RELATIVISTIC CORRECTIONS TO MANY ELECTRON ATOMIC LEVELS

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A general procedure is proposed for calculating the relativistic corrections to the levels of many-electron atoms in any order of perturbation theory. The part of the interaction due to the exchange of high-energy photons is taken into account by means of an effective potential. A mixed gauge is employed for the electromagnetic potentials. Concrete expressions for the level shift in the order α^3 Ry are presented.

1. INTRODUCTION

A very important success of contemporary quantum electrodynamics has been the calculation of the corrections to the levels of hydrogen-like atoms due to the interaction with the radiation field. The generalization of these results to many-electron atoms is a very complicated problem and has not, to our knowledge, been carried out in a systematic fashion. Araki[1] and Sucher[2] have calculated the corrections for two-electron atoms, but their methods are specific to the case of two electrons and cannot be generalized immediately to problems with a larger number of electrons. The difficulties in the calculation of the radiative corrections for many-electron atoms arise, on one hand, from the known troubles of quantum electrodynamics connected with the infrared divergencies and, on the other hand, from the complications specific to the many-electron problem which are connected with disconnected graphs and which do not allow one to write down simple equations of the Bethe-Salpeter type.

In the present paper we overcome these difficulties in, as it seems to us, the most simple and natural fashion. Not having an equation of the Bethe-Salpeter type at our disposal, we try to write down a Schrödinger type equation for our problem, with interaction potentials between the electrons among each other and the nucleus. In order to avoid the infrared divergencies, we divide the electromagnetic field into a soft and a hard part, as is often done. The interaction due to the hard component is taken into account by means of potentials. The interaction of the electrons with the soft component of the field is included explicitly in the Schrödinger equation. The resulting scheme of calculation is internally consistent and is in principle applicable in all orders of perturbation theory. However, the calculation of the corrections is practicable only in the lowest orders α^2 Ry and α^3 Ry. In the present paper we calculate the corrections in these orders, including also terms of the order $(m/M)\alpha^2$ Ry, where m is the mass of the electron, and M is the mass of the nucleus.

The total level shift of a many-electron atom is divided into two parts, one of which is the Bethe logarithm, while the second can be written as an average value over nonrelativistic wave functions of some effective interaction U:

$$\Delta E_n = \Delta E_n^{(B)} + U_{nn}, \tag{1}$$

where $\Delta E_n^{(B)}$ is the Bethe term,

$$\Delta E_n^{(B)} = \frac{2}{3}\frac{\alpha}{m^2}\sum_{n'}(E_n - E_{n'})|\mathbf{P}_{nn'}|^2 \ln\left|\frac{E_n - E_{n'}}{m\alpha^2}\right|, \qquad \mathbf{P} = \sum_{i=1}^{l}\mathbf{p}_i, \tag{2}$$

and the operator U is given by

$$U = \sum_{i<k=0}^{l} U_{ik} - \sum_{i=1}^{l}\frac{p_i^4}{8m^2}, \tag{3}$$

$$\begin{aligned} U_{0i} = {} & \frac{\alpha Z\pi}{2m^2}\delta^{(3)}(\mathbf{r}_i) + \frac{Z\sqrt{\alpha}}{2m}\Big\{\mu_i'[\mathbf{r}_i\mathbf{p}_i] \\ & - 2\frac{m}{M}(\mu_i[\mathbf{r}_i\mathbf{p}_0])\Big\}\frac{1}{r_i^3} + \frac{\sqrt{\alpha}}{m}(\mu_0[\mathbf{r}_i\mathbf{p}_i])\frac{1}{r_i^3} \\ & + \frac{Z\alpha}{2mM}\left(\mathbf{p}_i\mathbf{p}_0 + \frac{(\mathbf{p}_i\mathbf{r}_i)(\mathbf{p}_0\mathbf{r}_i)}{r_i^2}\right)\frac{1}{r_i} + \frac{8\pi}{3}\mu_i\mu_0\delta^{(3)}(\mathbf{r}_i) \\ & - \left(\mu_i\mu_0 - \frac{3(\mu_i\mathbf{r}_i)(\mu_0\mathbf{r}_i)}{r_i^2}\right)\frac{1}{r_i^3} + \frac{Z\alpha^2}{m^2}\left(\frac{38}{45} - \ln 2\alpha^2\right)\delta^{(3)}(\mathbf{r}_i) \end{aligned} \tag{4}$$

(in the center-of-inertia system $\mathbf{p}_0 = -\mathbf{P}$),

$$\begin{aligned} U_{ik} = {} & -\frac{\alpha\pi}{m^2}\delta^{(3)}(\mathbf{r}_{ik}) + \frac{\sqrt{\alpha}}{2m}\{\mu_k'[\mathbf{r}_{ik}\mathbf{p}_k] \\ & - \mu_i'[\mathbf{r}_{ik}\mathbf{p}_i] + 2(\mu_i[\mathbf{r}_{ik}\mathbf{p}_k]) - 2(\mu_k[\mathbf{r}_{ik}\mathbf{p}_i])\}\frac{1}{r_{ik}^3} \\ & - \frac{\alpha}{2m}\left(\mathbf{p}_i\mathbf{p}_k + \frac{(\mathbf{p}_i\mathbf{r}_{ik})(\mathbf{p}_k\mathbf{r}_{ik})}{r_{ik}^2}\right)\frac{1}{r_{ik}} - \frac{8\pi}{3}(\mu_i\mu_k)\delta^{(3)}(\mathbf{r}_{ik}) \\ & + \left(\mu_i\mu_k - \frac{3(\mu_i\mathbf{r}_{ik})(\mu_k\mathbf{r}_{ik})}{r_{ik}^2}\right)\frac{1}{r_{ik}^3} \\ & + \frac{\alpha^2}{m^2}\left(\frac{14}{3}\ln\alpha + \frac{43}{5} + \frac{5}{3}\sigma_i\sigma_k\right)\delta^{(3)}(\mathbf{r}_{ik}) \\ & - \frac{7}{6\pi}\frac{\alpha^2}{m^2}\{r_{ik}^{-3}(a) + 4\pi(\ln(m\alpha a) + C)\delta^{(3)}(\mathbf{r}_{ik})\} \quad (i,k \neq 0). \end{aligned} \tag{5}$$

Here we have used the following notation. The particles are numbered by the indices 0 to l, where 0 corresponds to the nucleus (coordinate $\mathbf{r}_0 = 0$), and i = 1, ..., l correspond to the electrons (coordinates $\mathbf{r}_i$); $\mathbf{r}_{ik} = \mathbf{r}_i - \mathbf{r}_k$; $\mathbf{p}_i$ (i = 0, ..., l) are the momenta of the particles; m is the mass of the electron, M is the mass of the nucleus, Z is the charge of the nucleus; μ_i are the magnetic moments of the particles (with account of the anomalous magnetic moments); σ_i are the Pauli matrices. For the electrons $\mu_i' = (\sqrt{\alpha}/2m)(1 + \alpha/\pi)\sigma_i$. Further, $r^{-3}(a) = \theta(r - a)r^{-3}$, where θ is the unit step function, and a is set equal to zero after calculation of the average

*$[\mathbf{r}_i\mathbf{p}_i] \equiv \mathbf{r}_i \times \mathbf{p}_i$.

value. C is the Euler constant. We have everywhere used units such that $\hbar = c = 1$.

2. GENERAL SCHEME OF CALCULATION

Let us consider the interaction of l Dirac particles (electrons) with the electromagnetic field. Our starting point is the l-particle Green's function

$$G = i^l \langle 0 | T\{\psi(x_1')\bar{\psi}(x_1), \ldots, \psi(x_l')\bar{\psi}(x_l)\} | 0\rangle,$$

which, in the momentum space, has a pole in the total energy of the particles at the point corresponding to the desired energy level. We try to choose a nonrelativistic Hamiltonian for the interaction of the l electrons which gives in each order of perturbation theory the corresponding contribution to the Green's function G and is thus convenient for the calculation of the energy level by standard nonrelativistic methods.

Let us consider the set of all Feynman graphs for G in momentum space. We divide the electron Green's functions (S) and the photon Green's functions (D) entering in these graphs into a soft (s) and a hard (h) component according to the following rules:

1. Lines connected with closed electron loops (i.e., electron lines in a loop or photon lines ending in a loop at least at one end) are not so divided.

2. The remaining electron lines are divided into a soft (electron) part S_s and a hard (positron) part S_h:

$$S_{s(h)}(\mathbf{p}, \varepsilon) = \frac{1}{2\sqrt{m^2+\mathbf{p}^2}} \frac{m + (-)\gamma_0\sqrt{m^2+\mathbf{p}^2} - \mathbf{p}\gamma}{\sqrt{m^2+\mathbf{p}^2} - (+)\varepsilon - i0}. \tag{7}$$

3. Photon lines beginning and ending at the same electron line are divided into a hard, Coulomb, and soft part:

$$D_h^{\alpha\beta} = \frac{1}{k^2}\theta(|\mathbf{k}| - \lambda) g_{\alpha\beta}. \tag{8}$$

$$D_c^{\alpha\beta} = -\frac{1}{\mathbf{k}^2}\theta(\lambda - |\mathbf{k}|) g_{\alpha 0} g_{\beta 0}, \tag{9}$$

$$D_s^{\alpha\beta} = \frac{1}{k^2}\theta(\lambda - |\mathbf{k}|)\left(g^{pq} + \frac{k^p k^q}{\mathbf{k}^2}\right) g_{\alpha p} g_{\beta q}. \tag{10}$$

Here $g^{\alpha\beta}$ is the metric tensor ($g^{00} = 1$, $g^{11} = g^{22} = g^{33} = -1$), p, q = 1, 2, 3.

4. Photon lines beginning and ending on different electron lines are divided into the same parts according to the formulas

$$D_h^{\alpha\beta} = \frac{1}{k^2}\theta(|\mathbf{k}| - \lambda)\left(g^{pq} + \frac{k^p k^q}{\mathbf{k}^2}\right) g_{\alpha p} g_{\beta q}, \tag{11}$$

$$D_c^{\alpha\beta} = -\frac{1}{\mathbf{k}^2} g_{\alpha 0} g_{\beta 0}, \tag{12}$$

$$D_s^{\alpha\beta} = \frac{1}{k^2}\theta(\lambda - |\mathbf{k}|)\left(g^{pq} + \frac{k^p k^q}{\mathbf{k}^2}\right) g_{\alpha p} g_{\beta q}. \tag{13}$$

After this division, we can consider the graphs with soft and hard parts separately. We shall regard the Coulomb lines and lines connected with closed loops as hard lines.

We call a connected graph irreducible if it is such that no nontrivial cut can be laid through it which intersects once each of the l electron lines connected with the ends of the graph, and goes only across soft lines. A cut is called nontrivial if it does not run only across external lines. If such a cut can be laid through the graph, the graph is called reducible. After the cut is laid through a reducible graph, the latter falls into two parts connected by soft electron and photon lines. These parts may in turn be reducible or irreducible. The whole set of graphs is obtained by taking the irreducible graphs and joining them by soft lines. It is easy to see that all graphs which are irreducible in our sense do not contain infrared divergencies and are therefore smooth functions of the electron energies ε_l in the neighborhood of the mass surface $\varepsilon_l = \sqrt{m^2 + \mathbf{p}^2}$. In first approximation we can therefore set $\varepsilon_l = \sqrt{m^2 + \mathbf{p}^2}$ for the external lines and $k^2 = 0$ for the photons in the irreducible graphs. Then these graphs no longer depend on the energy and take on the character of a potential.

The soft electron line (7) can be written in the form

$$S_s(\mathbf{p}, \varepsilon) = \sum_{i=1}^{2} \frac{u^i(\mathbf{p})\bar{u}^i(\mathbf{p})}{\sqrt{m^2+\mathbf{p}^2} - \varepsilon}. \tag{14}$$

Each irreducible graph, considered as a 4×4 matrix in the spinor indices of the i-th particle, stands between the four-spinors $u^i(\mathbf{p})$ and can be reduced to a two-component structure.

After this, the whole set of graphs will correspond to a theory in which the nonrelativistic electrons interact with a soft transverse photon field [the Green's functions of which correspond to formulas (10) and (13)] and with one another via a potential which in momentum space has a kernel equal to the sum of all irreducible graphs on the mass shell. In the exact theory the irreducible graphs depend on the energy. This dependence can be taken into account by writing the contribution of such a graph in the form

$$M = M_0 + M', \tag{15}$$

where M_0 is the contribution on the mass shell. The quantity M' contains a factor of the type $\varepsilon - \sqrt{\mathbf{p}^2 + m^2}$ or k^2. When multiplied by the corresponding soft line, they remove the pole from the latter. Such a line may be regarded as hard, and thus a previously reducible graph becomes irreducible of higher order than the irreducible graphs of which it is formed. With the new irreducible graph we can proceed as before in the same way. We divide it up according to (15). The second term gives rise to new irreducible graphs, etc. All these new irreducible graphs must be added to the potential.

We note that the spinors u^i in (14) do not depend on ε. The separation (15) can therefore be carried out in two- as well as in four-component form.

3. MASS AND CHARGE RENORMALIZATION

Since the expressions (8) to (13) for the photon Green's function are explicitly non-covariant, the renormalization of our theory cannot be carried through as simply as in the Feynman theory. We begin with the renormalization of the mass of the electron. We shall assume that the graphs contain an additional interaction with the vertex δm effecting this renormalization. If we write δm in the form of a sum of Feynman graphs, these graphs can also be divided into reducible and irreducible parts. The contribution from the reducible graphs is included explicitly by adding to the Hamiltonian for the interaction of the l electrons the necessary counter terms. They will be functions of the momentum of the corresponding particle and are deter-

mined by the obvious condition that in the absence of the other electrons, the interaction with the soft transverse photons must not lead to an energy shift for the free electron. The contribution from the irreducible graphs to δm will be taken into account, as usual, by subtracting from the graph for the self-energy of the electron its value on the mass shell.

Let us now turn to the renormalization of the charge. All lines connected with closed electron loops are regarded as hard lines and will not be divided into parts. We can therefore assume that the renormalization of the photon lines and of the graphs for the scattering of light by light has already been carried out from the very beginning. The vertices of the graphs then contain the quantity $e_0^2 Z_3$, i.e., the physical charge e^2. Hence, no additional renormalization is required. However, the graphs contain divergencies from the vertex parts and from the self-energy of the electron, which compensate each other, as is well known. In order to guarantee this compensation, we separate in each electron line the irreducible self-energy part and make the convention to regard one of the soft electron lines adjacent to it, for example the one to the right, as hard. This is natural, since after the mass renormalization the self-energy of the electron vanishes on the mass shell. Now the vertex parts will always appear in a sum with vertex parts of lower order and with self-energy parts adjacent to them on the left. The divergent terms of these expressions are relativistically invariant functions, since they arise from the integration over the region of large momenta of the particles, where expression (8) is relativistically invariant. Therefore they compensate each other in virtue of the Ward identity. For the non-invariant part there may, in principle, be no such compensation. This would only mean that the mutual compensation of the renormalizations of the vertex part and of the wave function of the electron does not take place independently in the low- and high-energy parts, and there occurs a partial intertwining of the two.

For the zeroth component of the vertex part (containing γ_0) this could lead to the appearance of spurious terms in the lower orders which do not vanish for zero momentum transfer and which disappear when the interaction with the soft photons is taken into account. However, we show now that such terms do not appear, i.e., the irreducible graphs for the zeroth component are completely renormalized. This is a consequence of an identity analogous to the usual Ward identity (and proved in the same way):

$$\frac{\partial}{\partial \varepsilon}\Sigma(\mathbf{p},\varepsilon) = \Lambda_0(\mathbf{p},\varepsilon;\mathbf{p},\varepsilon). \tag{16}$$

Here $\Sigma(\mathbf{p},\varepsilon)$ is the self-energy of the electron, and Λ_0 is the vertex function corresponding to the residue γ_0. Using (16), it is easy to show that the total account of the irreducible graphs of Λ_0 and of the corresponding graphs of Σ with the simple vertex γ_0 adjacent to the

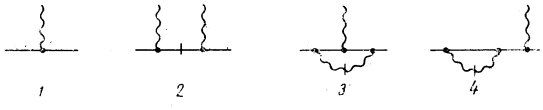

FIG. 1.

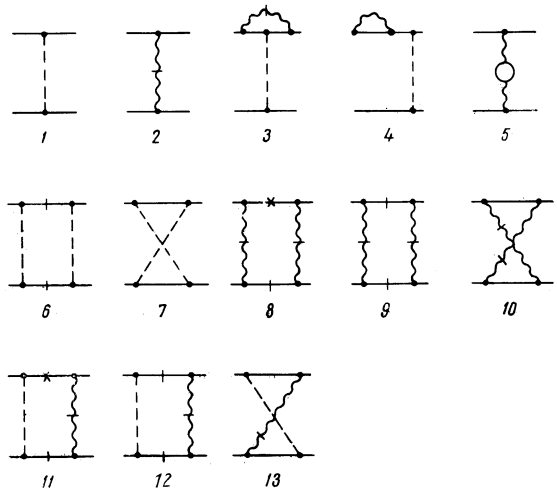

FIG. 2.

right leads to the usual renormalization of Λ_0, i.e., to the subtraction of its value for zero momentum of the phonon. For the space-like components of the vertex part this assertion will not, in general, be true, but this effect could show up only in corrections of order α^4 Ry.

4. CLASSIFICATION OF THE GRAPHS OF THE POTENTIAL

In this section we consider all irreducible graphs for the potential of the interaction of the $l+1$ particles (electrons plus nucleus) which lead to a level shift of an order not higher than α^3Ry or $mM^{-1}\alpha^2$Ry. It should be recalled that the order of the shift for a given graph depends on the value of the cut-off momentum λ. Clearly, the final result does not depend on the choice of λ. The most convenient choice is such that the inequalities

$$m\alpha \ll \lambda \ll m. \tag{17}$$

are fulfilled. Taking into account that the momentum of the electron in the atom has the order αm, we may conclude that if the potential behaves in momentum space like α^n for momenta of order α, then its contribution to the level shift will be of order α^{3+n} for $n<2$ and α^5 for $n \geq 2$.

After these introductory remarks we proceed now to the enumeration of the irreducible graphs for the potential.

We shall not write down the exchange graphs (obtained by interchanging the indices of the final states) since they are taken into account later through the antisymmetrization of the total wave function.

I. Single-particle potentials. These describe the interaction of a particle with the soft transverse field. The graphs making a contribution in orders up to α^3Ry or $mM^{-1}\alpha^2$Ry are shown in Fig. 1. Here and in the following we use the following notation. An electron line is represented by a solid line, a transverse photon line by a wavy line, and a Coulomb line by a dotted line. The cross denotes a hard line and the stroke denotes a soft line. The external lines are always soft.

In the graph 2 of Fig. 1, it is sufficient to include the terms independent of the momentum of the electron, and in the graph 1, 3 one may restrict oneself to the terms

which depend linearly on the momentum (anomalous magnetic moment).

II. Two-particle potentials. These describe the interaction of the particles with each other and with the soft transverse field. However, the graphs corresponding to the simultaneous interaction of the particles with one another and with the external field are small and can be disregarded. The remaining graphs are shown in Fig. 2. To these one must add the graph for two-photon exchange which takes account of the dependence of the graph 2, 2 on the energy variables and which has a structure analogous to 2, 8 but with two soft internal electron lines. The graphs 2, 3 to 13 all give contributions of order α^3Ry. In these graphs, the region of large momenta of the virtual photon plays the main role. They do not, therefore, depend on the momenta of the electrons and all reduce to potentials having a δ-function like character in x space (an exception is the magnetic term arising from the graph of Fig. 2, 3).

III. Three- and many-particle potentials. It is easy to see that these all lead to corrections of order α^4Ry and higher. The graphs without integrations of the type 3, 1 are small on account of the matrices between the hard and soft components of the electron Green's function. The graphs of the type 3, 2 are small since the Compton-type graph contained in them vanishes by the Thirring theorem when both Coulomb photons have zero momentum. Incidentally, for the same reason it is not necessary to take account of the graph of Fig. 4 in the two-particle potentials, although it formally leads also to corrections of the order α^3Ry.

In our approximation we must therefore only include the graphs of Figs. 1 and 2 for any number of particles. The concrete form of these potentials is derived in the next section.

5. HAMILTONIAN OF THE INTERACTION OF l ELECTRONS WITH ACCOUNT OF RELATIVISTIC CORRECTIONS

Let us now turn to the description of the separate terms of the general interaction of the particles with each other and with the soft transverse photon field **A**. We already have specifically in mind the case of l electrons numbered from 1 to l in the field of a nucleus, to which we assign the index 0. The total Hamiltonian H is taken of the form

$$H = H_A + \sum_{i=0}^{l} H_i^0 + H_I, \tag{18}$$

where

$$H_i^0 = \sqrt{m_i^2 + \mathbf{p}_i^2}, \quad m_0 = M, \quad m_i = m \quad (i = 1, \ldots, l), \tag{19}$$

$$H_A = \sum_{i=1}^{2} \int d^3k |\mathbf{k}| \theta(\lambda - |\mathbf{k}|) a_i^+(\mathbf{k}) a_i(\mathbf{k}), \tag{20}$$

and a_i^+ and a_i are the creation and annihilation operators for the soft photons. The term H_I contains the different terms corresponding to the graphs of the preceding section.

The sum of the graphs 1, 1 to 4 corresponds to the interaction with the electromagnetic field of a relativistic particle with a magnetic moment including the anomalous moment. This gives the following contribution to H_I:

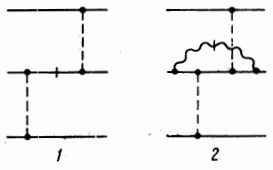

FIG. 3

FIG. 4.

$$H_I^{(1)} = \sum_{i=0}^{l} H_i^{(1)}, \tag{21}$$

$$H_i^{(1)} = -\frac{eZ_i}{m_i}(\mathbf{A}(\mathbf{r}_i)\mathbf{p}_i) - Z_i(\boldsymbol{\mu}_i[\nabla_i \mathbf{A}(\mathbf{r}_i)]) + \frac{Z_i^2 e^2}{2m}\mathbf{A}^2(\mathbf{r}_i). \tag{22}$$

Here $Z_0 = Z$, $Z_i = -1$ $(i = 1, \ldots, l)$; $Z\mu_0$ is the magnetic moment of the nucleus, and $(i = 1, \ldots, l)$

$$\boldsymbol{\mu}_i = \frac{e}{2m}\left(1 + \frac{\alpha}{2\pi}\right)\boldsymbol{\sigma}_i.$$

The graphs of Figs. 2, 1 and 2, 2 make a contribution to the interaction equal to

$$H_I^{(2,3)} = \sum_{i<k=0}^{l} H_{ik}^{(2,3)}, \tag{23}$$

respectively, where

$$H_{ik}^{(2)} = \frac{Z_i Z_k \alpha}{r_{ik}} + \bar{H}_{ik}^{(2)}. \tag{24}$$

The expressions for the potentials $H_{ik}^{(2)}$ and $H_{ik}^{(3)}$ are, in the momentum space,

$$\bar{H}_{ik}^{(2)}(\mathbf{p}_i', \mathbf{p}_k', \mathbf{p}_i, \mathbf{p}_k) = [(u^+(\mathbf{p}_i')u(\mathbf{p}_i))(u^+(\mathbf{p}_k')u(\mathbf{p}_k)) - 1]\frac{Z_i Z_k \alpha}{|\mathbf{p}_i' - \mathbf{p}_i|^2}. \tag{25}$$

$$H_{ik}^{(3)}(\mathbf{p}_i', \mathbf{p}_k', \mathbf{p}_i, \mathbf{p}_k) = [u^+(\mathbf{p}_i')u^+(\mathbf{p}_k')\boldsymbol{\alpha}_i\boldsymbol{\alpha}_k - \frac{(\boldsymbol{\alpha}_i(\mathbf{p}_i' - \mathbf{p}_i))(\boldsymbol{\alpha}_k(\mathbf{p}_i' - \mathbf{p}_i))}{|\mathbf{p}_i' - \mathbf{p}_i|^2})u(\mathbf{p}_i)u(\mathbf{p}_k)]\frac{Z_i Z_k \alpha}{|\mathbf{p}_i' - \mathbf{p}_i|^2}\theta(|\mathbf{p}_i' - \mathbf{p}_i| - \lambda). \tag{26}$$

If we regard the momenta of the electrons (nucleus) in (26) as small, we find, of course, the usual expression for the Breit operator with the only difference that the factor $\theta(|\mathbf{p}_i' - \mathbf{p}_i| - \lambda)$ appears, which leads to the appearance of oscillating functions in $H_{ik}^{(3)}$. As we shall see below, this difference disappears in the calculation of the shift, and we are left with the exact Breit operator. However, when taking account of the next order of perturbation theory, it is impossible to regard all electron momenta as small, and one must use the expressions (25) and (26).

The graphs 2, 3 and 2, 4 give the known corrections to the interaction due to the vertex part. With the help of the usual method of division into a soft and a hard part, they give the contribution[3]

$$H_I^{(4)} = \sum_{i<k=0}^{l} H_{ik}^{(4)}, \tag{27}$$

$$H_{ik}^{(4)} = -\delta^{(3)}(\mathbf{r}_{ik})\frac{\alpha^2}{m^2}\frac{8}{3}\left(\ln\frac{m}{2\lambda} + \frac{5}{6}\right) + \frac{\alpha^2}{4\pi m^2}\{(\sigma_i[\nabla \mathbf{p}_i]) - (\sigma_k[\nabla \mathbf{p}_k])\}\frac{1}{r_{ik}}, \tag{28}$$

$$H_{0i}^{(4)} = Z\delta^{(3)}(\mathbf{r}_i)\frac{\alpha^2}{m^2}\frac{4}{3}\left(\ln\frac{m}{2\lambda}+\frac{5}{6}\right)-\frac{Z\alpha^2}{4\pi m^2}(\sigma_i[\nabla \mathbf{p}_i])\frac{1}{r_i}, \quad (29)$$

where we have assumed that ∇ acts only on r_i^{-1} or r_{ik}^{-1}.

The graph of 2, 5 gives the usual corrections to the vacuum polarization:[3]

$$H_I^{(5)} = \sum_{i<k=0}^{l} H_{ik}^{(5)}, \quad (30)$$

$$H_{ik}^{(5)} = \frac{4}{15}Z_iZ_k\frac{\alpha^2}{m^2}\delta^{(3)}(\mathbf{r}_{ik}). \quad (31)$$

The remaining graphs for two-photon exchange all lead to δ-function-like potentials for the interaction of the electrons with one another, and yield together

$$H_I^{(6)} = \sum_{i<k=1}^{l} H_{ik}^{(6)}, \quad (32)$$

$$H_{ik}^{(6)} = \frac{\alpha^2}{m^2}\delta^{(3)}(\mathbf{r}_{ik})\left(-2\ln\frac{m}{\lambda}+2\ln 2+\frac{3}{2}\pi-\frac{2}{3}+\left(\frac{\pi}{3}+1\right)(\sigma_i\sigma_k)\right). \quad (33)$$

6. CALCULATION OF THE RELATIVISTIC CORRECTIONS TO THE LEVELS

After the Schrödinger equation for the system of electrons has been written down, there is in principle no difficulty to calculate the corrections. The account of the multitude of potential terms [in addition to (25) and (26)] reduces in our approximation to averaging them over the state ψ_n of interest to us.

We begin with the corrections on account of the exchange of soft photons. In our approximation it is sufficient to restrict oneself to the lowest order of perturbation theory and to include the one-photon intermediate states in the first two terms of (22) and the two-photon states in the third term of (22). Then one or two electrons take part in the interaction. It is natural that the considerations are similar to those encountered in the problem of the level shift for a single or two electrons. We shall therefore be very brief and refer to [1,3] for details.

The contribution from single-photon states has the general structure

$$\Delta_1 E_n = \frac{1}{(2\pi)^3}\int\frac{d^3k}{2k_0}\sum_{n'e}\frac{V_{nn'}V_{n'n}}{E_n-E_{n'}-k_0}\theta(\lambda-|\mathbf{k}|), \quad (34)$$

where

$$V_{nn'} = \sum_{i=1}^{l}(V_i)_{nn'},$$
$$V_i = \left\{-\frac{e}{m}\mathbf{p}_i\mathbf{e}-i([\mu_i\mathbf{k}]\mathbf{e})\right\}e^{i\mathbf{k}\mathbf{r}_i}, \quad (35)$$

and $\mathbf{e}$ is the polarization vector of the photon. As usual, we write

$$\frac{1}{E_n-E_{n'}-k_0} = -\frac{1}{k_0}+\frac{E_n-E_{n'}}{(E_n-E_{n'}-k_0)k_0} \quad (36)$$

and correspondingly, separate the shift into $\Delta_1^{(1)}E_n$ and $\Delta_1^{(2)}E_n$. Each of these terms can in turn be divided up into a sum of one-electron and two-electron parts, arising from the terms V_iV_i and V_iV_k ($i \neq k$):

$$\Delta_1^{(1)}E_n = \sum_i \Delta_1^{(1)}E_n^{(ii)} + \sum_{i\neq k}\Delta_1^{(1)}E_n^{(ik)}. \quad (37)$$

All terms $\Delta_1^{(1)}E_n^{(ii)}$ disappear on account of the renormalization of the mass (as in the one-electron problem). The terms of the type $\Delta_1^{(1)}E_n^{(12)}$ give

$$\Delta_1^{(1)}E_n^{(12)}+\Delta_1^{(1)}E_n^{(21)} = (\tilde{H}_{12}^{(3)})_{nn}, \quad (38)$$

where $\tilde{H}_{12}^{(3)}$ is the same expression as (26), except that it contains the factor $\theta(\lambda-|\mathbf{p}_1'-\mathbf{p}_1|)$. Summed with (26), it gives exactly the usual Breit operator.

Let us now turn to ΔE_n. In the integral over $\mathbf{k}$ we separate out the "supersoft region" $0 \leq |\mathbf{k}| \leq \kappa$, where $m\alpha^2 < \kappa < m\alpha$, $\kappa \ll \lambda$. In the supersoft region we can neglect the magnetic term in V_i and replace $e^{i\mathbf{k}\mathbf{x}}$ by unity. Then the contribution from the supersoft region gives terms which contain the known Bethe logarithm:

$$\Delta_1^{(3)}E_n = \frac{2}{3}\frac{\alpha}{\pi m^2}\sum_{n'}(E_n-E_{n'})|\mathbf{P}_{nn'}|^2\ln\left|\frac{E_n-E_{n'}}{\kappa}\right|, \quad (39)$$

where $\mathbf{P}$ is the total momentum of all electrons:

$$\mathbf{P} = \sum_{i=1}^{l}\mathbf{p}_i.$$

It is convenient to separate out the dependence on κ. Using the identity

$$\sum_{n'}(E_n-E_{n'})|A_{nn'}|^2 = -\tfrac{1}{2}[A[HA]]_{nn}, \quad (40)$$

we find

$$\Delta_1^{(3)}E_n = \frac{2}{3}\frac{\alpha}{\pi m^2}\sum_{n'}(E_n-E_{n'})|\mathbf{P}_{nn'}|^2\ln\left|\frac{E_n-E_{n'}}{m\alpha^2}\right| - \frac{4}{3}\frac{\alpha^2}{m^2}\ln\left(\frac{m\alpha^2}{\kappa}\right)Z\left(\sum_{i=0}^{l}\delta^{(3)}(\mathbf{r}_i)\right)_{nn}. \quad (41)$$

In the calculation of the contribution from the soft region $|\mathbf{k}| > \kappa$ we can neglect the difference $E_n - E_{n'}$ in the denominator and use (40) in carrying out the sum over n in the integral over $\mathbf{k}$. Let us consider the one- and two-electron terms separately.

After the renormalization of the mass the following contribution remains from the one-electron terms:

$$\Delta_1^{(4)}E_n = -\frac{4}{3}\frac{\alpha^2}{\pi m^2}\left(Z\sum_{i=1}^{l}\delta^{(3)}(\mathbf{r}_i)-\sum_{i\neq k=1}^{l}\delta^{(3)}(\mathbf{r}_{ik})\right)_{nn}\ln\frac{\kappa}{\lambda}. \quad (42)$$

The typical two-electron terms (from the pair of electrons 1 and 2) give

$$\Delta_1^{(5)}E_n^{(12)} = \frac{\alpha^2}{\pi m^2}\left(-\frac{8}{3}\pi\delta^{(3)}(\mathbf{r}_{12})\ln\frac{\kappa}{\lambda}+f(r_{12})\right)_{nn}, \quad (43)$$

where

$$f(r) = \frac{2}{3}\left(\frac{\cos\kappa r}{(\kappa r)^2}-\frac{\sin\kappa r}{(\kappa r)^3}-\frac{\cos\lambda r}{(\lambda r)^2}+\frac{\sin\lambda r}{(\lambda r)^3}\right). \quad (44)$$

The function f(r) is close to $-2r^{-3}/3$ in the physically interesting region $\kappa r \ll 1$, $\lambda r \gg 1$. However, it contains a δ-function-like singularity. It follows from the calculations of Araki[1] that f(r) can effectively be written in the form

$$f(r) = -\frac{2}{3}r^{-3}(a)-\frac{8\pi}{3}(\ln(m\alpha a)+C)\delta^{(3)}(\mathbf{r})+\left(\frac{32}{9}\pi+\frac{8\pi}{3}\ln\frac{m\alpha}{\lambda}\right)\delta^{(3)}(\mathbf{r}). \quad (45)$$

Here $r^{-3}(a) = r^{-3}$ for $r > a$ and $r^{-3}(a) = 0$ for $r < a$, where $a \to 0$; C is the Euler constant.

Let us now calculate the two-photon contribution, which can be written in the form

$$\Delta_2 E_n = \frac{2}{(2\pi)^6} \sum_{e_1 e_2} \sum_{n'} \int \frac{d^3k}{2k_0} \int \frac{d^3q}{2q_0} \frac{W_{nn'} W_{n'n}}{E_n - E_{n'} - k_0 - q_0}, \quad (46)$$

where $0 \leq |\mathbf{k}|, |\mathbf{q}| \leq \lambda$, and

$$W_{nn'} = \sum_{i=1}^{l} W^{(i)}_{nn'},$$
$$W^{(i)} = \frac{e^2}{2m} (\mathbf{e}_1 \mathbf{e}_2) e^{i(\mathbf{k}+\mathbf{q})\mathbf{r}_i}. \quad (47)$$

Using (36), we again obtain two terms, $\Delta_2^{(1)} E_n$ and $\Delta_2^{(2)} E_n$. None of the terms $\Delta_2^{(2)} E_n$ give a contribution in this case. Indeed, here the supersoft region does not contribute because of the smallness of the phase volume. In the soft region one can use formula (35). Since the $W^{(i)}$ do not depend on the momenta of the electrons, all the one-electron terms disappear after the renormalization of the mass, and the two-electron terms are zero by themselves.

Thus we are left with

$$\Delta_2^{(1)} E_n = -\frac{2}{(2\pi)^6} \sum_{e_1 e_2} \int \frac{d^3k}{2k_0} \frac{d^3q}{2q_0} (WW^+)_{nn} \frac{1}{k_0 + q_0}, \quad 0 \leq |\mathbf{k}|, |\mathbf{q}| \leq \lambda, \quad (48)$$

where the one-electron terms can again be disregarded —they disappear after renormalization. The two-electron terms yield together

$$\Delta_2^{(1)} E_n = -\frac{\alpha^2}{2\pi m^2} \sum_{i<k} (F(\mathbf{r}_{ik}))_{nn}, \quad (49)$$

where

$$F(\mathbf{r}) = \int \frac{d^3k\, d^3q}{(2\pi)^3} e^{i(\mathbf{k}+\mathbf{q})\mathbf{r}} \frac{1 + (\mathbf{kq})^2/k^2q^2}{k_0 q_0 (k_0 + q_0)}, \quad (50)$$

and the integration is, of course, taken over the region $0 \leq |\mathbf{k}|, |\mathbf{q}| \leq \lambda$. In the calculation of the average value of $F(\mathbf{r})$ one must take account of the δ-function-like singularities, as in the case of $f(\mathbf{r})$ (cf. [1]). Effectively,

$$F(\mathbf{r}) = r^{-3}(a) + 4\pi\delta^3(\mathbf{r}) \left[\frac{7}{3} (\ln 2 - 1) + \ln \frac{\lambda}{ma} + \ln(ma a) + C \right] \quad a \to 0. \quad (51)$$

It remains to include the contribution from the second order of perturbation theory in the potentials $\tilde{H}_I^{(2)}$ and $H_I^{(3)}$. In the order α^3 Ry, the contribution clearly comes only from the high-energy intermediate state in which the momenta of the pair of electrons are large. The corresponding correction to the energy is equal to

$$\Delta E = \sum_{i<k=1}^{l} \Delta E_{ik}, \quad (52)$$

$$\Delta E_{ik} = \frac{\alpha}{\pi} \int \frac{d^3k}{m - \sqrt{m^2 + \mathbf{k}^2}} (\delta^{(3)}(\mathbf{r}_{ik}) (\tilde{H}^{(2)}_{ik} + H^{(3)}_{ik})^2)_{nn}, \quad (53)$$

where $\tilde{H}^{(2)}_{ik}(\mathbf{k})$ and $H^{(3)}_{ik}(\mathbf{k})$ are the expressions (25) and (26) for $\mathbf{p}_i = \mathbf{p}_k = 0$ and $\mathbf{p}'_i = -\mathbf{p}'_k = \mathbf{k}$. A simple calculation yields

$$\Delta E_{ik} = \frac{\alpha^2}{m^2} \left[\delta^{(3)}(\mathbf{r}_{ik}) \left(3 - \frac{3}{2}\pi + \left(\frac{2}{3} - \frac{\pi}{3} \right) (\boldsymbol{\sigma}_i \boldsymbol{\sigma}_k) \right) \right]_{nn}. \quad (54)$$

Summing all contributions, we arrive at formulas (1) to (5) of the Introduction.

7. CONCLUSION

The method proposed in the present paper is useful for the calculation of the level shifts in atoms with an arbitrary number of electrons. We have determined the corrections of order α^3 Ry and $mM^{-1}\alpha^2$ Ry; the inclusion of the corrections in the subsequent orders increases the amount of numerical work, but does not lead to any essential difficulties. It is seen from the result that in the order investigated, the many-particle effects are all contained in the nonrelativistic wave functions and in the Bethe logarithm. The remaining terms are of the pair type.

In the case of two electrons our result can be compared with the work of Araki[1] and Sucher.[2] In the short communication of Sucher[2] no general formula for the level shift is given but only a particular result for a special form of the wave function. This makes a detailed comparison impossible but allows one to conclude that the coefficients of the contact terms of the interaction between the electrons do not agree between these two authors. The corresponding coefficients in our work differ both from the ones given by Araki and by Sucher. The difference to Araki is evidently connected with the circumstance that this author started from a different unperturbed equation containing Dirac operators instead of Schrödinger operators.

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