Relaxation effect and radiative corrections in many-electron atoms

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(Received 9 January 2004; published 21 May 2004)

We illuminate the importance of a self-consistent many-body treatment in calculations of vacuum polarization corrections to the energies of atomic orbitals in many-electron atoms. Including vacuum polarization in the atomic Hamiltonian causes a readjustment (relaxation) of the electrostatic self-consistent field. The induced change in the electrostatic energies is substantial for states with the orbital angular momentum $l > 0$. For such orbitals, the relaxation mechanism determines the sign and even the order of magnitude of the total vacuum polarization correction. This relaxation mechanism is illustrated with numerical results for the Cs atom.

Compared to hydrogenic one-electron systems, the calculation of radiative corrections for *many-electron* atoms brings in an additional layer of complexity: a strong Coulomb repulsion between the electrons. The problem is especially challenging for *neutral* many-electron atoms, where the interaction of an outer-shell electron with other electrons is comparable to its interaction with the nucleus. At the same time, a reliable calculation of radiative corrections for a heavy neutral system is required in evaluation of the parity nonconserving (PNC) amplitude in the 55-electron ^{133}Cs atom. Here it has been only recently realized that the sizes of radiative corrections [1–4] are comparable to the experimental error bar [5] of 0.35% and, together with the Breit correction [6], dramatically affect agreement (or disagreement [7]) with the standard model of elementary particles.

A systematic approach to the problem of radiative corrections in strongly correlated systems is to start from the Furry representation based on a self-consistent electronic potential [8]. This potential takes into account the fact that an electron moves in an average field created by both the nucleus and other electrons. Based on this idea, a program of calculating radiative corrections to PNC amplitudes have been put forth by Sapirstein *et al.* [9]. Kuchiev and Flambaum [3] and Milstein *et al.* [4] pursue a more qualitative approach using an independent-electron approximation. We believe that the question of an interplay between correlations and radiative corrections is yet to be addressed. While here we do not compute the PNC corrections, we illuminate a situation where disregarding correlations would lead to a substantial error in determining radiative correction: a radiative correction changes sign and even the order of magnitude when the presence of other electrons is accounted for.

In particular, we consider vacuum polarization (VP) corrections to energies of atomic states. To the leading order in αZ the VP may be accounted for by introducing the Uehling

potential $U_{\mathrm{VP}}(r)$ into the *atomic* Hamiltonian. This potential is attractive, and for a hydrogenlike ion the resulting VP corrections to the energies are always *negative*. For a complex atom, we find by contrast that, for orbitals with $l > 0$, the total correction is *positive*. Briefly, the reason for such a counterintuitive effect is due to a readjustment of atomic orbitals when the $U_{\mathrm{VP}}(r)$ potential is added to the self-consistent Dirac-Hartree-Fock (DHF) equations. The innermost $1s$ orbitals are "pulled in" by the short-ranged VP potential, leading to a decrease of the effective nuclear charge seen by the outer orbitals and thus to an increase of the electrostatic energy of these orbitals. Since for orbitals with $l > 0$ overlap with $U_{\mathrm{VP}}(r)$ and thus the lowest order correction are small, the resulting indirect "relaxation" contribution dominates the total VP correction to the energies. In the following we will present numerical results supporting this relaxation mechanism. Atomic units ($\hbar = |e| = m_e \equiv 1$) are used throughout.

Because of our interest in PNC in Cs, below we illustrate the relaxation effect with numerical results for this atom; however, the relaxation mechanism is also applicable in the cases of other many-electron atoms. We also notice that the relaxation mechanism described here is similar to that observed in calculations of the Breit corrections [10,11].

The conventional many-electron Hamiltonian may be represented as

$$H = \sum_i h_0(i) + \frac{1}{2}\sum_{i \neq j} \frac{1}{r_{ij}},\qquad(1)$$

where the single-particle Dirac Hamiltonian is

$$h_0(i) = c(\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i) + \beta_i c^2 + V_{\mathrm{nuc}}(r_i).\qquad(2)$$

The nuclear potential $V_{\mathrm{nuc}}(r)$ is obtained from the nuclear charge distribution $\rho_{\mathrm{nuc}}(r)$, which is what we approximate by the Fermi distribution

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TABLE I. Vacuum polarization corrections to binding energies in neutral Cs ($Z=55$). Here ε_{nl_j} are the DHF energies, $\delta\varepsilon_{nl_j}^{(1)}$ are the expectation values of the Uehling potential [Eq. (6)], and $\delta\varepsilon_{nl_j}^{\text{DHF}}$ are the VP corrections with the correlations included [Eq. (8)]. All quantities are given in atomic units, 1 a.u.$=27.211\ 38$ eV, and the notation $x[y]$ stands for $x \times 10^y$.

Orbital	ε_{nl_j}	$\delta\varepsilon_{nl_j}^{(1)}$	$\delta\varepsilon_{nl_j}^{\text{DHF}}$
	Core orbitals		
$1s_{1/2}$	-1330.396958	$-2.853[-1]$	$-2.782[-1]$
$2s_{1/2}$	-212.597116	$-3.392[-2]$	$-3.267[-2]$
$2p_{1/2}$	-199.428898	$-1.510[-3]$	$5.406[-4]$
$2p_{3/2}$	-186.434858	$-1.650[-4]$	$1.690[-3]$
$3s_{1/2}$	-45.976320	$-6.868[-3]$	$-6.581[-3]$
$3p_{1/2}$	-40.448097	$-3.339[-4]$	$1.987[-4]$
$3p_{3/2}$	-37.893840	$-3.719[-5]$	$4.609[-4]$
$3d_{3/2}$	-28.309043	$-1.839[-7]$	$4.531[-4]$
$3d_{5/2}$	-27.774710	$-4.370[-8]$	$4.425[-4]$
$4s_{1/2}$	-9.514218	$-1.457[-3]$	$-1.397[-3]$
$4p_{1/2}$	-7.446203	$-6.726[-5]$	$8.097[-5]$
$4p_{3/2}$	-6.920865	$-7.506[-6]$	$1.355[-4]$
$4d_{3/2}$	-3.485503	$-3.440[-8]$	$1.153[-4]$
$4d_{5/2}$	-3.396788	$-8.100[-9]$	$1.129[-4]$
$5s_{1/2}$	-1.490011	$-2.057[-4]$	$-2.050[-4]$
$5p_{1/2}$	-0.907878	$-7.773[-6]$	$2.035[-5]$
$5p_{3/2}$	-0.840312	$-8.395[-7]$	$2.757[-5]$
	Valence states		
$6s_{1/2}$	-0.127380	$-1.054[-5]$	$-1.159[-5]$
$6p_{1/2}$	-0.085616	$-1.942[-7]$	$2.284[-7]$
$6p_{3/2}$	-0.083785	$-2.180[-8]$	$4.513[-7]$
$7s_{1/2}$	-0.055190	$-2.896[-6]$	$-3.143[-6]$
$7p_{1/2}$	-0.042021	$-6.957[-8]$	$8.150[-8]$
$7p_{3/2}$	-0.041368	$-7.873[-9]$	$1.606[-7]$

$$\rho_{\text{nuc}}(r) = \frac{\rho_0}{1+\exp[(r-c)/a]}, \tag{3}$$

where ρ_0 is the normalization constant and c and a are the nuclear parameters. In our numerical example for ^{133}Cs, we use $c=5.6748$ fm and $a=0.52$ fm.

A common starting point for describing a multielectron atom is the self-consistent-field method. Here the many-body wave function is approximated by a Slater determinant constructed from single-particle orbitals (bispinors) $u_k(\boldsymbol{r})$. The orbitals are obtained by solving self-consistently the eigenvalue equations

$$(h_0 + U_{\text{DHF}})u_k(\boldsymbol{r}) = \varepsilon_k u_k(\boldsymbol{r}), \tag{4}$$

where U_{DHF} is the traditional DHF potential which depends on the orbitals occupied in the Slater determinant. The DHF energies for the core and several valence orbitals of Cs are listed in Table I.
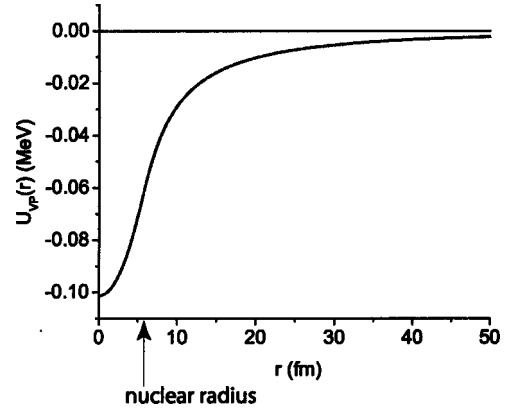

FIG. 1. Uehling potential for ^{133}Cs. Notice that the radius of the innermost $1s$ orbital is about 10^3 fm, much larger than the effective range of the VP potential.

The polarization of the vacuum by the nucleus modifies the nuclear electric field seen by the electrons. To the leading order in αZ, the VP may be conveniently described with the Uehling potential, which for a pointlike nucleus of charge Z reads (p.c. stands for point charge)

$$U_{\text{VP}}^{\text{p.c.}}(r) = \frac{2}{3\pi}\frac{\alpha Z}{r}\int_1^\infty dt\sqrt{t^2-1}\left(\frac{1}{t^2}+\frac{1}{2t^4}\right)\exp\left[-\frac{2r}{\alpha}t\right]. \tag{5}$$

This potential must be folded with the nuclear charge distribution,

$$U_{\text{VP}}(r) = \int d\boldsymbol{r}'\rho_{\text{nuc}}(|\boldsymbol{r}-\boldsymbol{r}'|)U_{\text{VP}}^{\text{p.c.}}(r'). \tag{}$$

We approximated $\rho_{\text{nuc}}(r)$ with the Fermi distribution, Eq. (3). In the numerical evaluation of the extended-nucleus Uehling potential, we employed the routine from Ref. [12]. The Uehling potential $U_{\text{VP}}(r)$ generated by the Cs nucleus is shown in Fig. 1. Notice that the actual range of this potential is a few nuclear radii (instead of Compton wavelength $\lambdabar_e \approx 384$ fm), because the potential for a pointlike charge, Eq. (5), diverges logarithmically as $r \to 0$; therefore the folded potential U_{VP} is dominated by the contributions accumulated inside the nucleus.

How does one compute the VP corrections $\delta\varepsilon_k$ to the energies of the atomic orbitals? Below we consider two possibilities: (i) the lowest-order perturbative treatment,

$$\delta\varepsilon_k^{(1)} = \langle u_k|U_{\text{VP}}|u_k\rangle, \tag{6}$$

and (ii) the self-consistent approach. Indeed, as in Ref. [2], the VP potential may be introduced into the DHF equations,

$$(h_0 + U_{\text{VP}} + U_{\text{DHF}}')u_k'(\boldsymbol{r}) = \varepsilon_k' u_k'(\boldsymbol{r}), \tag{7}$$

and a set of new energies ε_k' and orbitals $u_k'(\boldsymbol{r})$ is obtained. Notice that the DHF potential is modified as well, since it depends on the new set of the occupied orbitals $u_k'(\boldsymbol{r})$. The *correlated* VP correction to the energy of the orbital k is simply

$$\delta\varepsilon_k^{\mathrm{DHF}} = \varepsilon_k' - \varepsilon_k. \tag{8}$$

Additionally, we carried out an independent correlated calculation in the framework of the linearized coupled DHF approximation [13], which is equivalent to the random-phase approximation (RPA). This approximation describes a linear response of the atomic orbitals to the perturbing interaction, i.e., the VP potential. Numerical values obtained from the linearized coupled DHF calculations were in close agreement with the full DHF results.

The numerical results of our calculations are presented in Table I. While analyzing this table, we observe that the lowest order corrections, $\delta\varepsilon_k^{(1)}$, are always negative, reflecting the fact that the Uehling potential is attractive (see Fig. 1). Owing to the short-ranged nature of VP, and the fact that only the s orbitals have a significant overlap with the nucleus, the corrections to the energies of $l=0$ orbitals are much larger than those for $l>0$ orbitals. As to the correlated corrections, they differ quite substantially from the lowest order corrections. A comparison of Eq. (7) and Eq. (4) reveals the origin of this discrepancy: the perturbation, in addition to the Uehling potential, contains a difference between the two DHF potentials

$$\delta U = U_{\mathrm{VP}} + (U_{\mathrm{DHF}}' - U_{\mathrm{DHF}}). \tag{9}$$

For orbitals with $l>0$, where the first term above is small, the modification of the DHF potential contributes significantly to the VP energy corrections.

The modification of the DHF potential induced by the vacuum polarization is clearly a many-body effect, not present in a hydrogenlike system. Such an effect has been explored before, for example in calculations of the Breit corrections [10,11], and it is commonly referred to as a relaxation mechanism. Let us illustrate this relaxation mechanism. Denoting the correction to the occupied orbital wave functions as $\chi_a(\boldsymbol{r}) = u_a'(\boldsymbol{r}) - u_a(\boldsymbol{r})$, we write

$$(U_{\mathrm{DHF}}' - U_{\mathrm{DHF}})(\boldsymbol{r}) \approx \sum_a \int \chi_a^\dagger(\boldsymbol{r}') \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} u_a(\boldsymbol{r}') d\boldsymbol{r}'$$

$$+ \sum_a \int u_a^\dagger(\boldsymbol{r}') \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} \chi_a(\boldsymbol{r}') d\boldsymbol{r}'$$

$$- (\mathrm{exchange}),$$

where we discarded contributions nonlinear in $\chi_a(\boldsymbol{r})$, and "exchange" denotes a nonlocal part of the perturbation. The first two (direct) terms can be interpreted as an electrostatic potential produced by a perturbation $\delta\rho_{\mathrm{el}}(r)$ in the radial electronic density

$$\rho_{\mathrm{el}}(r) = -\frac{1}{4\pi r^2} \sum_a u_a^\dagger(\boldsymbol{r}) u_a(\boldsymbol{r}).$$

We plot both the electronic density $\rho_{\mathrm{el}}(r)$ and the VP-induced perturbation $\delta\rho_{\mathrm{el}}(r)$ in Fig. 2. The minima of $\rho_{\mathrm{el}}(r)$ correspond to positions of the electronic shells, marked on the plot by their values of principal quantum number n.
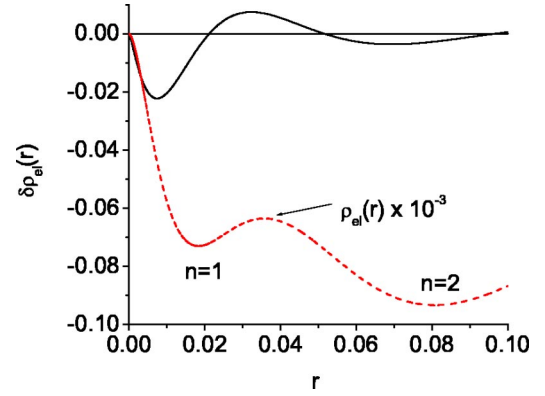

FIG. 2. Perturbation of the electronic radial charge distribution $\delta\rho_{\mathrm{el}}(r)$ (solid line) for the Cs atom due to vacuum polarization by the nucleus. We also show the unperturbed density $\rho_{\mathrm{el}}(r)$ multiplied by a factor of 10^{-3} (dashed line). The minima of $\rho_{\mathrm{el}}(r)$ correspond to positions of the electronic shells, marked on the plot by their values of the principal quantum number n.

Figure 2 may be interpreted in the following way: the s orbitals are "pulled in" by the attractive Uehling potential closer to the nucleus. As a result, screening of the nuclear charge by the inner orbitals becomes more efficient. For example, the modification of the effective charge felt by the $n=2$ electrons is simply the area under the $\delta\rho_{\mathrm{el}}(r)$ curve, accumulated between $r=0$ and the radius of the shell ($r \approx 0.08a_0$); from Fig. 2 it is clear that the induced modification of the effective charge for the $n=2$ shell has a negative sign. Such an enhanced screening leads to a reduced attraction of the electrons by the nucleus and to the *increase* in the energy of the outer electrons. From Table I we see that this indirect relaxation contribution to the energy may be well comparable to the direct VP correction, $\delta\varepsilon_k^{(1)}$. While for $l=0$ orbitals the direct correction gives a reasonable estimate, for all orbitals with $l>0$, the neglect of the relaxation would lead to an even qualitatively incorrect result. Moreover, the higher the orbital angular momentum, the smaller the direct correction, and the more important the relaxation mechanism is. For example, for $4d$ orbitals the VP correction in the lowest order is four orders of magnitude smaller than the correlated result.

To summarize, here we illuminated the importance of the self-consistent many-body treatment in calculations of vacuum polarization corrections. Including the VP Uehling potential into the atomic Hamiltonian causes a readjustment (relaxation) of the electrostatic self-consistent field. The induced change in the electrostatic energies is substantial for states with the orbital angular momentum $l>0$. As illustrated in our numerical results for Cs, the relaxation mechanism determines the sign and even the order of magnitude of the total VP correction for orbitals with $l>0$.

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