terms of Feynman graphs. Thus the approach could be a real alternative to perturbation theory. The purpose of this work has been to show that it is a prospective alternative.

Appendix. The present theory as a singular case of three interacting fields

Consider three interacting fields S, R, S′, to be governed by the Heisenberg equations

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi(\boldsymbol{x}, t) = \left(-\frac{\Delta}{2M} - eA(\boldsymbol{x}, t)\right)\psi(\boldsymbol{x}, t), \tag{A.1}$$

$$(\Box - \mu^2)A(\boldsymbol{x}, t) = -e\psi^\dagger(\boldsymbol{x}, t)\psi(\boldsymbol{x}, t) + e\psi'^\dagger(\boldsymbol{x}, t)\psi'(\boldsymbol{x}, t), \tag{A.2}$$

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi'(\boldsymbol{x}, t) = h\{eA(\boldsymbol{x}, t)\}\psi'(\boldsymbol{x}, t). \tag{A.3}$$

$\psi(\boldsymbol{x}, t)$ and $A(\boldsymbol{x}, t)$ as well as $\psi'(\boldsymbol{x}, t)$ and $A(\boldsymbol{x}, t)$ shall satisfy the commutation relations (1) and all commutators of operators referring to S and S′ shall vanish. S′ is therefore a second field of fermions of charge $e > 0$. For $e = 0$ the system 'decays' into three independent systems S, R, S′. We note that the quanta of S and S′ interact only by means of the quanta of R. Equation (A.2) tells us that both S and S′ constitute the 'source' of R whereas the field amplitude $A(\boldsymbol{x}, t)$ of R plays the role of a 'potential' for S as well as for S′ (cf (A.1), (A.3)). The Hilbert space of the interacting system is

obviously the product $\mathcal{H} := \mathcal{F}_S \otimes \mathcal{F}_R \otimes \mathcal{F}_{S'}$ of the Fock spaces of the interacting partners.

Assume now that S' is 'degenerate' so that its quanta can neither move nor react in any way on the quanta of R and S. This is obviously the case if $h\{eA(x, t)\} = 0$ so that the Heisenberg operator $\psi'(x, t)$ of the field amplitude of S' is equal to the Schrödinger operator $\psi'(x)$. So we get in (A.2) a stationary source term $e\psi'^{\dagger}(x)\psi'(x)$. In the Schrödinger picture, the condition $d\psi'(x, t)/dt = 0$ means that all Schrödinger amplitudes of any s' quanta of S' are independent of t. So, whatever the initial state $|\chi'\rangle$ of S', it remains in that state for ever. The 'accessible' part of the Hilbert space of the system (S, R, S') therefore is $\mathcal{F}_S \otimes \mathcal{F}_R \otimes |\chi'\rangle$. As soon as $|\chi'\rangle$ has been specified, S' behaves like a system with a one-dimensional Hilbert space in which every operator equals its expectation value. So we can replace in (A.2) the operator $e\psi^{\dagger}(x)\psi'(x)$ by its expectation value in $|\chi'\rangle$. If the latter is denoted by $Zej(x)$ we get (2), i.e. an 'external charge density', but we do not get an 'external potential' like (8). We note further that for a great manifold of states $|\chi'\rangle$ of S' the above expectation value $Zej(x)$ can be assumed square integrable. Point sources are quite unnatural in this connection.

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