

Radiative potential and calculations of QED radiative corrections to energy levels and electromagnetic amplitudes in many-electron atoms

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(Received 15 July 2005; published 30 November 2005)

We derive an approximate expression for a “radiative potential” which can be used to calculate QED strong Coulomb field radiative corrections to energies and electric dipole ($E1$) transition amplitudes in many-electron atoms with an accuracy of a few percent. The expectation value of the radiative potential gives radiative corrections to the energies. Radiative corrections to $E1$ amplitudes can be expressed in terms of the radiative potential and its energy derivative (the low-energy theorem): the relative magnitude of the radiative potential contribution is $\sim\alpha^3 Z^2 \ln(1/\alpha^2 Z^2)$, while the sum of other QED contributions is $\sim\alpha^3 (Z_i+1)^2$, where Z_i is the ion charge; that is, for neutral atoms ($Z_i=0$) the radiative potential contribution exceeds other contributions $\sim Z^2$ times. The advantage of the radiative potential method is that it is very simple and can be easily incorporated into many-body theory approaches: relativistic Hartree-Fock, configuration interaction, many-body perturbation theory, etc. As an application we have calculated the radiative corrections to the energy levels and $E1$ amplitudes as well as their contributions (-0.34% and $+0.43\%$, respectively) to the parity nonconserving (PNC) $6s-7s$ amplitude in neutral cesium ($Z=55$). Combining these results with the QED correction to the weak matrix elements (-0.41%) we obtain the total QED correction to the PNC $6s-7s$ amplitude, $(-0.32\pm 0.03)\%$. The cesium weak charge $Q_W = -72.66(29)_{\text{exp}}(36)_{\text{theor}}$ agrees with the Standard Model value $Q_W^{\text{SM}} = -73.19(13)$, the difference is $0.53(48)$.

DOI: [10.1103/PhysRevA.72.052115](https://doi.org/10.1103/PhysRevA.72.052115)

PACS number(s): 32.80.Ys, 31.30.Jv

I. INTRODUCTION

The precision of calculations and measurements of phenomena of heavy neutral atoms has reached the level where strong-field QED radiative corrections are observable. The most striking example is parity nonconservation (PNC) in the neutral cesium atom ($Z=55$) where the nuclear Coulomb field radiative corrections “saved” the standard model of particle physics (this dramatic story may be found, e.g., in the review of Ref. [1]; see also the original papers for the measurement [2,3] and calculations of strong-field radiative corrections [4–15]).

While there is an abundance of highly accurate calculations of radiative corrections to phenomena of single-electron or few-electron atoms, only a handful of calculations have been performed for atoms with many electrons. A proper account of the many-body effects in calculations of radiative corrections to phenomena of many-electron atoms, including the PNC amplitude, is lacking.

The first estimates of radiative corrections to energies of an external electron in heavy neutral atoms were performed more than 20 years ago [16]. A semiempirical formula for the s -wave radiative correction to energy levels (the Lamb shift) was derived. The relative magnitude of this correction is $\sim Z^2 \alpha^3 \ln(1/Z^2 \alpha^2)$. It rapidly increases with the nuclear charge Z and was important in making a very accurate prediction of the francium ($Z=87$) spectrum (measurements performed after the theoretical prediction [16] agree with the calculated energy levels to better than 0.1%). Calculations of the Lamb shift in alkali and coinage metal atoms were performed in Ref. [17] using local Dirac-Slater potentials; importantly, it was demonstrated that the ratio of energy shifts

arising from the Uehling potential and self-energy in neutral atoms is the same as that in hydrogenlike ions, verifying the authors’ earlier estimates [18] (see also, e.g., Ref. [19] where a similar approach, following from Welton’s semiclassical arguments [20], has been used successfully to estimate the self-energy in several-electron highly charged ions). Calculations of the Lamb shift in neutral alkali atoms were also performed in Ref. [21] using local atomic potentials. In our recent works [6] we used a parametric potential fitted to reproduce Lamb shifts in hydrogenlike ions to perform approximate numerical calculations of radiative corrections to the energy levels, electric dipole ($E1$) transition amplitudes, and a rough estimate of radiative corrections to the PNC amplitude in cesium. Recently, calculations of radiative corrections in local effective atomic potentials have been performed for $E1$ amplitudes in neutral alkalis in Ref. [22] and for the PNC amplitude in Cs in Ref. [14].

It is well known that many-body effects (exchange interaction, core relaxation and polarization, correlations) may be very important. For any perturbation located at small distances, e.g., the field (volume) isotopic shift, the matrix elements for an electron with orbital angular momentum $l>0$ are dominated by the many-body effects mentioned above. In this case one cannot guarantee the magnitude or even the sign of the shift when one does a model potential calculation. Moreover, even for the s wave, many-body corrections can change the results by a factor of 2. QED radiative corrections also come from small distances, and one may expect a similar situation. Therefore recent calculations of QED corrections in model atomic potentials cannot guarantee results of high accuracy. Indeed, in a recent work [23] the importance of a proper account of core relaxation in calculations of the

radiative shift due to the Uehling potential was demonstrated for neutral cesium.

In the present work we suggest a simple radiative potential approach that allows one to calculate radiative corrections to many-electron atoms including many-body effects. In particular, our method is valid for calculations of the Lamb shift and radiative corrections to $E1$ amplitudes. We claim an accuracy of a few percent for calculations of radiative corrections to s -wave energy levels, s - p intervals, and s - p $E1$ amplitudes for neutral cesium using the radiative potential approach. We believe that our approach is complementary to the direct Feynman diagram calculations in a model potential.

This paper is organized as follows. In Sec. II we derive an approximate *ab initio* formula for the radiative potential for $Z\alpha \ll 1$. Then we refine this potential to include higher orders in $Z\alpha$ using published results for hydrogenlike ions [24]. In Sec. III we describe the procedure for calculations of QED radiative corrections to electric dipole amplitudes. In Sec. III A we derive the low-energy theorem: the vertex and normalization corrections are expressed in terms of $\partial\Sigma/\partial E$ where Σ is the electron self-energy operator. The dominating contribution to the $E1$ amplitude is due to the radiative corrections to electron wave functions produced by the radiative potential (Sec. III B). The relative value of this contribution is $\sim \alpha^3 Z^2 \ln(1/\alpha^2 Z^2)$ both in ions and neutral atoms. It is shown in Sec. III C that the sum of all other terms [the vertex correction, the normalization correction, and part of the self-energy operator which can be presented as $\Sigma^A = (H-E)A + A(H-E)$ and does not contribute to the energy shifts] is $\sim \alpha^3 (Z_i + 1)^2$, where Z_i is the ion charge, H is the atomic electron Hamiltonian, and A is an operator defined in Sec. III C. Therefore in neutral atoms ($Z_i = 0$) this sum is Z^2 times smaller than the radiative potential contribution and may be neglected. As an application we calculate in Sec. IV the radiative corrections to the energy levels and $E1$ amplitudes in neutral cesium including many-body effects: core relaxation, core polarization by the external photon electric field, and correlation corrections. In Sec. V we calculate the radiative corrections to energy levels and $E1$ amplitudes contributing to the parity nonconserving $6s$ - $7s$ amplitude in Cs. Finally, the conclusion for the radiative potential approach for the calculations of the QED radiative corrections to energies, $E1$ amplitudes, and the PNC amplitude is given in Sec. VI.

II. RADIATIVE POTENTIAL

A. Derivation of the radiative potential; radiative shifts in H-like ions

We define a radiative potential \hat{L} such that its average value coincides with the radiative corrections to energies,

$$\delta E_n = \langle n | \hat{L} | n \rangle; \quad (1)$$

the radiative potential is nonlocal and energy dependent, $\hat{L} = \hat{L}(\mathbf{r}, \mathbf{r}', E)$, where E is the electron energy. It contains the nonlocal electron self-energy operator in the strong Coulomb field, $\hat{\Sigma}(\mathbf{r}, \mathbf{r}', E)$, and the local vacuum polarization operator

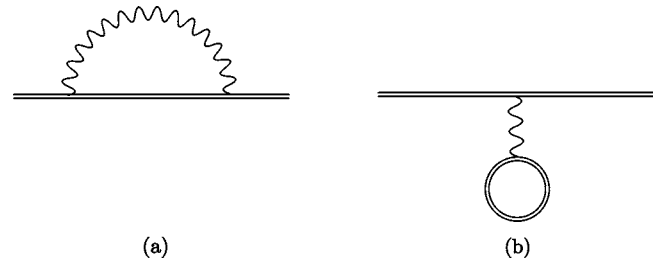


FIG. 1. Diagrams for radiative energy shifts (\hat{L}) corresponding to (a) the self-energy and (b) vacuum polarization. The double line denotes a bound electron; the wavy line denotes a photon.

comprised of the lowest-order in $Z\alpha$ Uehling potential $\Phi_U(r)$ and the higher-order Wichmann-Kroll potential. Diagrams for the radiative energy shifts are presented in Fig. 1.

The actual problem is the calculation of the self-energy $\Sigma(\mathbf{r}, \mathbf{r}', E)$. This calculation can be divided into two parts: one in which the electron interaction with virtual photons of high frequency is considered, and one in which virtual photons of low frequency is considered. In the high frequency case the external field (the nuclear Coulomb field) need only be included to first order (vertex diagram). In the case of a free electron the vertex diagram gives the electric $f(q^2)$ and magnetic $g(q^2)$ form factors presented, for example, in Ref. [25]. The calculations of the contributions of $f(q^2)$ and $g(q^2)$ to the radiative potential \hat{L} are similar to the calculation of the Uehling contribution presented in Ref. [25]. Therefore we present the calculations very briefly. We also present the well-known results for the Uehling potential for comparison with the $f(q^2)$ and $g(q^2)$ contributions calculated in this work.

In the momentum representation the high-frequency contribution to the radiative potential is equal to

$$\Phi_{\text{rad}}(\mathbf{q}) = Q_{\text{rad}}(\mathbf{q})\Phi(\mathbf{q}), \quad (2)$$

where Φ is the atomic potential which at small distances is equal to the unscreened nuclear electrostatic potential, and

$$Q_{\text{rad}}(\mathbf{q}) = -\frac{1}{\mathbf{q}^2} P(-\mathbf{q}^2) + \frac{g(-\mathbf{q}^2)}{2m} \boldsymbol{\gamma} \cdot \mathbf{q} + f(-\mathbf{q}^2) - 1. \quad (3)$$

Here the first term contains the polarization operator $P(-\mathbf{q}^2)$ and leads to the Uehling potential, $\boldsymbol{\gamma}$ are the Dirac matrices, and $m = 1/r_c$ where r_c is the Compton wavelength. We use units $\hbar = c = 1$ throughout, except where presented explicitly. In the coordinate representation [25]

$$\Phi_{\text{rad}}(r) = \frac{1}{4\pi^2 r} \text{Im} \int_{-\infty}^{\infty} \Phi_{\text{rad}}(-y^2) \exp(iy) y dy, \quad (4)$$

where $y = \sqrt{\mathbf{q}^2}$. A method to calculate this integral is suggested in Ref. [25]. After substitution of $P(-\mathbf{q}^2)$, $f(-\mathbf{q}^2)$, and $g(-\mathbf{q}^2)$ from Ref. [25] we obtain

$$\Phi_{\text{rad}}(r) = \Phi_U(r) + \Phi_g(r) + \Phi_f^\lambda(r). \quad (5)$$

The first term is the well-known Uehling potential

$$\Phi_U(r) = \frac{2\alpha}{3\pi} \Phi(r) \int_1^\infty dt \frac{\sqrt{t^2-1}}{t^2} \left(1 + \frac{1}{2t^2}\right) e^{-2trm}. \quad (6)$$

For the magnetic form-factor contribution we obtain

$$\Phi_g(r) = \frac{\alpha}{4\pi m} i\boldsymbol{\gamma} \cdot \nabla \left[\Phi(r) \left(\int_1^\infty dt \frac{1}{t^2 \sqrt{t^2-1}} e^{-2trm} - 1 \right) \right]. \quad (7)$$

A straightforward calculation for the electric form factor gives

$$\begin{aligned} \Phi_f^\lambda(r) = & -\frac{\alpha}{\pi} \Phi(r) \int_1^\infty dt \frac{1}{\sqrt{t^2-1}} \left[\left(1 - \frac{1}{2t^2}\right) \right. \\ & \left. \times [\ln(t^2-1) + \ln(4m^2/\lambda^2)] - \frac{3}{2} + \frac{1}{t^2} \right] e^{-2trm}. \quad (8) \end{aligned}$$

The expression for the electric form factor (8) contains a low-frequency cutoff parameter λ in the argument of the logarithm. In the standard calculation of the energy shift [25] this parameter is assumed to be in the interval $(Z\alpha)^2 m \ll \lambda \ll m$. After addition of the low-frequency contribution the parameter λ cancels out. To minimize the low-frequency contribution we select λ of the order of the electron binding energy in atoms, $\lambda \sim (Z\alpha)^2 m$, which is the smallest possible value that can be taken as the border for the high-frequency region [one can use free-electron Green's functions to calculate the electron form factors, used above, for frequencies $\omega \gg (Z\alpha)^2 m$]. This gives $\ln(4m^2/\lambda^2) = 4 \ln(1/Z\alpha) + \text{const}$, where the constant const does not depend on Z for $Z\alpha \ll 1$, $\text{const} \sim 1$. Therefore the high-frequency contribution allows us to determine the electric form-factor contribution with logarithmic accuracy. The uncertainty is due to the omitted low-frequency contribution for this term.

The constant in the electric form factor can be found from a comparison with calculations of the Lamb shift for the high-energy levels (principal quantum number $n \gg 1$) in hydrogenlike ions. Indeed, the energy of an external electron in a many-electron atom is extremely small, $E \sim 10^{-5} mc^2$. Therefore we need the self-energy operator $\Sigma(\mathbf{r}, \mathbf{r}', E \approx 0)$. The short-range character of Σ means that we can use unscreened Coulomb Green's functions to calculate it.

For very light atoms ($Z \sim 1$) the comparison can be made with the nonrelativistic calculations presented in Ref. [25], yielding $\text{const} \approx -0.63$. However, this result is not applicable for $Z \geq 10$. In this case we have to use the results of all orders in $Z\alpha$ calculations for hydrogenlike ions presented in Ref. [24]. To reproduce the results of Ref. [24] (and leave some room for a low-frequency contribution discussed below) we select this logarithm in the form $4 \ln(1/Z\alpha + 0.5)$, where a small constant 0.5 is added into the argument of the logarithm. This selection gives an accuracy $\sim 10\%$ for all important applications: the s -wave self-energy, s - p intervals (which are needed to calculate the parity violation effects), and fine structure intervals for any Z . However, the radiative shifts for p waves (and higher waves) are small and sensitive to the

low-frequency contribution. To make our calculation complete and improve the accuracy to 1% we should consider this contribution too.

A consistent calculation of the low-frequency contribution to the nonlocal self-energy operator $\Sigma(\mathbf{r}, \mathbf{r}', E)$ using Coulomb or parametric potential Green's functions is a complicated task. However, at the present level of experimental accuracy this low-frequency problem is not of immediate importance. It is much easier to fit this small low-frequency contribution using a parametric potential $\Phi_l(r)$. A typical frequency in the low-frequency contribution is $\sim E_{1s}$; therefore the range of this potential is about the size of the $1s$ orbital, a_B/Z . To reproduce the p -level radiative energy shifts we use the following expression for the low-frequency contribution:

$$\Phi_l(r) = -\frac{B(Z)}{e} Z^4 \alpha^5 mc^2 e^{-Zr/a_B}, \quad (9)$$

where e is the proton charge and $B(Z) = 0.074 + 0.35Z\alpha$ is a coefficient fitted to reproduce the radiative shifts for the high Coulomb p levels calculated in Ref. [24].

Finally, we should introduce one more correction which becomes important for very heavy atoms, $Z > 80$. The potential (8) is not applicable for very small distances, $r \ll Z\alpha r_c$. Indeed, we used an expression for the electric form factor of a free electron. However, at very small distances the electron potential energy $Z\alpha/r \gg m$ and we should use an expression for an off-mass-shell form factor $f(p, p')$ instead of $f(-q^2)$. The form factor $f(p, p')$ leads to a nonlocal expression $\Sigma(\mathbf{r}, \mathbf{r}', E)$ for $r \ll Z\alpha r_c$ instead of the local potential (8). Integration of an electron wave function ψ with a nonlocal operator $(f \Sigma(\mathbf{r}, \mathbf{r}', E) \psi(\mathbf{r}') d^3 r')$ makes the effective potential less singular. We take into account this fact by introducing a small distance cut-off coefficient $mr/(mr + 0.07Z^2\alpha^2)$. Our final expression for the electric formfactor contribution has the following form

$$\begin{aligned} \Phi_f(r) = & -A(Z, r) \frac{\alpha}{\pi} \Phi(r) \int_1^\infty dt \frac{1}{\sqrt{t^2-1}} \left[\left(1 - \frac{1}{2t^2}\right) \right. \\ & \left. \times [\ln(t^2-1) + 4 \ln(1/Z\alpha + 0.5)] - \frac{3}{2} + \frac{1}{t^2} \right] e^{-2trm}. \quad (10) \end{aligned}$$

Here the coefficient $A(Z, r) = (1.071 - 1.976x^2 - 2.128x^3 + 0.169x^4)mr/(mr + 0.07Z^2\alpha^2)$, where $x = (Z - 80)\alpha$; $A(Z, r)$ was found by fitting the radiative shifts for the high Coulomb s levels calculated in Ref. [24].

Thus we obtain the following expression for the complete radiative potential:

$$\Phi_{\text{rad}}(r) = \Phi_U(r) + \Phi_g(r) + \Phi_f(r) + \Phi_l(r) + \frac{2}{3} \Phi_{\text{WC}}^{\text{simple}}(r), \quad (11)$$

where $\Phi_U(r)$ is the Uehling potential (6), $\Phi_g(r)$ is the magnetic formfactor contribution (7), $\Phi_f(r)$ is the high-frequency electric form-factor contribution (10), and $\Phi_l(r)$ is the low-frequency contribution (9).

TABLE I. Difference (in %) between the results of the Mohr-Kim self-energy calculations in Ref. [24] and the radiative potential results $[(\text{Mohr}-g-f-l)/(\text{Mohr}-g)]$ for hydrogenlike ions.

Z	10	20	30	40	50	60	70	80	90	100	110
$5s_{1/2}$	0.0	0.4	0.5	0.3	0.0	-0.2	-0.2	0.0	0.1	0.1	0.0
$5p_{1/2}$	-0.8	-3.6	-2.8	-1.8	-1.1	-0.7	-0.3	0.1	0.8	1.8	3.3
$5p_{3/2}$	-2.5	-8.3	-8.9	-7.3	-5.2	-3.1	-1.1	0.4	1.4	1.7	0.8

To make the picture complete we added to the radiative potential a simplified form of the Wichmann-Kroll potential (higher-orders vacuum polarization) which has accurate short-range and long-range asymptotics [6]:

$$\Phi_{\text{WC}}^{\text{simple}}(r) = -\frac{2\alpha}{3\pi}\Phi(r)\frac{0.092Z^2\alpha^2}{1+(1.62r/r_c)^4}. \quad (12)$$

Accurate calculations of the Wichmann-Kroll contribution in hydrogenlike ions for $Z=30, 40, \dots, 100$ have been performed in Ref. [26]. To reproduce the Wichmann-Kroll s -wave shifts from Ref. [26] with a few percent accuracy one should take $\Phi_{\text{WC}}(r) = 2/3 \Phi_{\text{WC}}^{\text{simple}}(r)$. The Wichmann-Kroll potential (12) gives a very small contribution which may be noticeable ($\sim 1\%$) only for $Z > 80$. (This confirms our conclusion [6] that the contribution of higher orders into the vacuum polarization potential is so small that it is unobservable in neutral atoms: for the cesium atom the Wichmann-Kroll potential gives a contribution to s waves about 50 times smaller than the Uehling potential contribution; moreover, the Uehling potential itself gives only about 10% of the total radiative correction for s waves and a very small contribution for higher waves.)

Note that our fitting coefficient in the electric form-factor contribution $A(Z, r) \approx 1$ and the coefficient in the low-frequency contribution B is small, therefore the semiempirical radiative potential (11) is always close to the result of the direct Feynman diagram calculation $\Phi_U(r) + \Phi_g(r) + \Phi_f^\lambda(r)$. It may look surprising that the radiative potential obtained in the approximation $Z\alpha \ll 1$ gives energy shifts which are close to the all-orders results. However, the higher-order corrections to the energy shifts are mainly due to the relativistic electron wave functions which we take into account exactly when calculating the matrix elements. Indeed, the Dirac wave function diverges at small distances $r < a_B/Z$:

$$\frac{\psi_{p_{1/2}}^\dagger \psi_{p_{1/2}}}{Z^2 \alpha^2} \sim \psi_s^\dagger \psi_s \sim r^{-Z^2 \alpha^2} = \exp(-Z^2 \alpha^2 \ln r). \quad (13)$$

The radiative energy shifts originate from very small distances $r \sim r_c = \hbar/mc$. Thus we take into account the relativistic enhancement factor $[\psi^2(r_c)/\psi^2(a_B/Z)] \sim (a_B/Zr_c)^{Z^2 \alpha^2} = (1/Z\alpha)^{Z^2 \alpha^2} = \exp[Z^2 \alpha^2 \ln(1/Z\alpha)]$ in the $Z\alpha$ dependence of the matrix elements when we use the Dirac wave functions.

In Table I we compare the self-energy for $5s_{1/2}$, $5p_{1/2}$, and $5p_{3/2}$ levels in hydrogenlike ions calculated using the potential $\Phi_g(r) + \Phi_f(r) + \Phi_l(r)$ with those of Ref. [24]. It is seen that the radiative potential Φ_{rad} reproduces the self-energy within a few percent for all Z . The comparison is made for

the highest available principal quantum number $n=5$ in order to satisfy the condition $E \ll mc^2$ which is needed to calculate the radiative corrections in neutral atoms. However, in practice the results are good for any $n > 1$. Moreover, the potential $\Phi_{\text{rad}}(r)$ even gives the $1s$ energy with reasonable accuracy, $\sim 10\%$. Note that to calculate parity violation we mainly need to reproduce high s -level shifts in Cs ($Z=55$), Tl ($Z=81$), and Fr ($Z=87$); the p -level shifts are very small and not important.

The above calculations (and those of Ref. [24]) were performed in the Coulomb field of a pointlike nucleus $\Phi(r) = Ze/r$. The small correction due to finite nuclear size can be taken into account using integration over a realistic charge density for the nucleus, $\Phi_{\text{rad}}(\mathbf{r}) = \int \Phi_{\text{rad}}^{\text{point charge}}(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r}')d^3r'$. The finite nuclear size contribution is suppressed by a small parameter $r_n/r_c \sim 10^{-2}$. The results of our calculations for neutral cesium presented later in this work include this correction.

B. Radiative potential in atomic calculations

The radiative potential we have derived from radiative shifts in hydrogenlike ions can be used in calculations of radiative shifts in ions and neutral atoms for all Z and for any number of electrons.

Indeed, all electron wave functions with energy $E \ll mc^2$ are proportional to the zero-energy Coulomb wave functions in the area $r \sim r_c$, since the energy E may be neglected in the Dirac equation and the potential is unscreened in this region. Therefore the ratio of the matrix elements of the radiative potential will be equal to the ratio of the electron densities near the origin (at a given j, l). This is the reason why one may use parametric potentials fitted to reproduce Lamb shifts in hydrogenlike ions (for principal quantum numbers $n \gg 1$). Any potential of the range $\sim r_c$ will give the same results. The radiative potentials Eqs. (6) and (10) belong to this class. This also explains the conclusion of Ref. [17] that the ratio of the self-energy contribution to the Uehling contribution is the same in hydrogenlike ions and neutral atoms calculated in Dirac-Slater potentials.

The magnetic form-factor potential Eq. (7) is a long-range one. However, it decays rapidly and its matrix elements are still determined by small distances $r \sim a_B/Z$ where all the wave functions with principal quantum numbers $n \gg 1$ and given j, l are proportional (since the energy $|E_n| \ll |E_{1s}|$ and may be neglected in the area $r \sim a_B/Z$). Thus the radiative shifts at a given j, l are still proportional to the electron density in the vicinity of the nucleus ($1/n^3$ in the Coulomb case). Numerical data presented in Ref. [25] show that this state-

ment is accurate to a few percent for $n > 1$ (exact for $n \gg 1$).

Our semiempirical radiative potential was derived in the field of the nucleus. In atoms there is an electron density contribution to the radiative potential. This can be found by integration of the point-charge radiative potential over the electron density (as in the finite nuclear size calculation). It is easy to show that this contribution is very small. The electron density contribution is suppressed Z times relative to the nuclear charge contribution. Indeed, to find the energy shift we need to integrate the radiative potential with a squared external electron wave function $\psi^2(r)$. For the nuclear contribution $\psi^2 \sim \psi^2(r_c)$; for the electron charge contribution $\psi^2 \sim \psi^2(a_B)$, since the radius of the electron charge density is of the order of the Bohr radius a_B . For an external s -wave electron in a neutral atom the ratio $\psi^2(r_c)/\psi^2(a_B) \sim Z$. Thus the nuclear contribution is Z times larger than the electron density contribution. A more elaborate estimate using the WKB semiclassical electron wave function and the Thomas-Fermi electron density confirms this simple estimate.

Note that to estimate the electron density contribution to the self-energy operator we can use a semiclassical expression for Σ derived in Ref. [27]:

$$\Sigma(r, r', E) = \frac{\alpha}{3\pi m^2} \ln \frac{mc^2}{|e\Phi(r) + E|} \nabla^2(-e\Phi(r)) \delta(\mathbf{r} - \mathbf{r}'). \quad (14)$$

Here $\nabla^2(-e\Phi(r)) = 4\pi e^2 n_e(r)$, $n_e(r)$ is the electron number density. This semiclassical expression is valid for $r > a_B/Z$. Again, an estimate based on Eq. (14) shows that the electron density contribution is Z times smaller than the nuclear charge contribution.

Another conclusion from Eq. (14) is that the self-energy operator is not sensitive to the energy of a valence electron in the area $r \sim a_B/Z$ [the small-distance boundary of the applicability of Eq. (14)] where $e\Phi(a_B/Z) \sim (Z^2 \alpha^2) mc^2 \gg E \sim \alpha^2 mc^2$. The logarithm in this area is equal to $\ln(1/Z^2 \alpha^2)$, it is the same value that appears in the pure Coulomb case [cf. Eq. (10)]. An estimate of the energy dependence in this area may be characterized by the ratio

$$\frac{\frac{\partial \Sigma}{\partial E}}{(\Sigma/E)} \sim \frac{1}{Z^2} \quad (15)$$

which is very small in neutral atoms. In ions this ratio is $\sim (Z_i + 1)^2 / Z^2$, where Z_i is the ion charge [for a valence electron in an ion $E \sim (Z_i + 1)^2 \alpha^2 mc^2$]. We shall recall these conclusions during the discussion of the low-energy theorem for an electric dipole amplitude.

C. Asymptotics of the radiative potential

It may be useful to present long-range and short-range asymptotics of the radiative potentials. For $mr \gg 1$

$$\Phi_U(r) = \frac{\alpha}{4\sqrt{\pi}(mr)^{3/2}} e^{-2mr} \Phi(r), \quad (16)$$

$$\Phi_f(r) \sim \frac{\alpha}{4\sqrt{\pi}(mr)^{1/2}} (\ln mr + 4 \ln Z\alpha) e^{-2mr} \Phi(r). \quad (17)$$

Note that the asymptotics of the high-frequency contribution to $\Phi_f(r)$ are presented as an illustration only. A correct (long-range) expression for large r is determined by the contribution of low frequencies. However, numerically this long-range contribution is not significant. Indeed, the radiative corrections to s -wave energies are proportional to $1/n^3$ (ψ^2 near the origin) to an accuracy $\sim 1\%$ (see Refs. [24,25]). This can be considered as an estimate of the contribution of the long-range tail and the energy dependence of $\Sigma(\mathbf{r}, \mathbf{r}', E)$.

The form factor g at large distances gives a contribution which describes the interaction of the electron anomalous magnetic moment with the atomic electrostatic potential Φ [25]:

$$\Phi_g = -i \frac{\alpha \hbar}{4\pi mc} \boldsymbol{\gamma} \cdot \nabla \Phi. \quad (18)$$

This long-range potential decreases faster than $1/r^2$ since the nuclear electrostatic potential is screened by atomic electrons. It gives an especially important contribution for orbitals with $l > 0$. The long-range character of this interaction guarantees that it is not very sensitive to higher order in $Z\alpha$ corrections which are produced by the strong Coulomb field at $r \sim r_c$.

The short-range asymptotics of the radiative potentials, $mr \ll 1$, are the following:

$$\Phi_U(r) = \frac{2\alpha}{3\pi} \ln(1/mr) \Phi(r), \quad (19)$$

$$\Phi_f(r) = -\frac{\alpha}{\pi} \ln(1/mr) [\ln(1/mr) + \ln(m^2/\lambda^2)] \Phi(r), \quad (20)$$

$$\Phi_g(r) = i \frac{\alpha}{2\pi} mr \ln(1/mr) \boldsymbol{\gamma} \cdot \mathbf{n} \Phi(r). \quad (21)$$

We see that the area $mr < 1$ is not important for the magnetic form-factor contribution.

As we pointed out in Sec. II A, the expression (20) for the electric form-factor contribution is not applicable for $mr \ll Z\alpha$. Indeed, the short-range asymptotics (20) can be obtained very easily using high-energy asymptotics of the vertex operator $\Gamma^\mu(p, p', q)$ where p and p' are initial and final electron four-momenta, and q is the photon four-momentum. These asymptotics can be found, e.g., in Ref. [25]. In the case $|q^2| \gg p^2 = p'^2 = m^2$,

$$\Gamma^\mu(p, p', q) = \gamma^\mu \exp \left[-\frac{\alpha}{4\pi} \ln \frac{|q^2|}{m^2} \left(\ln \frac{|q^2|}{m^2} + 2 \ln \frac{m^2}{\lambda^2} \right) \right]. \quad (22)$$

To obtain the result in the coordinate representation we should substitute $q \sim 1/r$. This gives the correction (20) to the Coulomb potential. However, in the area $|q^2| \gg p^2, p'^2 \gg m^2$,

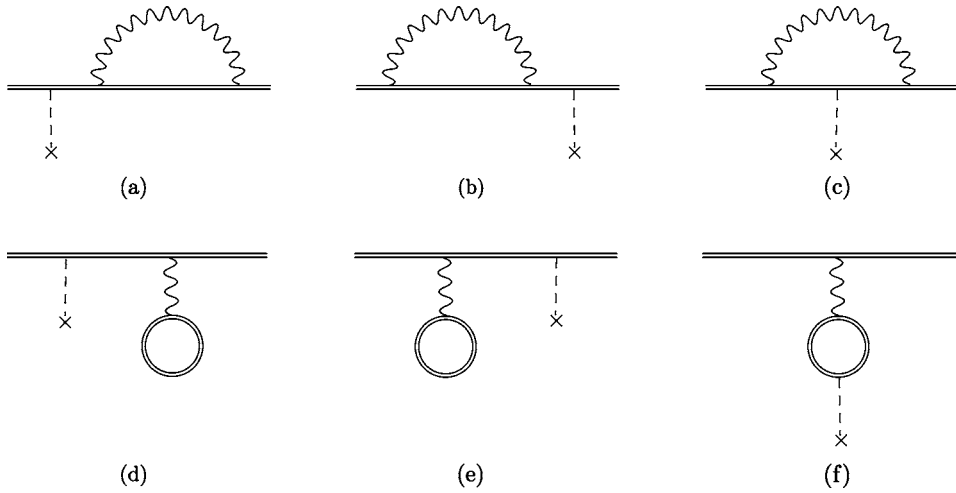


FIG. 2. Diagrams for radiative corrections to the $E1$ amplitude: (a),(b) self-energy; (c) vertex; (d),(e) vacuum polarization; and (f) external photon polarization operator. Notations are the same as in Fig. 1; the dashed line with the cross denotes the laser driven external photon field.

$$\Gamma^\mu(p, p', q) = \gamma^\mu \exp\left(-\frac{\alpha}{2\pi} \ln \frac{|q^2|}{p^2} \ln \frac{|q^2|}{p'^2}\right). \quad (23)$$

Here we have an explicit dependence on both electron momenta, therefore in the coordinate representation we obtain the nonlocal correction to the potential. This corresponds to the area where the Coulomb potential $Z\alpha/r \gg m$.

The radiative shift for the $p_{1/2}$ orbital is a special case. This orbital has a lower Dirac component penetrating to the region $r \sim r_c$; see Eq. (13). The relative contribution of the short-distance area $r \sim r_c$ increases as $\sim Z^2 \alpha^2$. This leads to a cancellation of $\Phi_f(r)$ and $\Phi_g(r)$ contributions at $Z \sim 40$. For very large Z the short-range contribution dominates and the radiative corrections for $p_{1/2}$ become comparable to that for $s_{1/2}$. At $Z=110$ the $p_{1/2}$ shift is only three times smaller than the $s_{1/2}$ shift.

For electron angular momentum $j > 1/2$, the short-range contributions of $\Phi_U(r)$ and $\Phi_f(r)$ are suppressed. The dominating contribution is given by the long-range $\Phi_g(r)$. The result is also sensitive to the low-frequency contribution described by $\Phi_l(r)$.

III. ELECTROMAGNETIC $E1$ AMPLITUDES

Diagrams for radiative corrections to the electric dipole ($E1$) transition amplitude are presented in Fig. 2. The magnitude of different QED contributions to $E1$ amplitudes depends on the virtual photon gauge. Corrections to $E1$ amplitudes in hydrogenlike ions have been calculated with logarithmic accuracy [$\sim \alpha^3 Z^2 \ln(1/\alpha^2 Z^2)$] in Ref. [28]. It is pointed out there that in the Yennie gauge it is enough to take into account only those corrections to the nonrelativistic electron wave functions produced by the nonrelativistic radiative potential [containing $\delta(r)$].

In neutral atoms there is an additional small parameter suppressing the external photon vertex contribution [Fig. 2(c)]. The binding energies of the valence electron and the external photon frequency are extremely small in comparison with typical virtual photon frequencies. This makes corrections to the electric dipole operator (from the electron anomalous magnetic moment) and all contributions proportional to $\partial \Sigma / \partial E$ negligible [see Eq. (15)].

Therefore the radiative potential approach should work in neutral atoms even better than in hydrogenlike ions. One has only to add the radiative potential to the atomic potential, calculate the electron wave functions, and use them to calculate electric dipole matrix elements. It is convenient to perform the calculations in the length form for the electric dipole operator ($\mathbf{D} = e\mathbf{r}$).

In the following section (Sec. III A) we derive the low-energy theorem for the $E1$ amplitude (expressing the vertex contribution in terms of the self-energy). In Sec. III B we explain the suppression of the vertex corrections and the validity of the radiative potential approach. In Sec. III C we perform a standard subtraction to remove ultraviolet divergences from the radiative corrections to the amplitude and estimate different contributions.

A. Derivation of the low-energy theorem

For the contribution of the high-frequency virtual photons the low-energy theorem follows from the Ward identity [25]

$$\Gamma^\mu(p, p, 0) = \frac{\partial G^{-1}(p)}{\partial p_\mu}, \quad (24)$$

where Γ^μ is the vertex operator, $G^{-1} = \gamma^\mu p_\mu - m - M(p)$ is the inverse electron Green's function, and $M(p)$ is the mass (self-energy) operator in the momentum representation. In the length form for the electric dipole operator we only need the zero component of the Ward identity [$\Gamma^0 = \gamma^0 - \partial M(p) / \partial E$] since the electron-photon interaction in this case is described by $H_{\text{int}} \approx e \gamma^0 \Gamma^0 \phi$, where $\phi = \mathbf{r} \cdot \mathbf{E}$ and \mathbf{E} is the photon field. Therefore the sum of the usual $E1$ amplitude and the vertex correction is

$$\langle 1 | r - \frac{1}{2} \left(r \frac{\partial \Sigma}{\partial E} + \frac{\partial \Sigma}{\partial E} r \right) | 2 \rangle, \quad (25)$$

where $\Sigma \equiv \gamma^0 M$. Here it is assumed that the transformation of the mass operator from the momentum representation to the coordinate representation is accompanied by the antisymmetrization of the operators r and M since, generally speaking, they do not commute (actually, this noncommutativity exists for the low-frequency contribution only). There is also some

difference in definitions of the mass operator M in Ref. [25] and the self-energy operator Σ used in this work (extra Dirac matrix γ^0 ; the matrix elements in Ref. [25] are defined using $\bar{\psi} = \psi^\dagger \gamma^0$, we use $\psi^\dagger \Sigma \psi$). Note that this low-energy theorem for the high-frequency contribution is valid in any order of perturbation theory (including all orders in $Z\alpha$) and holds for the renormalized operators (similar to the Ward identity). One should add to Eq. (25) the QED corrections to the wave functions $|1\rangle$ and $|2\rangle$ which are not shown there explicitly.

To prove the low-energy theorem for the low-frequency contribution we can use a nonrelativistic expression for the QED correction to the electric dipole amplitude presented, e.g., in Ref. [29]:

$$\delta\langle 1|z|2\rangle = \frac{2\alpha}{3\pi m^2} \int_0^\kappa \omega d\omega \operatorname{Re} f(\omega), \quad (26)$$

$$f(\omega) = \sum_{n,k} \frac{\langle 1|z|n\rangle \langle n|p_i|k\rangle \langle k|p_i|2\rangle}{(E_2 - E_n)'(E_2 - E_k - \omega)} + \sum_{n,k} \frac{\langle 1|p_i|n\rangle \langle n|p_i|k\rangle \langle k|z|2\rangle}{(E_1 - E_n - \omega)(E_1 - E_k)'} \quad (27)$$

$$+ \sum_{n,k} \frac{\langle 1|p_i|n\rangle \langle n|z|k\rangle \langle k|p_i|2\rangle}{(E_1 - E_n - \omega)(E_2 - E_k - \omega)} \quad (28)$$

$$- \frac{\langle 1|z|2\rangle}{2} \sum_n \left(\frac{\langle 1|p_i|n\rangle \langle n|p_i|1\rangle}{(E_1 - E_n - \omega)^2} + \frac{\langle 2|p_i|n\rangle \langle n|p_i|2\rangle}{(E_2 - E_n - \omega)^2} \right). \quad (29)$$

The typical frequency ω of a virtual photon is large in comparison with the difference of excitation energies of the valence electron. Therefore we can simplify the vertex contribution [Eq. (28)] by replacing E_n by E_k , since $(E_k - E_n) \ll \omega$, and summing over n (closure). We repeat this procedure by replacing E_k by E_n and summing over k . The result for the vertex contribution can be presented in a symmetric form (to cancel the first-order correction in $(E_k - E_n)/\omega$ and the commutator $[z, p_i]$),

$$\frac{1}{2} \sum_n \left(\frac{\langle 1|z p_i|n\rangle \langle n|p_i|2\rangle}{(E_2 - E_n - \omega)^2} + \frac{\langle 1|p_i|n\rangle \langle n|p_i z|2\rangle}{(E_1 - E_n - \omega)^2} \right). \quad (30)$$

Here we neglected the small difference $E_2 - E_1$. Now we see that the vertex contribution is indeed proportional to $z(\partial\Sigma/\partial E)$ [$\Sigma \propto p_i|n\rangle \langle n|p_i/(E_1 - E_n - \omega)$, $\partial\Sigma/\partial E_1 \propto -p_i|n\rangle \langle n|p_i/(E_1 - E_n - \omega)^2$]. Combining all terms and using the definition of Σ ,

$$\Sigma(E_1) = \frac{2\alpha}{3\pi m^2} \int_0^\kappa \omega d\omega \operatorname{Re} \sum_n \frac{p_i|n\rangle \langle n|p_i}{(E_1 - E_n - \omega)}, \quad (31)$$

we obtain the low-energy theorem for the radiative correction to the electromagnetic amplitude:

$$\langle 1|D|2\rangle_{\text{rad}} = \sum_n \frac{\langle 1|D|n\rangle \langle n|\Sigma(E_2)|2\rangle}{E_2 - E_n} + \sum_n \frac{\langle 1|\Sigma(E_1)|n\rangle \langle n|D|2\rangle}{E_1 - E_n} \quad (32)$$

$$- \frac{1}{2} \langle 1|D \frac{\partial\Sigma}{\partial E} + \frac{\partial\Sigma}{\partial E} D|2\rangle \quad (33)$$

$$+ \frac{1}{2} \langle 1|D|2\rangle \left(\langle 1|\frac{\partial\Sigma}{\partial E}|1\rangle + \langle 2|\frac{\partial\Sigma}{\partial E}|2\rangle \right). \quad (34)$$

Note that we can extend this derivation to include the high-frequency contribution. We just have to use the relativistic radiation operator $\gamma^\mu \exp(i\mathbf{k} \cdot \mathbf{r})$ instead of the momentum operator p_i . [One should start from the relativistic expression for the amplitude [30–32] instead of Eqs. (26)–(29).]

In this derivation we used the long-range character of the electric dipole operator \mathbf{r} . Indeed, we assumed that the matrix element $\langle n|z|k\rangle$ in the sum over n and k is dominated by states with $|E_n - E_k| \ll \omega$. This is certainly correct for the states located at distances comparable to the radius of the valence electron where $|E_n| \sim |E_k| \sim |E_1| \sim |E_2|$. For short-range operators (e.g., weak or hyperfine interactions) the contribution of states $|E_n| \sim |E_k| \gg |E_1| \sim |E_2|$ may be important.

B. Enhancement of the self-energy contribution

The contribution of the electron self-energy Σ to the $E1$ amplitude [Eq. (32)] is enhanced by the small energy denominator $E_{1,2} - E_n$ corresponding to the excitation of an external electron. The vertex (33) and normalization (34) contributions are not enhanced since $\partial\Sigma/\partial E \sim \Sigma/\omega$, where $\omega \gg E_{1,2} - E_n$ is a typical virtual photon frequency. One may conclude that the vertex and normalization contributions are suppressed relative to the self-energy contribution by a small factor $(E_{1,2} - E_n)/\omega$. Moreover, the vertex and normalization contributions usually have opposite signs and partially cancel each other. This is seen if we introduce complete sums $\sum_n |n\rangle \langle n|$ between the operators D and $\partial\Sigma/\partial E$ in the first and second terms in Eq. (33); the large diagonal contributions in these sums ($|n\rangle = |1\rangle$ in the first term and $|n\rangle = |2\rangle$ in the second) cancel exactly the normalization contribution Eq. (34).

There is another way to explain the suppression of the vertex contribution. The product $r[\partial\Sigma(r, r', E)/\partial E]$ is small everywhere inside a neutral atom. The matrix element of r typically comes from the distance $r \sim a_B$. At this distance the nuclear Coulomb field is screened, $Z_{\text{eff}} \sim 1$; therefore in this region $\partial\Sigma(r, r', E)/\partial E$ cannot have Z^2 enhancement. On the other hand, at small distances where the nuclear charge is unscreened, r is small. This can also be seen from the vertex diagram itself where the operator r is locked inside the virtual photon loop located at a small distance from the nucleus. There is no such suppression for the radiative correction to the electron wave function. The radiative potential changes the energy of the electron. This in turn changes the large distance asymptotics of the electron wave function and the matrix element of r .

In the approximate expression for the radiative potential we use in this work $\partial\Sigma(r, r', E)/\partial E = 0$ and so there are no vertex or normalization contributions. The first two terms in the radiative correction Eq. (32) can be presented in terms of corrections to the wave functions produced by Σ :

$$|1_{\Sigma}\rangle = \sum_n \frac{\langle 1|\Sigma(E_1)|n\rangle\langle n|}{E_1 - E_n}, \quad |2_{\Sigma}\rangle = \sum_n \frac{\langle 2|\Sigma(E_2)|n\rangle\langle n|}{E_2 - E_n}, \quad (35)$$

$$\langle 1|D|2\rangle_{\Sigma} = \langle 1_{\Sigma}|D|2\rangle + \langle 1|D|2_{\Sigma}\rangle. \quad (36)$$

We have checked that our approximate expression for the radiative potential gives correct diagonal matrix elements of Σ (radiative shifts). Here we need the nondiagonal matrix elements $\langle 1, 2|\Sigma|n\rangle$. However, the main contribution to the matrix element of $D=er\sim ea_B$ is given by the states with $E_n \sim \hbar^2/(ma_B^2) \sim E_{1,2} \ll \omega$, where ω is the virtual photon energy. Therefore our approximate radiative potential should give such matrix elements $\langle 1, 2|\Sigma|n\rangle$ correctly. Note, once again, that this statement is incorrect for the radiative corrections to the matrix elements of short-range operators like the weak and hyperfine interactions. In this case the states with $E_n \sim \hbar c/r_{\text{typical}} > \omega$ give a significant contribution and use of the radiative potential designed to give matrix elements between low-energy electron states is not justified.

The derivation (and result) of the low-energy theorem we have presented above is similar to that of the low-energy theorem for correlation corrections to the electric dipole amplitude in our work [33]. The vertex (structural radiation) and normalization correlation corrections are also proportional to $\partial\Sigma/\partial E$ and suppressed by a factor $E_{\text{valence}}/E_{\text{core}} \sim 1/10$ where E_{valence} and E_{core} are ionization energies for the valence and core electrons. It is interesting to note that for the correlation corrections the vertex and normalization contributions were found to be numerically small for both long-range (electric dipole) and short-range (weak, hyperfine) operators.

There is also a certain similarity between this theorem and the low-energy theorem (the Low theorem) for Bremsstrahlung (see, e.g., Ref. [25]). The main radiation comes from the external particle ends of the scattering diagram and is expressed in terms of the elastic scattering amplitude. The structural radiation (from inside the scattering vertex) is small and is expressed in terms of the derivative of the elastic amplitude. In our case we consider the radiation of a weakly bound electron ($E < 0$) which is not so different from the radiation of an unbound particle ($E > 0$) if the energy E is small.

C. Estimates of different QED corrections

All terms in Eqs. (26)–(29) and (32)–(34) are divergent as κ tends to infinity. Therefore we have to perform a subtraction of a standard counterterm in the expression for the self-energy operator,

$$\frac{p_i|n\rangle\langle n|p_i}{(E - E_n - \omega)} - \frac{p_i|n\rangle\langle n|p_i}{(-\omega)} = \frac{p_i|n\rangle\langle n|p_i(E - E_n)}{\omega(E - E_n - \omega)}, \quad (37)$$

to cancel the linear divergence in Eqs. (26) and (27) and regroup other terms to cancel the logarithmic divergences. After the subtraction and commutation $p_i(E_2 - H) = -[p_i, H] + (E_2 - H)p_i = i\nabla_i(-e\Phi) + (E_2 - H)p_i$ the first term in Eq. (27)

can be transformed as follows [we use the operator form of Eq. (27) for brevity]:

$$\frac{z}{2\omega(E_2 - H)} \left(i\nabla_i(-e\Phi) \frac{1}{(E_2 - H - \omega)} p_i - p_i \frac{1}{(E_2 - H - \omega)} i\nabla_i(-e\Phi) \right) \quad (38)$$

$$+ \frac{1}{2\omega}(zp_i - z|2\rangle\langle 2|p_i) \frac{1}{(E_2 - H - \omega)} p_i. \quad (39)$$

The second term in Eq. (27) gives a similar contribution.

All terms containing $i\nabla_i(-e\Phi)$ are combined to give a low-frequency contribution to the radiative potential. In particular, the large- ω contribution in Eq. (38) gives a well-known local term in Σ ,

$$\Sigma(\mathbf{r}, \mathbf{r}', E) = \frac{\alpha}{3\pi m^2} \ln \frac{\kappa}{E_{\text{min}}} \nabla^2(-e\Phi(r)) \delta(\mathbf{r} - \mathbf{r}') \quad (40)$$

which cancels the low-energy cutoff parameter κ in the high-frequency contribution proportional to $\ln(m/\kappa)$ (from the form factor f ; see Ref. [34]). Here $\nabla^2(-e\Phi(r)) = 4\pi e^2 Z \delta(\mathbf{r})$. It is easy to estimate the contribution of Σ to the QED radiative corrections to $\langle s|z|p\rangle$ [see Eq. (32)]. The nonrelativistic density of an s -wave valence electron is $\psi^2(0) \sim (Z_i + 1)^2 Z/a_B^3$, where Z_i is the ion charge ($Z_i = 0$ for a neutral atom and $Z_i = Z - 1$ for a hydrogenlike ion), the energy $E_1 \sim (Z_i + 1)^2 \alpha^2 mc^2$. Therefore the relative value of the QED correction produced by Σ is $\sim \langle s|\Sigma|s\rangle/E_1 \sim \alpha^3 Z^2 \ln(1/\alpha^2 Z^2)$.

The terms in Eq. (39) are combined with the vertex and normalization contributions to produce equations that do not contain ultraviolet divergences. The terms proportional to zp_i [see Eq. (39)] and $p_i z$ combined with the vertex contribution (28) give the following QED radiative correction to $\langle 1|z|2\rangle$:

$$\begin{aligned} \langle 1|z|2\rangle_{\text{vertex}} = & -\frac{\alpha}{3\pi m^2} \sum_{n,k} \langle 1|p_i|n\rangle\langle n|z|k\rangle \\ & \times \langle k|p_i|2\rangle \frac{E_n - E_1 + E_k - E_2}{E_n - E_1 - E_k + E_2} \ln \left| \frac{E_n - E_1}{E_k - E_2} \right|. \end{aligned} \quad (41)$$

The energy-dependent factor in this equation is always of the order of unity (it varies from 2 to $\ln|E_n/E_k|$). The ratio v/c for a valence electron is $p/mc \sim (Z_i + 1)\alpha$. Therefore the relative correction from the vertex term is $\sim (Z_i + 1)^2 \alpha^3$. A more sophisticated estimate based on closure gives the same result: $\alpha \langle 1|p_z p|2\rangle/m^2 = \alpha \langle 1|p^2 z + z p^2|2\rangle/m^2 = 2\alpha \langle 1|(E_1 + e\Phi)z + z(E_2 + e\Phi)|2\rangle/m \sim \alpha^2 (Z_i + 1)/m \sim \alpha^3 (Z_i + 1)^2 \langle 1|z|2\rangle$. For hydrogenlike ions this correction is $Z^2 \alpha^3$, comparable to the radiative potential contribution [$\sim \alpha^3 Z^2 \ln(1/\alpha^2 Z^2)$]. However, for neutral atoms this correction is $\sim \alpha^3$, i.e., it is extremely small.

The terms proportional to $z|2\rangle\langle 2|p_i$ and $p_i|1\rangle\langle 1|z$ combined with the normalization contribution (29) give the following QED radiative correction to $\langle 1|z|2\rangle$:

$$\langle 1|z|2\rangle_{\text{norm}} = -\frac{\alpha}{3\pi m^2} \langle 1|z|2\rangle [\langle 1|p^2|1\rangle + \langle 2|p^2|2\rangle]. \quad (42)$$

For a valence electron $p/m \sim (Z_i+1)\alpha c$, therefore the relative QED correction can be estimated as $\sim (Z_i+1)^2\alpha^3$, of the same order as the vertex contribution.

Finally, the contribution of the external photon polarization operator [Fig. 2(f)] also does not have the Z^2 enhancement since it comes from distances $r \sim a_B$. Thus the only important contribution in neutral atoms is that of the radiative potential.

IV. APPLICATIONS TO NEUTRAL CESIUM

In this section we apply the radiative potential method to calculate radiative corrections to energy levels and electromagnetic amplitudes in the neutral cesium atom. We limit our consideration to the s and p levels of the external electron which are important for the parity violation calculation. All calculations are performed taking into account finite nuclear size.

A. Energies

To calculate the radiative corrections to the energy levels we add the radiative potential to the nuclear Coulomb potential and calculate the self-consistent direct and exchange potentials obtained using Dirac-Hartree-Fock (DHF) equations for the electron core. This DHF potential includes the potential δV (“core relaxation”) which arises from the change in the core electron wave functions due to the radiative potential. Then we calculate the energy levels of the external electron in this DHF potential produced by the core electrons. The next step is to include the correlation corrections. It is convenient to calculate these corrections using the correlation potential method [33,35] which takes into account all second-order correlation corrections and three dominating series of higher-order diagrams (screening of the electron-electron interaction, the hole-particle interaction, and iteration of the correlation self-energy) to all orders in the residual Coulomb interaction. The nonlocal and energy-dependent correlation potential $\hat{\Sigma}^{corr}(\mathbf{r}, \mathbf{r}', E)$ is defined by the equation for the correlation correction to the electron energy $\delta E_n^{corr} = \langle n | \hat{\Sigma}^{corr}(\mathbf{r}, \mathbf{r}', E) | n \rangle$; it is defined in an analogous way to the radiative potential, Eq. (1). We add $\hat{\Sigma}^{corr}$ to the Dirac-Hartree-Fock potential to include it to all orders. The results of calculations for the radiative corrections are presented in Table II.

TABLE II. Radiative corrections to ionization energies in Dirac-Hartree-Fock field without relaxation $[(\text{DHF})_0]$, with relaxation included $[(\text{DHF})_0 + \delta V]$, and with correlation corrections included $[(\text{DHF})_0 + \delta V + \hat{\Sigma}^{corr}]$; units cm^{-1} .

Level	$6s_{1/2}$	$7s_{1/2}$	$6p_{1/2}$	$7p_{1/2}$	$8p_{1/2}$	$9p_{1/2}$
$(\text{DHF})_0$	15.5	4.3	0.2	0.07	0.03	0.02
$(\text{DHF})_0 + \delta V$	15.9	4.3	-0.8	-0.3	-0.1	-0.07
$(\text{DHF})_0 + \delta V + \hat{\Sigma}^{corr}$	17.6	4.1	-0.4	-0.1	-0.05	-0.03

It is seen that the many-body corrections change the result for the s levels by $\sim 10\%$ and they change the sign and magnitude for p levels. Our results for Uehling relaxation (not explicitly presented) are in perfect agreement with those of Ref. [23].

The results are in agreement with our previous calculations [6] and lie within the range spanned by model potential calculations of the $6s$ Lamb shift performed in Ref. [17] (from 15 to 27 cm^{-1}) and Ref. [21] (from 13 to 23 cm^{-1}). However, the accuracy of our present work is higher, $\sim 1\%$ for s levels.

B. $E1$ amplitudes

We use a similar method as that for the energies to calculate the radiative corrections to the electromagnetic amplitudes between the s and p levels. First, we calculate the external electron wave functions including the radiative potential and the core relaxation δV . Then we use these wave functions to calculate the radiative corrections to the electromagnetic amplitudes in the Dirac-Hartree-Fock approximation. At the second step we calculate the effect of the electron core polarization by the external photon electric field using the time-dependent Hartree-Fock method. These core polarization corrections are often called the RPAE (random-phase approximation with exchange) corrections. At the final step we use the correlation potential method [33,35] to calculate the correlation corrections to the radiative corrections. In fact, to the required accuracy it is enough to add $\hat{\Sigma}^{corr}$ to the Dirac-Hartree-Fock equations and calculate the external electron wave functions. Other correlation corrections are proportional to $\partial \hat{\Sigma}^{corr} / \partial E$ and contribute about 1% only (the low-energy theorem; we mentioned this at the end of Sec. III B). The results of the calculations for the radiative corrections are presented in Table III. Following Ref. [22], we present the results in terms of the dimensionless relative ra-

TABLE III. Relative radiative corrections R_{sp} to the electromagnetic amplitudes $\langle s_{1/2} | r | p_{1/2} \rangle = \langle s_{1/2} | r | p_{1/2} \rangle_0 [1 + (\alpha/\pi) R_{sp}]$ in Dirac-Hartree-Fock field with relaxation included (DHF), with RPAE corrections included (DHF+RPAE), and with correlation corrections included (DHF+RPAE+ $\hat{\Sigma}^{corr}$).

Transition	$6s-6p$	$6s-7p$	$6s-8p$	$6s-9p$	$7s-6p$	$7s-7p$	$7s-8p$	$7s-9p$
DHF	0.266	-2.90	-4.62	-5.68	-0.451	0.270	-2.07	-3.21
DHF+RPAE	0.286	-4.39	-11.9	-29.7	-0.432	0.270	-2.20	-3.60
DHF+RPAE+ $\hat{\Sigma}^{corr}$	0.265	-2.91	-6.25	-10.3	-0.340	0.231	-1.60	-2.52

diative corrections R to the electromagnetic amplitude defined by the relation

$$\langle s|r|p\rangle = \langle s|r|p\rangle_0 \left(1 + \frac{\alpha}{\pi} R_{sp}\right). \quad (43)$$

Note that the radiative corrections for the $6s_{1/2}-7p_{1/2}$, $8p_{1/2}$, $9p_{1/2}$ amplitudes are large since the amplitudes are small and sensitive to any corrections to the DHF potential.

Unfortunately, we calculated but did not present the radiative corrections to the electromagnetic amplitudes in our previous paper [6]; we presented only their total contribution to the parity violating amplitude. Anyway, the accuracy in our present work is higher ($\sim 1\%$).

In a recent work [22], direct calculations of the radiative corrections to $E1$ amplitudes in the neutral alkali atoms were performed. In particular, the radiative correction to the $6s-6p$ amplitude in Cs was calculated using the local Kohn-Sham potential. In this approach, the nonlocal exchange interaction is replaced by a semiempirical local term that depends on the electron density. Ref. [22] also does not take into account many-body corrections: core relaxation, RPAE, and correlation corrections. Nevertheless, $6s-6p$ is a large ‘‘resonance’’ amplitude, and the many-body effects should not be very significant here. Indeed, our Dirac-Hartree-Fock value $R = 0.266$ is very close to the result of Ref. [22]: $R = 0.261$. We select our Dirac-Hartree-Fock value for comparison since it is the lowest-order approximation we use (no RPAE or correlation corrections) and most similar to that of Ref. [22]. However, the very small difference between the results is accidental. The result of Ref. [22] does not include the Uehling potential contribution ($\sim -10\%$), and one may also expect some difference due to the core relaxation effect and the different treatment of the exchange interaction.

V. RADIATIVE CORRECTIONS TO THE PNC AMPLITUDE IN CESIUM

Now we can calculate the QED radiative corrections to the PNC $6s-7s$ amplitude in Cs. It is convenient to use the results of the sum-over-states approach of Ref. [36]:

$$\begin{aligned} E_{PNC} &= \sum_n \frac{\langle 7s|D|np\rangle \langle np|\hat{H}_W|6s\rangle}{E_{6s} - E_{np}} + \frac{\langle 7s|\hat{H}_W|np\rangle \langle np|D|6s\rangle}{E_{7s} - E_{np}} \\ &= (1.908 - 1.352 - 0.070 - 0.020 + \dots) + (-1.493 \\ &\quad + 0.120 + 0.010 + 0.003 + \dots) = -0.894 + \dots \end{aligned} \quad (44)$$

The units are $iea_B(-Q_W/N) \times 10^{-11}$, where Q_W is the nuclear weak charge and N is the number of neutrons. 98% of the sum is given by the terms $n=6, 7, 8, 9$ explicitly presented above. The result includes the many-body corrections to all matrix elements.

A. Contributions of energies and $E1$ amplitudes

Now it is very easy to calculate the contributions to the PNC amplitude from radiative corrections to the energy intervals and electromagnetic amplitudes. Using the last line of

Table II (with all many-body corrections included) we find that the radiative corrections to the energy intervals change the PNC amplitude by -0.34% . Using the last line of Table III (with all many-body corrections included) we find that the radiative corrections to the $E1$ amplitudes $\langle 6s, 7s|D|np_{1/2}\rangle$ change the PNC amplitude by $+0.43\%$.

Note that in Cs these two corrections nearly cancel each other, the sum of the two contributions is $\Delta = (0.43 - 0.34)\% = 0.09\%$. This cancellation was noted in our work [6] where these corrections in the DHF approximation were estimated to be 0.33% ($E1$) and -0.29% (energies). The difference between our old and current results is mainly because in Ref. [6] we used only three dominating terms in the sum (44) while in the present work we use eight terms. The fact that in Ref. [6] we used a different (and less accurate) radiative potential is not so significant. The contribution of the radiative corrections to the omitted terms $n > 9$ in the sum (44) is estimated in the present work (using an asymptotic formula) to be $\sim 0.01\%$.

To estimate the error we also performed another calculation. We neglected the low-frequency contribution $\Phi_f(r)$ and set the coefficient $A(Z, r) = 1$ in $\Phi_f(r)$. This variation changes the s -wave shifts by a few percent only. However, the p -wave shifts change several times since they are small and sensitive to the low-frequency contribution $\Phi_f(r)$. In this case the $E1$ contribution is 0.44% and the energy contribution is -0.35% ; the sum $\Delta = 0.09\%$ does not change. Thus the value of Δ is very stable and practically does not depend on the choice of the (short-range) radiative potential if this potential gives correct energy shifts. We estimate the uncertainty in $\Delta = 0.09\%$ as $\sim 0.01\%$.

B. Weak matrix elements

The self-energy and vertex QED radiative corrections to the weak matrix elements have been calculated in Refs. [8–13]) using Coulomb wave functions. However, all neutral atom wave functions near the nucleus are proportional to the Coulomb wave functions since the screening of the nuclear Coulomb potential and the electron energy may be neglected here. Therefore the relative magnitude of the QED radiative corrections for an external electron in a neutral atom is the same for all weak matrix elements $\langle np_{1/2}|\hat{H}_W|n's\rangle$ and coincides with the Coulomb case for $n, n' \gg 1$. Moreover, even the many-body corrections do not influence this statement since these corrections are proportional to the weak matrix elements $\langle np_{1/2}|\hat{H}_W|n's\rangle$ and are multiplied by the same factor (equal to the relative QED correction for the weak matrix element) which does not depend on n and n' . This means that we can use the Coulomb results of Refs. [8–13] to find the contribution of the QED corrections to the weak matrix elements. The results of calculations for the self-energy and vertex contribution are the following (in %): $-0.73(20)$ [8] (all orders in $Z\alpha$, using approximate relation); -0.6 [9] (lowest order); $-0.9(1)$ [9,11] (lowest order and estimate of higher orders); -0.85 [10,12] (lowest order and higher orders in the logarithmic approximation); -0.815 [13] (all orders $2s-2p$). Note that even for $n=2$ the binding energy to mass

ratio is $E_n/mc^2=0.02$ and the relative radiative correction should be very close to the large n limit (i.e., one may expect a difference with the large n limit result $\sim E_n/mc^2=2\%$). Based on these results we assume the correction equal to $(-0.82\pm 0.03)\%$ which is in agreement with all calculations.

The Uehling potential contribution is easy to find and the error is negligible. According to Refs. [4–7,11] the Uehling contribution to the weak matrix element is 0.42% (note that the Uehling contribution to the weak matrix element is practically the same as its contribution to E_{PNC} since the sum of the Uehling contributions from the energies and electromagnetic amplitudes is about -0.01%). The Wichmann-Kroll contribution is very small, -0.005% [6,14].

Thus the sum of all radiative corrections to the weak matrix elements contributes $(-0.82+0.42-0.005)\% \approx (-0.41\pm 0.03)\%$ to E_{PNC} .

C. PNC amplitude

The sum of all QED radiative corrections to E_{PNC} is -0.34% (energies)+ 0.43% ($E1$) -0.41% (weak) $=-0.32\pm 0.03\%$. All three contributions (energies, $E1$, weak) are equally important here, and the $E1$ contribution is the largest. The error $\sim 0.01\%$ in $\Delta=-0.34\%$ (energies)+ 0.43% ($E1$) gives a small contribution to the error in E_{PNC} if added in quadrature.

Note that the low-energy theorem may be extended to E_{PNC} if we treat the weak potential as part of the nuclear potential and assume that all electron orbitals contain small components produced by the weak interaction [i.e., $\psi=\psi_0+\delta\psi_W$; the effects of the QED corrections to the weak matrix elements and energy levels must also be included into $\delta\psi_W$, which may be presented as $\delta\psi_W=\sum_n|n\rangle\langle n|W|0\rangle/(E_0-E_n)$]. Then one can calculate the PNC amplitude including QED and many-body corrections in the same way as was done for the calculations of the usual $E1$ amplitudes. This argument justifies the calculation of the PNC amplitude using the radiative potential approach.

Recently, calculations of radiative corrections to the PNC amplitude in Cs were performed in Ref. [14] in an effective atomic potential. The result is $(-0.27\pm 0.03)\%$. Our result $(-0.32\pm 0.03)\%$ is slightly different possibly due to the many-body corrections which have not been calculated in the work [14]. Note that the net effect of the many-body corrections in Cs is not very large because of the accidental cancellations of different many-body corrections. One can see these cancellations between the RPAE and correlation contributions in Table III for the radiative corrections to the $E1$ amplitudes. A strong accidental cancellation happens also for the main PNC amplitude where there are four large correlation corrections, up to $\pm 20\%$ each, and the sum of all correlation corrections is 2% only [6,35]; such a cancellation does not take place, for example, in the PNC amplitude for Tl, where the total contribution of the many-body corrections is large.

The many-body calculations of the PNC amplitude produced by the electron-nucleus weak interaction are described in detail in our review [1] where one can also find numerous references (see also the original papers for calculations of

atomic structure [6,35–37] and Breit corrections [6,37–40]). The contribution of the weak electron-electron interaction is very small, within the standard model it is equal to 0.04% [41]. Therefore the PNC amplitude is proportional to the nuclear weak charge Q_W . Using the most precise many-body calculation [6] (which includes the Breit correction and the neutron skin correction), we obtain the following result for the PNC amplitude with the radiative corrections $(-0.32\pm 0.03)\%$ calculated in the present work:

$$E_{PNC} = -0.898(1 \pm 0.5\%) \times 10^{-11} i e a_B (-Q_W/N). \quad (45)$$

From the measurement of the PNC amplitude [2] we obtain

$$Q_W = -72.66(29)_{\text{exp}}(36)_{\text{theor}}. \quad (46)$$

The difference with the standard model value $Q_W^{\text{SM}} = -73.19(13)$ [42] is

$$Q_W - Q_W^{\text{SM}} = 0.53(48), \quad (47)$$

adding the errors in quadrature.

Note that in the experiment [2] it is the ratio E_{PNC}/β that was measured, where β is the vector transition polarizability. To extract Q_W we used $\beta=26.99(5)a_B^3$ obtained in Ref. [6] as the statistical average of the two most accurate values of β . For comparison with the two values of Q_W presented in Ref. [14] we also present Q_W for each β . Using $\beta=26.957(51)a_B^3$ from Refs. [3,43] we obtain $Q_W = -72.57(29)_{\text{exp}}(36)_{\text{theor}}$. Using $\beta=27.15(11)a_B^3$ from Refs. [6,44,45] we obtain $Q_W = -73.09(39)_{\text{exp}}(37)_{\text{theor}}$. These results coincide exactly with those of Ref. [14]. The exact coincidence is accidental since our QED radiative corrections are slightly different. This difference (0.05%) has been cancelled by some tiny corrections (-0.08% from the momentum dependence of the weak charge at $q\sim 30$ MeV [12] and 0.04% from the weak electron-electron interaction [41]) which we prefer not to include into our present results since they are much smaller than the omitted many-body corrections in the calculation of the main PNC amplitude [6]. Another argument to omit these tiny corrections is that they are not proportional to Q_W and violate the convenient relation $E_{PNC} = \text{const} \times Q_W$.

VI. SUMMARY AND CONCLUSION

We suggest to calculate radiative corrections to energy levels and electromagnetic amplitudes using the simple radiative potential

$$\Phi_{\text{rad}}(r) = \Phi_U(r) + \Phi_g(r) + \Phi_f(r) + \Phi_l(r) + \frac{2}{3}\Phi_{\text{WC}}^{\text{simple}}(r), \quad (48)$$

where $\Phi_U(r)$ is the Uehling potential (6), $\Phi_g(r)$ is the magnetic form-factor contribution (7), $\Phi_f(r)$ is the electric form-factor contribution (10), $\Phi_l(r)$ is the low-frequency contribution (9). The simplified Wichmann-Kroll potential $\Phi_{\text{WC}}^{\text{simple}}(r)$ [Eq. (12)] gives a very small contribution which may be noticeable ($\sim 1\%$) only for $Z > 80$.

The results obtained using this radiative potential are in good agreement (few percent) with the radiative corrections

to the s , $p_{1/2}$, and $p_{3/2}$ energy levels calculated in Ref. [24] for the hydrogenlike ions. The advantage of the radiative potential method is that it is very simple and can be used in many-electron atoms and molecules.

To calculate radiative corrections to electric dipole amplitudes we suggest use of the low-energy theorem derived in Sec. III A. It is applicable because the ionization energy of an external (valence) electron E_{ex} and the external photon frequency ω_{ex} are small in comparison with the typical frequency of a virtual photon ω_{ν} ; $E_{\text{ex}}, \omega_{\text{ex}} \ll \omega_{\nu}$. The vertex and normalization corrections are expressed in terms of the energy derivative of the electron self-energy operator. The dominating contribution is given by the corrections to the electron wave functions produced by the radiative potential. The relative contributions of the remaining corrections are small, $\sim 1/Z^2$ in neutral atoms and $\sim (Z_i+1)^2/Z^2$ in ions.

The radiative potential method allows us to take into account many-body effects. First, Φ_{rad} is added to the Dirac-Hartree-Fock Hamiltonian (i.e., the potential $V=V_{\text{DHF}}+\Phi_{\text{rad}}$ is used) and a new self-consistent field is obtained which includes a correction to the Dirac-Hartree-Fock potential δV_{DHF} due to the change of the internal electron orbitals produced by Φ_{rad} (the relaxation effect). The relaxation effect is always significant. For a short-range potential Φ_{rad} it is larger than the direct radiative shift for electron angular momenta $j > 1/2$. Then the new electron energy levels and DHF orbitals can be used to calculate the correlation corrections applying the many-body theory methods which are described, for example, in Ref. [6].

We applied the radiative potential method to calculate the radiative corrections to energy levels and electromagnetic amplitudes in the neutral Cs atom and demonstrated the importance of many-body effects in such calculations. The many-body effects change the s -level radiative shifts by $\sim 10\%$, and they change the sign and magnitude of the

p -level shifts. Many-body effects in the radiative corrections to the electromagnetic amplitudes are also very significant. The RPAE (core polarization) corrections usually enhance the radiative correction. The effect is especially significant for the small amplitudes where we observed the RPAE enhancement up to six times. The correlation corrections usually act in the opposite direction and are equally significant.

Finally, we calculated the contributions of the radiative energy shifts and radiative corrections for the electromagnetic amplitudes to the PNC $6s$ - $7s$ amplitude in cesium. The radiative corrections to the weak matrix elements have been calculated in previous works. The sum of all QED radiative corrections to E_{PNC} is -0.34% (energies) $+0.43\%$ ($E1$) -0.41% (weak) $=(-0.32 \pm 0.03)\%$. Note that all three contributions are equally important here, and the $E1$ contribution is the largest. Using this radiative correction and previous many-body calculations we obtain the PNC amplitude $E_{\text{PNC}} = -0.898(1 \pm 0.5\%) \times 10^{-11} \text{iea}_B(-Q_W/N)$. From the measurements of the PNC amplitude [2] we extract the Cs weak charge $Q_W = -72.66(29)_{\text{exp}}(36)_{\text{theor}}$. The difference with the standard model value $Q_W^{\text{SM}} = -73.19(13)$ [42] is $Q_W - Q_W^{\text{SM}} = 0.53(48)$.

ACKNOWLEDGMENTS

We are grateful to M. Kuchiev and A. Yelkhovsky for useful discussions. We are also grateful to M. Kuchiev for providing MATHEMATICA code for calculations of the relativistic Coulomb wave functions and to V. Dzuba for an improved version of the Dzuba-Flambaum-Sushkov code for atomic many-body calculations. This work was supported by the Australian Research Council. J.G. acknowledges support from an Avadh Bhatia Women's Fellowship and from Science and Engineering Research Canada while at University of Alberta. J.G. is grateful to University of Alberta for kind hospitality on a subsequent visit funded by a UNSW Faculty of Science grant.

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