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Quantum electrodynamics of high-Z few-electron atoms

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Relativistic quantum electrodynamic perturbation theory is applied to the high-Z few-electron system. Interaction of the bound electrons with the radiation field is treated as a perturbation that results in the electron-electron interaction and radiative corrections. The leading perturbations, of order α, are examined. For two-electron atoms, a precise evaluation of the one-exchanged-photon correction in the $1\,^1S_0$, $2\,^3S_1$, $2\,^3P_0$, and $2\,^3P_2$ states is made.

I. INTRODUCTION

This paper examines high-Z few-electron atoms from the point of view of quantum electrodynamic perturbation theory in the bound-interaction picture. The purpose is to provide a consistent framework for the relativistic calculation of the structure of these atoms including the effects of radiative corrections. The perturbation theory considered here is an expansion about basis states of noninteracting Dirac electrons bound in the static Coulomb field of the nucleus. Radiative corrections and electron-electron interactions are perturbations produced by interactions of the electrons with the quantized radiation field. For a few strongly bound electrons in a high-Z Coulomb field, these perturbations are small compared to the binding energy, and the perturbation expansion converges rapidly. In particular, the relevant expansion parameter is $1/Z$, and this method provides a generalization of the $1/Z$ expansion methods of Layzer and Bahcall[1] and of Dalgarno and Stewart[2] to include higher-order relativistic effects and radiative corrections.

This approach to high-Z two-electron atoms has been briefly discussed by Bethe and Salpeter[3] and by Sucher;[4] it is of renewed interest due to the rapid rise of experimental activity in this area. More recent studies of electron-interaction corrections in this framework have been made, for example, by Ivanov, Ivanova, and Safronova.[5]

The present paper gives a consistent discussion of all the leading corrections, including radiative effects, to provide the groundwork for a study of the higher-order corrections. Precise calculations are carried out for the electron-electron interaction in two-electron atoms.

In Sec. II, the basic formalism is reviewed. The leading corrections, of order α, are derived in Sec. III. The one-exchanged photon-correction is examined in Sec. IV, and a precise numerical evaluation is made for the $1\,^1S_0$, $2\,^3S_1$, $2\,^3P_0$, and $2\,^3P_2$ states of two-electron atoms. Concluding remarks are made in Sec. V.

II. FORMULATION

Energy levels of high-Z few-electron atoms are described here within the framework of the Furry bound-interaction picture of quantum electrodynamics.[6] The zeroth-order basis states are the eigenfunctions of the Dirac equation

$$[-i\boldsymbol{\alpha}\cdot\nabla+V(x)+\beta-E_n]\phi_n(\mathbf{x})=0 \tag{1}$$

for an external Coulomb potential with source charge Ze

$$V(x)=-\frac{Z\alpha}{x}\ . \tag{2}$$

Units are chosen such that $c=\hbar=m=1$, where m is the electron mass, and the γ matrices are given by

$$\boldsymbol{\gamma}=\beta\boldsymbol{\alpha},\ \ \gamma^0=\beta,\ \ \boldsymbol{\alpha}=\begin{bmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{bmatrix},\ \ \beta=\begin{bmatrix}I & 0\\ 0 & -I\end{bmatrix}, \tag{3}$$

where $\boldsymbol{\sigma}$ are the Pauli matrices. In the Furry picture, the electron-positron field operator $\psi(x)$ is expanded in terms of electron annihilation operators a_n and positron creation operators $b_n^\dagger$ as

$$\begin{aligned}\psi(x)&=\sum_{E_n(>0)}a_n\phi_n(x)+\sum_{E_n(<0)}b_n^\dagger\phi_n(x)\\ &=\sum_n(a_n+b_n^\dagger)\phi_n(x)\ ,\end{aligned} \tag{4}$$

where

$$\phi_n(x)=\phi_n(\mathbf{x})e^{-iE_nt} \tag{5}$$

and where the creation and annihilation operators are defined so that

$$\begin{aligned}&a_n \text{ and } a_n^\dagger=0 \text{ if } E_n<0\ ,\\ &b_n \text{ and } b_n^\dagger=0 \text{ if } E_n>0\ .\end{aligned} \tag{6}$$

In Eq. (4) the summation symbol is understood to mean summation over the discrete spectrum and integration over the continuous spectrum. The subscript n denotes the complete set of quantum numbers $\{n,l,j,m\}$ needed to specify the state. The principal quantum number n is replaced by the energy E for states in the continuous spectrum; l determines the parity $P=(-1)^l$ and is the orbital-angular-momentum quantum number in the nonrelativistic limit, j is the total-angular-momentum quantum number, and m is the z component of the total angular momentum.

The anticommutation relations among the creation and annihilation operators are

$$\begin{aligned} &\{a_n,a^{\dagger}_{n'}\}=\delta^{+}_{nn'}\ ,\\ &\{b_n,b^{\dagger}_{n'}\}=\delta^{-}_{nn'}\ ,\\ &\{a_n,a_{n'}\}=\{a^{\dagger}_n,a^{\dagger}_{n'}\}=0\ ,\\ &\{b_n,b_{n'}\}=\{b^{\dagger}_n,b^{\dagger}_{n'}\}=0\ , \end{aligned} \tag{7}$$

where

$$\delta^{\pm}_{nn'}=\theta(\pm E_n)\delta_{nn'}\delta_{ll'}\delta_{jj'}\delta_{mm'} \tag{8a}$$

if n and n' correspond to states in the discrete spectrum,

$$\delta^{\pm}_{nn'}=\theta(\pm E)\delta(E-E')\delta_{ll'}\delta_{jj'}\delta_{mm'} \tag{8b}$$

if n and n' correspond to states in the continuous spectrum, and

$$\delta^{\pm}_{nn'}=0 \tag{8c}$$

if one index refers to a state in the discrete spectrum and the other refers to a state in the continuous spectrum.

Zeroth-order electron states are given by electron creation operators acting on the Coulomb field vacuum $|0\rangle$ that has the property

$$a_n\,|0\rangle=b_n\,|0\rangle=0 \quad \text{for all } n\ . \tag{9}$$

The one-electron states are given by

$$|\,nljm\,\rangle=a^{\dagger}_{nljm}\,|0\rangle\ . \tag{10}$$

Two-electron states with weak singlet-triplet mixing and well-defined total-angular-momentum quantum numbers J and M are given by

$$|\,nljn'l'j'JM\,\rangle=\sum_{m,m'}\langle jmj'm'\,|\,jj'JM\,\rangle a^{\dagger}_{nljm}a^{\dagger}_{n'l'j'm'}\,|0\rangle \tag{11a}$$

for $\{n,l,j\}\neq\{n',l',j'\}$, and

$$|\,nljnljJM\,\rangle=\frac{1}{\sqrt{2}}\sum_{m,m'}\langle jmjm'\,|\,jjJM\,\rangle a^{\dagger}_{nljm}a^{\dagger}_{nljm'}\,|0\rangle\ . \tag{11b}$$

The zeroth-order Hamiltonian is

$$H_0=\sum_n(a^{\dagger}_na_n-b^{\dagger}_nb_n)E_n\ . \tag{12}$$

A direct calculation shows that the eigenvalues of H_0 are given by

$$\begin{aligned} &H_0\,|\,nljm\,\rangle=E_n\,|\,nljm\,\rangle\ ,\\ &H_0\,|\,nljn'l'j'JM\,\rangle=(E_n+E_{n'})\,|\,nljn'l'j'JM\,\rangle\ . \end{aligned} \tag{13}$$

Thus the zeroth-order energy level is the sum of the Dirac energies of the individual orbitals

$$E_n=\left[1+\frac{(Z\alpha)^2}{\{n-(j+\frac{1}{2})+[(j+\frac{1}{2})^2-(Z\alpha)^2]^{1/2}\}^2}\right]^{-1/2}mc^2\ . \tag{14}$$

The interaction between the electron-positron field and the radiation field is determined by the interaction Hamiltonian density

$$H_I(x)=j^{\mu}(x)A_{\mu}(x)-\delta M(x)\ , \tag{15}$$

where

$$j^{\mu}(x)=-\frac{e}{2}[\,\bar{\psi}(x)\gamma^{\mu},\psi(x)] \tag{16}$$

is the electromagnetic current, $A_{\mu}(x)$ is the vector potential operator for the radiation field, and

$$\delta M(x)=\tfrac{1}{2}\delta m[\,\bar{\psi}(x),\psi(x)] \tag{17}$$

is the mass-renormalization counter term. The commutators in (16) and (17) refer only to creation and annihilation operators, i.e., the Dirac wave functions and the γ matrices are always in the order shown.

The prescription of Gell-Mann and Low is employed here to obtain an expression for the bound-state level shifts in perturbation theory.[7] Sucher has written an equivalent expression in terms of the S matrix to which the standard renormalization prescription may be applied:[4]

$$\Delta E=\lim_{\substack{\lambda\to 1\\ \epsilon\to 0}}\tfrac{1}{2}i\epsilon\frac{\partial\langle S_{\epsilon,\lambda}\rangle_c/\partial\lambda}{\langle S_{\epsilon,\lambda}\rangle_c}\ . \tag{18}$$

The subscript c denotes the fact that only connected Feynman graphs are included in the matrix element. In (18), $S_{\epsilon,\lambda}$ is the adiabatic S matrix defined by

$$S_{\epsilon,\lambda}=1+\sum_{j=1}^{\infty}S^{(j)}_{\epsilon,\lambda}\ , \tag{19}$$

where

$$S^{(j)}_{\epsilon,\lambda}=\frac{(-i\lambda)^j}{j!}\int d^4x_j\cdots\int d^4x_1 e^{-\epsilon|t_j|}\cdots e^{-\epsilon|t_1|}\times T[H_I(x_j)\cdots H_I(x_1)]\ . \tag{20}$$

In (20), T is the Wick time-ordering operator.

These equations provide the basic formulation of bound-state quantum electrodynamics. In the next section the leading corrections, of order α, are examined.

III. LEADING CORRECTIONS

To second order in H_I, Eq. (18) yields

$$\Delta E = \lim_{\epsilon\to 0} \tfrac{1}{2} i\epsilon[\langle S_\epsilon^{(1)}\rangle_c + 2\langle S_\epsilon^{(2)}\rangle_c - (\langle S_\epsilon^{(1)}\rangle_c)^2 + \cdots] , \tag{21}$$

where

$$\langle S_\epsilon^{(j)}\rangle_c = \langle S_{\epsilon,\lambda}^{(j)}\rangle_c \,|_{\lambda=1} . \tag{22}$$

To order α, only the first two terms in (21) are relevant. The term δM is of order α and contributes through the first matrix element in (21). We have

$$\langle S_\epsilon^{(1)}\rangle_c = i \int d^4x\, e^{-\epsilon|t|} \langle \delta M(x)\rangle_c \tag{23}$$

and

$$\langle S_\epsilon^{(2)}\rangle_c = -\tfrac{1}{2} \int d^4x_2 \int d^4x_1 e^{-\epsilon|t_2|} e^{-\epsilon|t_1|} \langle T[j^{\mu_2}(x_2)A_{\mu_2}(x_2) j^{\mu_1}(x_1)A_{\mu_1}(x_1)]\rangle_c + O(\alpha^2) . \tag{24}$$

It is convenient to employ the relations

$$\delta M(x) = {:}\delta M(x){:} - \delta m \,\mathrm{Tr}[S_F(x,x)] \tag{25}$$

and

$$j^\mu(x) = {:}j^\mu(x){:} + e\,\mathrm{Tr}[\gamma^\mu S_F(x,x)] , \tag{26}$$

where Tr denotes the trace in the 4×4 Dirac matrix space, and the dots denote normal order. The propagation function S_F is given by

$$\begin{aligned} S_F(x_2,x_1) &= \langle 0 | T[\psi(x_2)\bar{\psi}(x_1)] | 0\rangle \\ &= \sum_{n,m} \phi_n(x_2)\bar{\phi}_m(x_1)[\delta_{nm}^{+}\theta(t_2-t_1) \\ &\qquad - \delta_{nm}^{-}\theta(t_1-t_2)] \\ &= \frac{1}{2\pi i}\int_{-\infty}^{\infty} dz \sum_n \frac{\phi_n(\mathbf{x}_2)\bar{\phi}_n(\mathbf{x}_1)}{E_n - z(1+i\delta)} e^{-iz(t_2-t_1)} , \end{aligned} \tag{27}$$

where the θ function is defined so that $\theta(0)=\frac{1}{2}$. The second term on the right-hand side of (25) corresponds to a Feynman diagram with a disconnected closed loop and is neglected. The second term on the right-hand side of (26) corresponds to a vacuum polarization loop and is retained.

In the following we consider only zeroth-order states consisting of a well-defined number of electrons in bound states. In this case

$$\langle \delta M\rangle_c = \langle {:}\delta M{:}\rangle_c = \delta m \sum_{n,m} \bar{\phi}_n(x)\phi_m(x)\langle a_n^\dagger a_m\rangle , \tag{28}$$

and since

$$\int_{-\infty}^{\infty} dt\, e^{-\epsilon|t|} e^{-i(E_m-E_n)t} = \frac{2}{\epsilon}\delta(E_n,E_m) + O(\epsilon) , \tag{29}$$

where

$$\delta(E_n,E_m) = \begin{cases} 1 & \text{if } E_n = E_m , \\ 0 & \text{if } E_n \neq E_m , \end{cases} \tag{30}$$

the lowest-order mass term is

$$\langle S_\epsilon^{(1)}\rangle_c = \frac{2i}{\epsilon}\delta m \sum_{n,m} \int d\mathbf{x}\, \bar{\phi}_n(x)\phi_m(x)\delta(E_n,E_m) \times \langle a_n^\dagger a_m\rangle + O(\epsilon) . \tag{31}$$

In the second-order term

$$\langle T[j^{\mu_2}(x_2)A_{\mu_2}(x_2)j^{\mu_1}(x_1)A_{\mu_1}(x_1)]\rangle_c = \langle T[j^{\mu_2}(x_2)j^{\mu_1}(x_1)]\rangle_c g_{\mu_2\mu_1} D_F(x_2-x_1) , \tag{32}$$

where D_F is the photon propagator

$$\begin{aligned} g_{\mu_2\mu_1} D_F(x_2-x_1) &= \langle 0 | T[A_{\mu_2}(x_2)A_{\mu_1}(x_1)] | 0\rangle \\ &= -g_{\mu_2\mu_1}\frac{i}{(2\pi)^4}\int d^4k \frac{e^{-ik(x_2-x_1)}}{k^2+i\delta} . \end{aligned} \tag{33}$$

From (26),

$$\begin{aligned} \langle T[j^{\mu_2}(x_2)j^{\mu_1}(x_1)]\rangle_c &= \langle T[{:}j^{\mu_2}(x_2){:}\,{:}j^{\mu_1}(x_1){:}]\rangle_c + e\,\mathrm{Tr}[\gamma^{\mu_2}S_F(x_2,x_2)]\langle {:}j^{\mu_1}(x_1){:}\rangle_c \\ &\quad + e\,\mathrm{Tr}[\gamma^{\mu_1}S_F(x_1,x_1)]\langle {:}j^{\mu_2}(x_2){:}\rangle_c + \mathscr{D} , \end{aligned} \tag{34}$$

where $\mathscr{D}$ corresponds to a diagram with two vacuum polarization loops which in this order is a disconnected diagram. With the aid of the identities

$$\begin{aligned} \langle T[{:}j^{\mu_2}(x_2){:}\,{:}j^{\mu_1}(x_1){:}]\rangle_c &= e^2 \sum_{n,m} \bar{\phi}_n(x_2)\gamma^{\mu_2}\phi_m(x_2) \sum_{k,l} \bar{\phi}_k(x_1)\gamma^{\mu_1}\phi_l(x_1)\langle a_n^\dagger a_k^\dagger a_l a_m\rangle \\ &\quad + e^2 \sum_{n,l} \bar{\phi}_n(x_2)\gamma^{\mu_2}S_F(x_2,x_1)\gamma^{\mu_1}\phi_l(x_1)\langle a_n^\dagger a_l\rangle \\ &\quad + e^2 \sum_{k,m} \bar{\phi}_k(x_1)\gamma^{\mu_1}S_F(x_1,x_2)\gamma^{\mu_2}\phi_m(x_2)\langle a_k^\dagger a_m\rangle \end{aligned} \tag{35}$$

and

$$\langle :j^{\mu}(x): \rangle_c = -e \sum_{n,m} \bar{\phi}_n(x)\gamma^{\mu}\phi_m(x)\langle a_n^{\dagger}a_m \rangle \tag{36}$$

we have

$$\begin{aligned}\langle S_{\epsilon}^{(2)} \rangle_c = -e^2 \int d^4x_2 \int d^4x_1 e^{-\epsilon|t_2|}e^{-\epsilon|t_1|}D_F(x_2-x_1) \\ \times \Bigg[\frac{1}{2}\sum_{n,m} \bar{\phi}_n(x_2)\gamma_{\mu}\phi_m(x_2) \sum_{k,l} \bar{\phi}_k(x_1)\gamma^{\mu}\phi_l(x_1)\langle a_n^{\dagger}a_k^{\dagger}a_l a_m \rangle \\ + \sum_{n,m} \bar{\phi}_n(x_2)\gamma_{\mu}S_F(x_2,x_1)\gamma^{\mu}\phi_m(x_1)\langle a_n^{\dagger}a_m \rangle \\ - \mathrm{Tr}[\gamma_{\mu}S_F(x_2,x_2)] \sum_{n,m} \bar{\phi}_n(x_1)\gamma^{\mu}\phi_m(x_1)\langle a_n^{\dagger}a_m \rangle \Bigg] + O(\alpha^2) \; .\end{aligned} \tag{37}$$

For small ϵ, the integration over t_2 and t_1 is simplified by employing the relation

$$\begin{aligned}\int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_1 e^{-\epsilon|t_2|}e^{-\epsilon|t_1|}e^{-iz(t_2-t_1)}e^{-i\Delta E_{mn}t_2}e^{-i\Delta E_{lk}t_1} \\ = \frac{2\epsilon}{[\epsilon^2+(z+\Delta E_{mn})^2]} \frac{2\epsilon}{[\epsilon^2+(z-\Delta E_{lk})^2]} \\ = \delta(\Delta E_{mn}, -\Delta E_{lk})\frac{2\pi}{\epsilon}\delta(z+\Delta E_{mn}) + O(1) \\ = \delta(E_n+E_k, E_l+E_m)\frac{1}{\epsilon}\int_{-\infty}^{\infty} d(t_2-t_1)e^{-iz(t_2-t_1)}e^{-i\Delta E_{mn}t_2}e^{-i\Delta E_{lk}t_1} + O(1) \; ,\end{aligned} \tag{38}$$

where $\Delta E_{ij} = E_i - E_j$, in the first term of (37), and the relation

$$\int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{\infty} dt_1 e^{-\epsilon|t_2|}e^{-\epsilon|t_1|}e^{-iz(t_2-t_1)}e^{iE_nt_2}e^{-iE_mt_1} = \delta(E_n,E_m)\frac{1}{\epsilon}\int_{-\infty}^{\infty} d(t_2-t_1)e^{-iz(t_2-t_1)}e^{iE_nt_2}e^{-iE_mt_1} + O(1) \tag{39}$$

in the second term. Equation (29) applies to the third term. We thus have for the level shift of order α ($e^2 = 4\pi\alpha$),

$$\begin{aligned}E^{(2)} = -4\pi i\alpha \int d(t_2-t_1) \int d\mathbf{x}_2 \int d\mathbf{x}_1 D_F(x_2-x_1) \\ \times \Bigg[\frac{1}{2}\sum_{n,m} \bar{\phi}_n(x_2)\gamma_{\mu}\phi_m(x_2) \sum_{k,l} \bar{\phi}_k(x_1)\gamma^{\mu}\phi_l(x_1)\delta(E_n+E_k,E_l+E_m)\langle a_n^{\dagger}a_k^{\dagger}a_l a_m \rangle \\ + \sum_{n,m} \bar{\phi}_n(x_2)\gamma_{\mu}S_F(x_2,x_1)\gamma^{\mu}\phi_m(x_1)\delta(E_n,E_m)\langle a_n^{\dagger}a_m \rangle \\ - \mathrm{Tr}[\gamma_{\mu}S_F(x_2,x_2)] \sum_{n,m} \bar{\phi}_n(x_1)\gamma^{\mu}\phi_m(x_1)\delta(E_n,E_m)\langle a_n^{\dagger}a_m \rangle \Bigg] \\ -\delta m \sum_{n,m} \int d\mathbf{x} \bar{\phi}_n(x)\phi_m(x)\delta(E_n,E_m)\langle a_n^{\dagger}a_m \rangle \; .\end{aligned} \tag{40}$$

This expression for the level shift applies to any zeroth-order basis state consisting of a well-defined number of electrons. The electron-electron interaction term (first) in (40) agrees with the result of Brown derived with a time-dependent formalism,[8] and with the earlier results of Breit[9] and Oppenheimer.[10] The self-energy (second) and vacuum polarization (third) terms in (40) agree with the well-known single-electron expressions. This is shown explicitly by considering the level shift for a single electron in state i, according to Eq. (10). In that case

$$\begin{aligned}\langle a_n^{\dagger}a_k^{\dagger}a_l a_m \rangle = 0 \; , \\ \langle a_n^{\dagger}a_m \rangle = \delta_{ni}\delta_{mi} \; ,\end{aligned} \tag{41}$$

and

$$E^{(2)} = E_{\mathrm{SE}}^{(2)} + E_{\mathrm{VP}}^{(2)} \; , \tag{42}$$

where

$$E^{(2)}_{\mathrm{SE}}=-4\pi i\alpha \int d(t_2-t_1)\int d\mathbf{x}_2\int d\mathbf{x}_1 D_F(x_2-x_1)\bar{\phi}_i(x_2)\gamma_\mu S_F(x_2,x_1)\gamma^\mu\phi_i(x_1)-\delta m\int d\mathbf{x}\,\bar{\phi}_i(x)\phi_i(x) \tag{43}$$

and

$$E^{(2)}_{\mathrm{VP}}=4\pi i\alpha\int d(t_2-t_1)\int d\mathbf{x}_2\int d\mathbf{x}_1 D_F(x_2-x_1)\,\mathrm{Tr}[\gamma_\mu S_F(x_2,x_2)]\bar{\phi}_i(x_1)\gamma^\mu\phi_i(x_1)\ . \tag{44}$$

The Feynman diagrams corresponding to (43) and (44) appear in Fig. 1.

For a two-electron state of the form

$$\sum_{i,j} C_{ij}a_i^\dagger a_j^\dagger\,|\,0\rangle \tag{45}$$

we have

$$\begin{gathered}\langle a_n^\dagger a_k^\dagger a_l a_m\rangle=(C^*_{kn}-C^*_{nk})(C_{lm}-C_{ml})\ ,\\ \langle a_n^\dagger a_m\rangle=\sum_k (C^*_{kn}-C^*_{nk})(C_{km}-C_{mk})\ .\end{gathered} \tag{46}$$

The two-electron second-order level shift is written as the sum

$$E^{(2)}=E^{(2)}_{\mathrm{PE}}+E^{(2)}_{\mathrm{SE}}+E^{(2)}_{\mathrm{VP}} \tag{47}$$

corresponding to the three Feynman diagrams in Fig. 2. The exchanged-photon term $E^{(2)}_{\mathrm{PE}}$ arises from the first term of (40) and is given by

$$\begin{aligned}E^{(2)}_{\mathrm{PE}}=-4\pi i\alpha\int d(t_2-t_1)\int d\mathbf{x}_2\int d\mathbf{x}_1 D_F(x_2-x_1)\sum_{k,n}C^*_{kn}\frac{1}{\sqrt{2}}[\,\bar{\phi}_k(x_2)\bar{\phi}_n(x_1)-\bar{\phi}_n(x_2)\bar{\phi}_k(x_1)]\gamma_\mu^{(2)}\gamma^{\mu(1)}\\ \times\sum_{l,m}C_{lm}\frac{1}{\sqrt{2}}[\phi_l(x_2)\phi_m(x_1)-\phi_m(x_2)\phi_l(x_1)]\\ \times\delta(E_n+E_k,E_l+E_m)\ .\end{aligned} \tag{48}$$

To evaluate the self-energy and vacuum polarization terms we confine our attention to two-electron states that are linear combinations of products of hydrogenic states with well-defined parity, total angular momentum, and z component of angular momentum. We further restrict our attention to states of the form of Eq. (11) so that the C's in (45) can be written as

$$C_{nn'}=\delta_{\beta\beta_1}\delta_{\beta'\beta_2}D_{\sigma\sigma'}\ , \tag{49}$$

where β denotes the subset of quantum numbers $\{n,l,j\}$ and σ denotes the remaining quantum number $\{m\}$. Equation (49) simply reflects the fact that in this case the summation in Eq. (45) extends over the magnetic quantum numbers σ and σ' for fixed β and β'. Then in the last three terms in (40),

$$\begin{aligned}\sum_{n,m}Q_{nm}\langle a_n^\dagger a_m\rangle&=\sum_n Q_{nn}\sum_k[C^*_{kn}(C_{kn}-C_{nk})+C^*_{nk}(C_{nk}-C_{kn})]\\ &=\sum_\beta Q_{\beta\beta}\sum_\sigma\sum_{\beta',\sigma'}[\delta_{\beta\beta_2}\delta_{\beta'\beta_1}D^*_{\sigma'\sigma}(D_{\sigma'\sigma}-\delta_{\beta_1\beta_2}D_{\sigma\sigma'})+\delta_{\beta'\beta_2}\delta_{\beta\beta_1}D^*_{\sigma\sigma'}(D_{\sigma\sigma'}-\delta_{\beta_1\beta_2}D_{\sigma'\sigma})]\\ &=\sum_{\beta=\beta_1,\beta_2}Q_{\beta\beta}\ .\end{aligned} \tag{50}$$

The result in (50) takes into account the fact that the operators represented by Q_{nm} are diagonal in the specified basis, and that they are independent of σ. The last equality in (50) follows from the normalization of the C's,

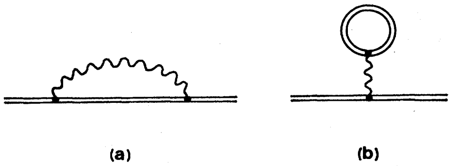

FIG. 1. Feynman diagrams for the (a) self-energy and (b) vacuum polarization in one-electron atoms.

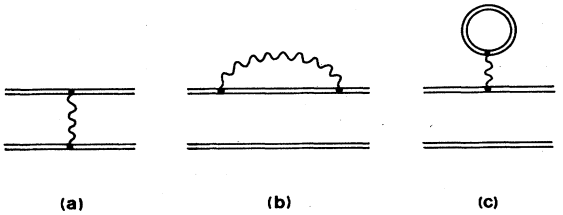

FIG. 2. Feynman diagrams for the (a) one-exchanged-photon correction, (b) self-energy, and (c) vacuum polarization in two-electron atoms.

$$\sum_{i,j} C_{ij}^{*}(C_{ij}-C_{ji})=\sum_{\sigma,\sigma'} D_{\sigma\sigma'}^{*}(D_{\sigma\sigma'}-\delta_{\beta_1\beta_2}D_{\sigma'\sigma})=1 \ . \tag{51}$$

Hence the self-energy term $E_{\mathrm{SE}}^{(2)}$ in (47) is

$$E_{\mathrm{SE}}^{(2)}=-4\pi i\alpha \int d(t_2-t_1) \int d\mathbf{x}_2 \int d\mathbf{x}_1 D_F(x_2-x_1) \sum_{\beta} \bar{\phi}_{\beta}^{\sigma}(x_2)\gamma_{\mu}S_F(x_2,x_1)\gamma^{\mu}\phi_{\beta}^{\sigma}(x_1)-\delta m \sum_{\beta} \int d\mathbf{x}\bar{\phi}_{\beta}^{\sigma}(x)\phi_{\beta}^{\sigma}(x) \tag{52}$$

and the vacuum polarization term $E_{\mathrm{VP}}^{(2)}$ is

$$E_{\mathrm{VP}}^{(2)}=4\pi i\alpha \int d(t_2-t_1) \int d\mathbf{x}_2 \int d\mathbf{x}_1 D_F(x_2-x_1)\,\mathrm{Tr}[\gamma_{\mu}S_F(x_2,x_2)] \sum_{\beta} \bar{\phi}_{\beta}^{\sigma}(x_1)\gamma^{\mu}\phi_{\beta}^{\sigma}(x_1) \ . \tag{53}$$

In (52) and (53), the summation over β extends over the hydrogenic orbitals that comprise the two-electron state, and σ can have any value in each orbital. For the ground state, the summation introduces a factor of 2.

The self-energy and vacuum polarization corrections of order α for the two-electron atom in the present perturbation approach are just the sums of the corresponding hydrogenic corrections. The exchanged-photon correction is considered in more detail in the next section.

IV. ONE-EXCHANGED-PHOTON CORRECTION

In this section we examine the one-exchanged-photon correction in Eq. (48) for states of the form of Eq. (11), and give precise numerical results over a wide range of Z. It is convenient to express the correction as the sum of a direct term E_d and an exchange term E_e,

$$E_{\mathrm{PE}}^{(2)}=E_d+E_e \tag{54}$$

with

$$E_d=-4\pi i\alpha \int d(t_2-t_1) \int d\mathbf{x}_2 \int d\mathbf{x}_1 D_F(x_2-x_1)\Phi^{\dagger}(\mathbf{x}_2,\mathbf{x}_1)\alpha_{\mu}^{(2)}\alpha^{\mu(1)}\Phi(\mathbf{x}_2,\mathbf{x}_1) \tag{55}$$

and

$$E_e=4\pi i\alpha \int d(t_2-t_1) \int d\mathbf{x}_2 \int d\mathbf{x}_1 D_F(x_2-x_1)e^{i\eta(t_2-t_1)}\Phi^{\dagger}(\mathbf{x}_2,\mathbf{x}_1)\alpha_{\mu}^{(2)}\alpha^{\mu(1)}\Phi(\mathbf{x}_1,\mathbf{x}_2) \ , \tag{56}$$

where

$$\Phi(\mathbf{x}_2,\mathbf{x}_1)=\sum_{\sigma,\sigma'} D_{\sigma\sigma'}\phi_{\beta_2}^{\sigma}(\mathbf{x}_2)\phi_{\beta_1}^{\sigma'}(\mathbf{x}_1) \tag{57}$$

and

$$\eta=E_{\beta_2}-E_{\beta_1} \ . \tag{58}$$

Integration over the time difference in (56) yields

$$\int d(t_2-t_1)D_F(x_2-x_1)e^{i\eta(t_2-t_1)}=\frac{ie^{i|\eta|x_{21}}}{4\pi x_{21}} \tag{59}$$

with $x_{21}=|\mathbf{x}_2-\mathbf{x}_1|$. We thus have for the direct term

$$E_d=\alpha \int d\mathbf{x}_2 \int d\mathbf{x}_1 \Phi^{\dagger}(\mathbf{x}_2,\mathbf{x}_1)\frac{1}{x_{21}}\alpha_{\mu}^{(2)}\alpha^{\mu(1)}\Phi(\mathbf{x}_2,\mathbf{x}_1) \ , \tag{60}$$

and for the real part of the exchange term

$$\mathrm{Re}(E_e)=-\alpha \int d\mathbf{x}_2 \int d\mathbf{x}_1 \Phi^{\dagger}(\mathbf{x}_2,\mathbf{x}_1)\frac{\cos(\eta x_{21})}{x_{21}} \times\alpha_{\mu}^{(2)}\alpha^{\mu(1)}\Phi(\mathbf{x}_1,\mathbf{x}_2) \ . \tag{61}$$

The imaginary part of the exchange term corresponds to a partial width of the excited-state resonance associated with decay to the ground state. The remainder of the natural width arises from the imaginary part of the self-energy. We are concerned here only with the real part of the level shift. Equations (60) and (61) give the Feynman gauge form of the one-exchanged photon correction. By direct calculation, this can be shown to be equal to the Coulomb gauge expression which consists of a static Coulomb interaction plus an exchanged transverse photon.[3] The latter term with retardation neglected ($\eta=0$) gives the well-known Breit interaction.

An accurate evaluation of $E_{\mathrm{PE}}^{(2)}$ for high-Z two-electron atoms is given here for the $1\,{}^1S_0$, $2\,{}^3S_1$, $2\,{}^3P_0$, and $2\,{}^3P_2$ states both as a power series in $(Z\alpha)^2$ and numerically. The level shift, understood to mean the real part, is expressed as

$$E_{\mathrm{PE}}^{(2)}=\alpha(Z\alpha)P(Z\alpha)mc^2 \ , \tag{62}$$

where $P(Z\alpha)$ can be expanded as

$$P(Z\alpha)=p_1+p_3(Z\alpha)^2+p_5(Z\alpha)^4+p_7(Z\alpha)^6+\cdots \ . \tag{63}$$

TABLE I. Values of the coefficients p_1.

State	p_1
$1\,{}^1S_0$	$\frac{5}{8}$
$2\,{}^3S_1$	$\frac{137}{729}$
$2\,{}^3P_0$	$\frac{1481}{6561}$
$2\,{}^3P_2$	$\frac{1481}{6561}$

TABLE II. Values of the coefficients p_3.

State	p_3
$1\,^1S_0$	$1-\frac{3}{4}\ln 2$
$2\,^3S_1$	$\frac{2075}{4374}+\frac{592}{729}\ln 2-\frac{2549}{2916}\ln 3$
$2\,^3P_0$	$\frac{17801}{39366}+\frac{6104}{6561}\ln 2-\frac{20957}{26244}\ln 3$
$2\,^3P_2$	$\frac{28223}{98415}+\frac{5848}{6561}\ln 2-\frac{13759}{17496}\ln 3$

The leading term p_1 corresponds to the nonrelativistic Coulomb interaction of the electrons. For completeness, these well-known coefficients are listed in Table I. The next term gives the leading relativistic correction in the electron-electron interaction. The coefficient p_3 was given for the $1\,^1S_0$ state numerically by Wu and Tauber[11] and exactly by Dalgarno and Stewart.[12] Stewart calculated the exact value of p_3 for the $2\,^3S_1$ state,[13] and Doyle gave accurate numerical values for p_3 for the $2\,^3P_0$ and $2\,^3P_2$ states.[14] The latter two authors considered other states as well.

We have calculated the coefficients p_1, p_3, and p_5 exactly for the states of interest. The procedure followed was first to carry out the integration over coordinate angles in Eqs. (60) and (61) to arrive at expressions for the sum in terms of radial integrals. These integrals are displayed in the Appendix. The remainder of the calculation was done with the aid of the algebraic computation program MACSYMA basically as follows. The integrands in the radial integrals were expanded in a Taylor series in η up to fourth order. The Γ-function integral over the variable y, defined in Eq. (A5), was formally evaluated. The integrand of the remaining integral was expanded in Taylor series in $Z\alpha$, and finally the integral over r, defined in Eq. (A5), was evaluated. The results for p_3 and p_5 are listed in Tables II and III, respectively. The values obtained for p_3 are in agreement with the previous work already mentioned. The expressions for p_5 include the dilogarithm function L of argument $-\frac{1}{2}$ where[15]

$$L(-\tfrac{1}{2})=\sum_{n=1}^{\infty}\frac{1}{n^2}(-\tfrac{1}{2})^n=-0.448\,414\,21\ldots \tag{64}$$

To provide values for the level shift $\Delta E_{\rm PE}^{(2)}$ for large Z and as a consistency check, we calculated the function $P(Z\alpha)$ numerically for the states of interest for $Z=10,20,\ldots,110$. Gaussian quadrature was applied for each of the variables r and y in (A5), with 60 and 100 integration points, respectively. The numerical precision was estimated by varying the number of integration points in each dimension. The results are given in Table IV. All figures shown in that table are significant.

By fitting a sixth- or seventh-degree polynomial in $(Z\alpha)^2$ to the first seven or eight calculated values of $[P(Z\alpha)-p_1]/(Z\alpha)^2$ we estimate the first few coefficients of the power series in $(Z\alpha)^2$. With the full calculated accuracy (more than shown in Table IV) of the values for $P(Z\alpha)$, the corresponding coefficients p_3 and p_5 agree with the analytic results to about nine and seven figures past the decimal point, respectively. In addition, a numerical estimate for the next coefficient p_7, apparently accurate to more than four figures past the decimal point, is obtained. The estimated values appear in Table V. Previous estimates of coefficients in (63) based on polynomial fits to numerical calculations have been made. An earlier estimate of $\Delta p_5=0.10$ for the $2\,^3S_1-2\,^3P_0$ splitting by Mohr is in agreement with the current results.[16] An estimate of p_5 and p_7 by Safronova is consistent with the present results for the $1\,^1S_0$ state but not for the excited states.[17] Results of a numerical calculation of $P(Z\alpha)$ for the $2\,^3S_1$, $2\,^3P_0$, and $2\,^3P_2$ states for $Z=14,16,17$ by Cheng are in complete agreement with the values given by Eq. (63).[18] Grant has estimated p_5 for the $2\,^3P_0$ and $2\,^3P_2$ states based on a numerical fit to results of a multiconfiguration Dirac-Hartree-Fock calculation.[19] His results $p_5(2^3P_0)=0.143\,282$ and $p_5(2\,^3P_2)=-0.001\,691\,2$ are in reasonable agreement with the values in Table III. Drake has calculated numerical values for p_5 that are in agreement with the results given here.[20]

The power series for the level shift provides an accurate approximation to the function $P(Z\alpha)$ for Z not too large.

TABLE III. Values of the coefficients p_5.

State	p_5
$1\,^1S_0$	$\frac{109}{32}-\frac{\pi^2}{16}-\frac{51}{16}\ln 2-\frac{3}{4}\ln^2 2$
$2\,^3S_1$	$\frac{29845}{104976}-\frac{181}{17496}\pi^2-\frac{958}{2187}\ln 2+\frac{57667}{69984}\ln 3$ $-\frac{181}{5832}\ln^2 2+\frac{2549}{2916}\ln 2\ln 3-\frac{2549}{2916}\ln^2 3$ $+\frac{3}{4}L(-\frac{1}{2})$
$2\,^3P_0$	$\frac{129731}{157464}+\frac{1411}{157464}\pi^2+\frac{643}{729}\ln 2-\frac{441845}{629856}\ln 3$ $-\frac{17021}{52488}\ln^2 2+\frac{29149}{26244}\ln 2\ln 3-\frac{20957}{26244}\ln^2 3$ $+\frac{3}{4}L(-\frac{1}{2})$
$2\,^3P_2$	$-\frac{1712371}{9447840}+\frac{1667}{314928}\pi^2-\frac{39623}{39366}\ln 2+\frac{4458869}{4199040}\ln 3$ $-\frac{42461}{104976}\ln^2 2+\frac{16831}{17496}\ln 2\ln 3-\frac{13759}{23328}\ln^2 3$ $+\frac{3}{8}L(-\frac{1}{2})$

TABLE IV. Numerical values of the function $P(Z\alpha)$.

Z	$1\,^1S_0$	$2\,^3S_1$	$2\,^3P_0$	$2\,^3P_2$
10	0.627 563	0.188 340	0.226 902	0.225 944
20	0.635 328	0.189 587	0.230 475	0.226 593
30	0.648 533	0.191 718	0.236 601	0.227 672
40	0.667 603	0.194 816	0.245 561	0.229 179
50	0.693 209	0.199 010	0.257 799	0.231 114
60	0.726 364	0.204 496	0.273 996	0.233 478
70	0.768 597	0.211 564	0.295 189	0.236 279
80	0.822 278	0.220 657	0.323 008	0.239 535
90	0.891 270	0.232 481	0.360 135	0.243 284
100	0.982 380	0.248 242	0.411 348	0.247 598
110	1.109 168	0.270 240	0.486 234	0.252 618

This is in contrast to the self-energy correction where the convergence is poor numerically. The power series expressions are summarized as

$$P(Z\alpha)=\tfrac{5}{8}+0.480\,140(Z\alpha)^2+0.219\,653(Z\alpha)^4+0.1507(Z\alpha)^6+\cdots \quad \text{for } 1\,^1S_0\ , \tag{65a}$$

$$P(Z\alpha)=\tfrac{137}{729}+0.076\,935(Z\alpha)^2+0.043\,223(Z\alpha)^4+0.0281(Z\alpha)^6+\cdots \quad \text{for } 2\,^3S_1\ , \tag{65b}$$

$$P(Z\alpha)=\tfrac{1481}{6561}+0.219\,768(Z\alpha)^2+0.142\,891(Z\alpha)^4+0.1070(Z\alpha)^6+\cdots \quad \text{for } 2\,^3P_0\ , \tag{65c}$$

$$P(Z\alpha)=\tfrac{1481}{6561}+0.040\,639(Z\alpha)^2-0.001\,882(Z\alpha)^4+0.0037(Z\alpha)^6+\cdots \quad \text{for } 2\,^3P_2\ . \tag{65d}$$

TABLE V. Estimated values for the coefficient p_7.

State	p_7
$1\,^1S_0$	0.1507
$2\,^3S_1$	0.0281
$2\,^3P_0$	0.1070
$2\,^3P_2$	0.0037

V. CONCLUSION

We have made a direct application of bound-state quantum electrodynamics to the high-Z few-electron system to derive all corrections of order α to the energy levels. The corrections are the exchanged-photon correction, the one-electron self-energy, and the one-electron vacuum polarization. In this approach it is clear how to proceed to higher-order corrections in a consistent way. Calculation of the next-order corrections, which include two-exchanged-photon and screened-Lamb-shift corrections, should be feasible within the present framework.

Accurate numerical values for the two-electron exchanged-photon correction are given here, and the one-electron corrections at high Z have been reviewed elsewhere.[21] For a stringent test of quantum electrodynamics, however, higher-order corrections in α or equivalently $1/Z$ are needed. A tentative comparison of theory and experiment, based on partial knowledge of the higher-order terms, yields satisfactory agreement.[22]

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APPENDIX

Integration over coordinate angles in Eqs. (60) and (61) yields the following expressions for the one-exchanged-photon level shift:

$$E_{\mathrm{PE}}^{(2)}=\alpha\int_0^\infty dx_2x_2^2\int_0^\infty dx_1x_1^2\left\{[g_r^2(x_2)+f_r^2(x_2)][g_r^2(x_1)+f_r^2(x_1)]\frac{1}{x_>}+\tfrac{8}{3}g_r(x_2)f_r(x_2)g_r(x_1)f_r(x_1)\frac{x_<}{x_>^2}\right\} \quad \text{for } 1\,^1S_0\ , \tag{A1}$$

$$\begin{aligned}E_{\mathrm{PE}}^{(2)}=\alpha\int_0^\infty dx_2x_2^2\int_0^\infty dx_1x_1^2\bigg\{&[g_r^2(x_2)+f_r^2(x_2)][g_s^2(x_1)+f_s^2(x_1)]\frac{1}{x_>}-\tfrac{8}{9}g_r(x_2)f_r(x_2)g_s(x_1)f_s(x_1)\frac{x_<}{x_>^2}\\&+[g_r(x_2)g_s(x_2)+f_r(x_2)f_s(x_2)][g_r(x_1)g_s(x_1)+f_r(x_1)f_s(x_1)]\eta j_0(\eta x_<)y_0(\eta x_>)\\&+\tfrac{1}{3}[g_r(x_2)f_s(x_2)g_s(x_1)f_r(x_1)+f_r(x_2)g_s(x_2)f_s(x_1)g_r(x_1)\\&\qquad-5g_r(x_2)f_s(x_2)f_s(x_1)g_r(x_1)-5f_r(x_2)g_s(x_2)g_s(x_1)f_r(x_1)]\\&\times\eta j_1(\eta x_<)y_1(\eta x_>)\bigg\} \quad \text{for } 2\,^3S_1\ ,\end{aligned} \tag{A2}$$

$$\begin{aligned}E_{\mathrm{PE}}^{(2)}=\alpha\int_0^\infty dx_2x_2^2\int_0^\infty dx_1x_1^2\bigg[&[g_r^2(x_2)+f_r^2(x_2)][g_p^2(x_1)+f_p^2(x_1)]\frac{1}{x_>}-\tfrac{8}{3}g_r(x_2)f_r(x_2)g_p(x_1)f_p(x_1)\frac{x_<}{x_>^2}\\&+[g_r(x_2)g_p(x_2)+f_r(x_2)f_p(x_2)][g_r(x_1)g_p(x_1)+f_r(x_1)f_p(x_1)]\eta j_1(\eta x_<)y_1(\eta x_>)\\&-[g_r(x_2)f_p(x_2)g_p(x_1)f_r(x_1)+f_r(x_2)g_p(x_2)f_p(x_1)g_r(x_1)\\&\quad+3g_r(x_2)f_p(x_2)f_p(x_1)g_r(x_1)]\eta j_0(\eta x_<)y_0(\eta x_>)\\&-\tfrac{1}{3}f_r(x_2)g_p(x_2)g_p(x_1)f_r(x_1)\\&\quad\times\eta[j_0(\eta x_<)y_0(\eta x_>)+8j_2(\eta x_<)y_2(\eta x_>)]\bigg]\quad\text{for } 2\,{}^3P_0\,,\end{aligned}\tag{A3}$$

$$\begin{aligned}E_{\mathrm{PE}}^{(2)}=\alpha\int_0^\infty dx_2x_2^2\int_0^\infty dx_1x_1^2\bigg[&[g_r^2(x_2)+f_r^2(x_2)][g_q^2(x_1)+f_q^2(x_1)]\frac{1}{x_>}-\tfrac{16}{15}g_r(x_2)f_r(x_2)g_q(x_1)f_q(x_1)\frac{x_<}{x_>^2}\\&+[g_r(x_2)g_q(x_2)+f_r(x_2)f_q(x_2)][g_q(x_1)g_r(x_1)+f_q(x_1)f_r(x_1)]\eta j_1(\eta x_<)y_1(\eta x_>)\\&+\tfrac{1}{5}[g_r(x_2)f_q(x_2)g_q(x_1)f_r(x_1)+f_r(x_2)g_q(x_2)f_q(x_1)g_r(x_1)\\&\quad-9g_r(x_2)f_q(x_2)f_q(x_1)g_r(x_1)]\eta j_2(\eta x_<)y_2(\eta x_>)\\&-f_r(x_2)g_q(x_2)g_q(x_1)f_r(x_1)\\&\quad\times\eta[\tfrac{4}{3}j_0(\eta x_<)y_0(\eta x_>)+\tfrac{7}{15}j_2(\eta x_<)y_2(\eta x_>)]\bigg]\quad\text{for } 2\,{}^3P_2\,.\end{aligned}\tag{A4}$$

In (A1)—(A4), g and f are the Dirac radial wave functions, the subscripts r, s, p, and q refer to the $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$ states, respectively, and $x_< = \min(x_2,x_1)$ and $x_> = \max(x_2,x_1)$. To evaluate the integrals in (A1)—(A4) it is convenient to make the change of variables

$$\int_0^\infty dx_2\int_0^\infty dx_1F(x_2,x_1)=\int_0^\infty dy\,y\int_0^1 dr[F(ry,y)+F(y,ry)]\tag{A5}$$

where $y=x_>$ and $ry=x_<$.

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