

Accurate vacuum-polarization calculations

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A numerical scheme for evaluating the part of the one-photon vacuum-polarization effect not accounted for by the Uehling potential (the Wichmann-Kroll effect) is presented. The method can be used with an arbitrary atomic model potential describing the bound electrons. Benchmark results for this effect are presented for hydrogenlike levels using a uniform nuclear-charge distribution. The effect of direct and exchange electron screening on the vacuum polarization are discussed in connection with the accurately measured $2p_{1/2}$ - $2s_{1/2}$ transition in lithiumlike uranium.

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I. INTRODUCTION

For bound electrons the dominant QED effect is the one-photon self-energy [see Fig. 1(a)]. Recently developed methods can now accurately determine the self-energy for highly charged ions [1–9]. In view of current level of interest for these highly charged ions, more accurate theoretical calculations of the vacuum polarization [see Fig. 1(b)], which is the second most important contribution, are desirable.

In the case of free electrons, the completely filled sea of negative-energy electrons has no observable effects. However, if we place a charged nucleus in the Dirac sea there is an observable effect. This is due to the fact that a virtual electron-positron pair created in a Coulomb field behaves in such a way that the electrons tend to be attracted to the nucleus while the positrons tend to escape from the nucleus. As a result the net charge observed at large but finite distances is smaller than the bare charge of the nucleus. The correction to a model where this observed charge is confined in the nucleus is referred to as the vacuum polarization. The total vacuum-polarization charge is thus zero with, roughly, a negative charge density outside the nucleus and a positive charge density inside the nucleus.

The first nonzero term in the $(Z\alpha)$ expansion of the one-photon vacuum polarization, the Uehling potential, was derived already in 1935 by Uehling [10] using results of Heisenberg [11]. The remaining part of the one-photon vacuum polarization we will refer to as the Wichmann-Kroll potential. The main emphasis in this work will be given this remaining part. The effect of the Wichmann-Kroll potential has been evaluated by several authors in various approximations [12–14]. The most accurate so far is the calculation by Soff and Mohr [14]. In our present work we will follow their suggested renormalization scheme. It is based on the potential expansion of the unrenormalized vacuum polarization into a zero-potential, a one-potential, and a many-potential term. Our numerical implementation of their scheme is completely different, though. We have been able to achieve better numerical stability and improve the numerical ac-

curacy substantially. Our method is also applicable for any atomic potential describing the bound electrons.

Certain two-photon vacuum-polarization effects that have an extra factor of α in their scaling law have also been evaluated in the literature. These are the so-called Källén-Sabry terms [15–17]. [The corresponding diagrams are shown in Figs. 3(j) and 3(k) in the last section.]

This paper is organized as follows. In Sec. II we derive unrenormalized expressions for the vacuum-polarization diagram in Fig. 1(b) and for the one-potential part of this. The finite renormalized contribution from this one-potential part corresponds to the Uehling potential. We then discuss the scheme for evaluating the finite part of the many-potential term corresponding to the Wichmann-Kroll potential. In Sec. III we discuss the numerical implementation of this scheme. Finally, in Sec. IV we present numerical results for hydrogenlike levels. We also discuss screening effects on the vacuum polarization in connection with the accurately measured $2p_{1/2}$ - $2s_{1/2}$ transition in lithiumlike uranium [18].

II. THEORY

The QED diagram for the one-photon vacuum-polarization (VP) effect is shown in Fig. 1(b). The corresponding energy shift for a state a can be expressed in terms of a vacuum-polarization potential, U_{VP} (note that

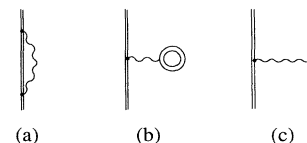


FIG. 1. Different one-photon processes. The double lines denote electrons propagating in an atomic potential field, and the wavy line a propagating photon. (a) gives rise to the electron self-energy, (b) describes the vacuum-polarization effect, and (c) the interaction between two bound electrons.

we do not factor out the electron charge), by writing

$$\Delta E_{\text{VP}}(a) = \int d^3 \mathbf{x}_1 \Phi_a^\dagger(\mathbf{x}_1) U_{\text{VP}}(\mathbf{x}_1) \Phi_a(\mathbf{x}_1). \quad (2.1)$$

Using standard Feynman rules and integrating over the time variables we have,

$$U_{\text{VP}}(\mathbf{x}_1) = -ie^2 c \int d^3 \mathbf{x}_2 \int_{-\infty}^{\infty} \frac{dz}{2\pi} \times \alpha^\nu D_{F\nu\mu}(\mathbf{x}_2 - \mathbf{x}_1, 0) \text{Tr}[\alpha^\mu S_F(\mathbf{x}_2, \mathbf{x}_2, z)], \quad (2.2)$$

where the time-independent Feynman photon propagator is given by

$$D_{F\nu\mu}(\mathbf{x}_2 - \mathbf{x}_1, z) = -\frac{c}{\epsilon_0} g_{\nu\mu} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2 - \mathbf{x}_1)}}{z^2 - c^2 \mathbf{k}^2 + i\eta} \quad (2.3)$$

and the time-independent Feynman electron propagator

$$S_F(\mathbf{x}_2, \mathbf{x}_1, z) = \sum_t \frac{\Phi_t(\mathbf{x}_2) \Phi_t^\dagger(\mathbf{x}_1)}{z - E_t(1 - i\eta)} \quad (2.4)$$

is a sum over all positive- and negative-energy states t for the electron moving in an atomic potential field V .

There is an energy parameter z associated with each propagator. Since the time integrations have been performed we have energy conservation at each vertex. Therefore the energy parameter is zero in the photon propagator while z is a free parameter in the electron propagator for our considered diagram. The z integration is over the real axis and the η that occurs in the propagators is a small positive number that adjust the poles to the correct side of the real axis. In the electron propagator the factor $(1 - i\eta)$ is formal and should be interpreted as to move the poles originating from the negative energy spectrum to the upper half plane and the ones originating from positive energy spectrum (also the ones with negative energy) to the lower half plane.

By performing the trace in Eq. (2.2), integrating over the angular part of \mathbf{k} and using the partial-wave expansion

$$\frac{1}{z - \hat{h}_{\text{bou}}(1 - i\eta)} = \frac{1}{z - \hat{h}_{\text{free}}(1 - i\eta)} + \frac{1}{z - \hat{h}_{\text{free}}(1 - i\eta)} V \frac{1}{z - \hat{h}_{\text{free}}(1 - i\eta)} + \frac{1}{z - \hat{h}_{\text{free}}(1 - i\eta)} V \frac{1}{z - \hat{h}_{\text{bou}}(1 - i\eta)} V \frac{1}{z - \hat{h}_{\text{free}}(1 - i\eta)}. \quad (2.9)$$

Here \hat{h}_{bou} and \hat{h}_{free} are the bound and free Dirac operators, respectively. This is an exact identity that allows us to write the vacuum polarization as a sum of three terms as shown in Fig. 2. We shall refer to these terms as the zero-potential term (U_0), the Uehling term (U_1), and the Wichmann-Kroll term (U_2).

A. The zero-potential term

The Furry theorem states that the contribution of any closed free-electron loop with an odd number of vertices

$$\frac{\sin[k|(\mathbf{x}_2 - \mathbf{x}_1)|]}{k|(\mathbf{x}_2 - \mathbf{x}_1)|} = \sum_{l=0}^{\infty} (2l+1) j_l(kr_1) j_l(kr_2) \mathbf{C}^l(1) \cdot \mathbf{C}^l(2), \quad (2.5)$$

we obtain

$$U_{\text{VP}}(\mathbf{x}_1) = -\frac{ie^2}{4\pi\epsilon_0} \frac{2}{\pi} \int d^3 \mathbf{x}_2 \int_0^\infty dk \int_{-\infty}^\infty \frac{dz}{2\pi} \times \sum_{l=0}^{\infty} (2l+1) j_l(kr_1) \mathbf{C}^l(1) \alpha^\mu(1) \times \sum_t \frac{\Phi_t^\dagger(\mathbf{x}_2) j_l(kr_2) \mathbf{C}^l(2) \alpha_\mu(2) \Phi_t(\mathbf{x}_2)}{z - E_t(1 - i\eta)}, \quad (2.6)$$

where one has to remember the scalar product between the \mathbf{C}^l tensors, which are related to the spherical harmonics as $C_m^l = \sqrt{4\pi/(2l+1)} Y_m^l$. Since we sum over all orientations m of j_κ for a specific κ in the $t=(n, \kappa, m)$ summation, one can show that l and μ have to be zero for nonvanishing contributions ($\mathbf{C}^0 = 1$ and α^0 is an identity matrix). Performing the z integration, which picks up half-pole contributions, and summing over m we finally obtain

$$U_{\text{VP}}(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{\pi} \int_0^\infty dk j_0(kr) \times \sum_{n,\kappa} (2j_\kappa + 1) \text{sgn}(E_{n,\kappa}) \langle n, \kappa | j_0(kr_2) | n, \kappa \rangle. \quad (2.7)$$

Equation (2.7) is a formal expression that contains the infinite unrenormalized charge and is divergent. In order to treat the divergency problem, we start with an expansion of the intermediate electron propagator,

$$S_F(\mathbf{x}_2, \mathbf{x}_1, z) = \sum_t \frac{\Phi_t(\mathbf{x}_2) \Phi_t^\dagger(\mathbf{x}_1)}{z - E_t(1 - i\eta)} = \left\langle \mathbf{x}_2 \left| \frac{1}{z - \hat{h}_{\text{bou}}(1 - i\eta)} \right| \mathbf{x}_1 \right\rangle = \left\langle \mathbf{x}_2 \left| \frac{1}{z - (\hat{h}_{\text{free}} + V)(1 - i\eta)} \right| \mathbf{x}_1 \right\rangle, \quad (2.8)$$

in terms of the atomic potential V ,

vanishes. Thus the first term in the potential expansion is zero. The expression for this zero-potential term is given by Eq. (2.7) with the only modification that the summation is over free electron states. With this partial-wave expansion there is an exact cancellation between the positive and negative energy states for the free-electron spectra with a given $|\kappa|$ value. To be specific, in the case when $|\kappa| = 1$ the cancellation takes place between the positive (negative) spectra of the $s_{1/2}$ angular symmetry and the negative (positive) spectra of the $p_{1/2}$ angular

symmetry. For bound spectra the cancellation is not exact giving rise to the divergent expression for U_{VP} .

B. The Uehling term

The second term in the potential expansion, the Uehling term, contains a divergency of the photon self-energy type and a finite part corresponding to the Uehling potential. The expression for the Uehling term is derived by replacing the electron propagator S_F in Eq. (2.2) with the one-potential term from the expansion in Eq. (2.9). Performing the trace and using the partial-wave expansion Eq. (2.5) we obtain the expression

$$U_1(\mathbf{x}_1) = -\frac{ie^2}{4\pi\epsilon_0} \frac{2}{\pi} \int d^3\mathbf{x}_2 \int d^3\mathbf{x}_3 \int_0^\infty dk \int_{-\infty}^\infty \frac{dz}{2\pi} \sum_{l=0}^\infty (2l+1) j_l(kr_1) \mathbf{C}^l(1) \alpha^\mu(1) \times \sum_{r,s} \frac{\Phi_r^\dagger(\mathbf{x}_2) j_l(kr_2) \mathbf{C}^l(2) \alpha_{\mu}(2) \Phi_r(\mathbf{x}_2) \Phi_s^\dagger(\mathbf{x}_3) V(\mathbf{x}_3) \Phi_s(\mathbf{x}_3)}{[z - E_r(1 - i\eta)][z - E_s(1 - i\eta)]}, \quad (2.10)$$

where we now sum over free electron states r and s . In principle we should integrate over the continuous spectra for r and s , but when evaluating the the Uehling term we shall use numerical “free” electron spectra for electrons confined in a box chosen to be large enough not to affect the numerical results. The integrations then go over to summations.

The expression in Eq. (2.10) for U_1 corresponds to Eq. (2.6) for U_{VP} . As for that expression only $l = \mu = 0$ gives a nonzero contribution. If r, s are both positive (negative) states, we can close the z integration in the upper (lower) plane and get zero contribution. Only the situation with one positive (+) and one negative (−) state thus contributes in the r, s summation. Performing the z integration then gives

$$U_1(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{4}{\pi} \int_0^\infty dk \sum_{\kappa} j_0(kr) (2j_{\kappa} + 1) \times \sum_p^+ \sum_{p'}^- \frac{\langle p, \kappa | j_0(kr_2) | p', \kappa \rangle \langle p', \kappa | V | p, \kappa \rangle}{E_{p,\kappa} - E_{p',\kappa}}, \quad (2.11)$$

where we have summed over the m quantum numbers and used that $r = (p, \kappa, m)$ and $s = (p', \kappa, m)$ must have the same κ and m . The extra factor of 2 occurs since we have restricted r to be a positive-energy state.

The Uehling potential can be derived from Eq. (2.11) by removing the charge divergency. Despite that there was no clear formulation of the charge renormalization, Uehling derived this finite contribution already in 1935 [10] using results achieved by Heisenberg [11]. The first deduction that was completely satisfactory from a theoretical standpoint was given by Schwinger in 1949 [19]. For a detailed and rigorous discussion of the Uehling potential the reader is referred to the book by Greiner, Müller, and Rafelski [20]. Here we shall just quote the result for the Uehling (Ue) potential in the coordinate

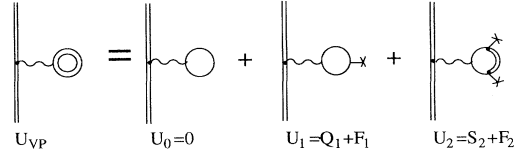


FIG. 2. The unrenormalized bound-state vacuum polarization potential (U_{VP}) decomposed into the zero-potential term ($U_0=0$), the Uehling term ($U_1 = Q_1 + F_1$), and the Wichmann-Kroll term ($U_2 = S_2 + F_2$). F_1 and F_2 denote the finite parts, Q_1 the charge divergency, and S_2 the spurious gauge-dependent part of U_2 .

representation without any mathematical justification

$$U_{Ue}(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{\alpha}{\pi} \int_0^\infty dr' 4\pi r'^2 \rho(r') \times \int_1^\infty dt \sqrt{t^2 - 1} \left(\frac{2}{3t^2} + \frac{1}{3t^4} \right) \times \frac{\sinh(2tr_{<}/\lambda_C)}{2tr_{<}/\lambda_C} \frac{\exp(-2tr_{>}/\lambda_C)}{r_{>}}, \quad (2.12)$$

where $r_{<}$ is the lesser and $r_{>}$ the greater of r and r' and $\rho(r')$ is the probability distribution for the charge generating the atomic potential V , that is here assumed to be spherically symmetric. The electron Compton wavelength (divided by 2π) $\lambda_C = \hbar/(mc)$ that occurs in this expression is the characteristic length for the induced vacuum-polarization charge. We will use this expression for the Uehling potential to evaluate the finite contribution denoted by F_1 in Fig. 2.

C. The Wichmann-Kroll term

The last term in the potential expansion given in Eq. (2.9) is the Wichmann-Kroll (WK) term. To obtain the correct finite part F_2 from this term we adopt the subtraction scheme suggested by Soff and Mohr [14],

$$F_2 = U_{VP} - U_1 - S_2, \quad (2.13)$$

where we have used the notations introduced in Fig. 2. S_2 is a spurious gauge-noninvariant piece that must be removed in order to obtain the correct result. This term has been discussed by many authors [12,13,21]. By making a partial-wave expansion of the S_2 term, each partial wave contribution can be shown to vanish [14]. Thus, performing a spherical-wave decomposition of Eq. (2.13) yields

$$F_2 = \sum_{\kappa} U_{VP}^{\kappa} - U_1^{\kappa} \quad (2.14)$$

TABLE I. Wichmann-Kroll vacuum-polarization effects on hydrogenlike levels in Xe and U expressed in terms of H where $\Delta E = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n^3} Hmc^2$. Only terms with $|\kappa| \leq 5$ are included in the values presented in this table. A spherical shell model for the nucleus is used in the first four lines and a uniform charge distribution in the last two lines.

	R_{rms} (fm)	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
^{54}Xe	4.826 shell	0.005899	0.006402	0.000448	0.000110
		0.0059 ^a	0.0064 ^a	0.0004 ^a	0.0001 ^a
^{92}U	5.751 shell	0.020659	0.027232	0.006795	0.000736
		0.0207 ^a	0.0272 ^a	0.0068 ^a	0.0007 ^a
^{92}U	5.751 uniform	0.020675	0.027254	0.006798	0.000736
^{92}U	5.860 uniform	0.020640	0.027203	0.006791	0.000736

^aSoff and Mohr [14].

if the summation is truncated after a finite number of terms. In terms of vacuum-polarization potentials we can write the finite potential contribution U_{WK} corresponding to F_2 as

$$U_{\text{WK}}(r) = U_{\text{VP}}(r) - U_1(r), \quad (2.15)$$

with the partial-wave expansions for U_{VP} and U_1 given by Eq. (2.7) and Eq. (2.11), respectively. The total renormalized one-photon vacuum-polarization potential is then the sum of the Uehling (U_{Ue}) and Wichmann-Kroll (U_{WK}) potentials.

III. NUMERICAL APPROACH

The Uehling term described by Eq. (2.12) is straightforward to implement numerically and we restrict here the numerical discussion to the Wichmann-Kroll term. To evaluate this term, we employ the outlined scheme in Eq. (2.15) evaluating (renormalizing) each partial-wave contribution separately. In calculating the Wichmann-Kroll term in this explicit form, we can use the numerical tools developed for the self-energy calculation [8,9]. Since there are no poles in the momentum integration we employ Gaussian quadrature. For the radial integration we use the method with discrete numerical spectra for electrons confined in a box [22] with the boundary condition that the orbitals vanishes outside the box. Both bound spectra, for which the electrons move in an atomic potential V , and “free” spectra ($V=0$) are used. The radius of the box has to be chosen large enough not to affect the numerical result. Considering effects for a bound state,

this implies that the corresponding wave function has to be small enough at the radius of the box. A typical value for lithiumlike uranium is one Bohr radius.

There is one ambiguity which has to do with the numerical spectra used. If we consider the partial-wave expansion of the zero-potential term it vanishes, as discussed in Sec. II A, due to exact cancellations between the positive and negative free electron states for each $|\kappa|$ value. In a similar manner there are cancellations (but not exact) for the main term for a given $|\kappa|$ value. To correctly obtain these cancellations numerically, one has to be very careful with the boundary conditions in the box. This was not achieved exactly in our calculation. Therefore, to purify our numerical spectra we employ, as in the self-energy calculation, the concept of subtracting a counter term. When we calculate the main term for a specific value of $|\kappa|$, we subtract also the corresponding contribution to the zero-potential term. (In principle we shall then re-add the zero-potential term calculated analytically, but this is just exactly zero.) This results in a stable and accurate evaluation of the main term. By also subtracting the Uehling term evaluated with the same numerical grids, we obtain a high numerical accuracy. Our numerical scheme, for evaluating the Wichmann-Kroll potential (F_2) is thus

$$F_2 = \sum_{|\kappa|=1}^{|\kappa_{\text{max}}|} U_{\text{VP}}^{|\kappa|} - U_0^{|\kappa|} - U_1^{|\kappa|}, \quad (3.1)$$

where we calculate each $|\kappa|$ separately up to a $|\kappa_{\text{max}}|$ and then extrapolate get the κ tail contribution. The partial-wave expansion in Eq. (2.7) is used for the U_{VP}

TABLE II. Wichmann-Kroll vacuum-polarization effects on hydrogenlike levels for various atoms expressed in terms of H (see Table I). A uniform charge distribution for the nucleus is used.

	R_{rms} (fm)	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
^{36}Kr	4.230	0.0027418	0.0028337	0.0000834	0.0000280
^{54}Xe	4.826	0.0059211	0.0064231	0.0004548	0.0001142
^{70}Yb	5.273	0.0102488	0.0228636	0.0015179	0.0002817
^{82}Pb	5.505	0.0150482	0.0185794	0.0034731	0.0004935
^{92}U	5.860	0.0206789	0.0272515	0.0068240	0.0007494
^{100}Fm	5.976	0.0269434	0.0377244	0.0118317	0.0010235
^{170}X	7.100	0.52639	0.77519	3.81914	0.01747

TABLE III. A comparison between the Wichmann-Kroll (WK) and the Uehling (Ue) vacuum-polarization effects on the lowest hydrogenlike levels for various atoms using a uniform charge density for the nucleus (eV).

	R_{rms} (fm)		$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
36Kr	4.230	Ue	-1.35582	-0.17798	-0.00348	-0.00053
		WK	0.01550	0.00200	0.00006	0.00002
54Xe	4.826	Ue	-7.3250	-1.0234	-0.0492	-0.0056
		WK	0.1695	0.0230	0.0016	0.0004
70Yb	5.273	Ue	-23.4016	-3.5384	-0.3121	-0.0252
		WK	0.8283	0.1198	0.0153	0.0028
82Pb	5.505	Ue	-50.6976	-8.2702	-1.0781	-0.0638
		WK	2.2900	0.3534	0.0660	0.0094
92U	5.860	Ue	-93.5868	-16.4610	-2.9055	-0.1266
		WK	4.9863	0.8214	0.2057	0.0226
100Fm	5.976	Ue	-152.071	-28.654	-6.405	-0.209
		WK	9.069	1.587	0.498	0.043
170X	7.100	Ue	-12413.0	-2380.5	-11051.0	-6.76
		WK	1479.8	272.4	1342.0	6.14

and U_0 terms using bound and free electron spectra, respectively, and for the U_1 term Eq. (2.11) is used involving free electron spectra.

IV. NUMERICAL RESULTS AND DISCUSSION

To check our numerical method for evaluating the WK contribution to the vacuum-polarization we compare in Table I our results for hydrogenlike levels in Xe and U with the calculation by Soff and Mohr [14]. They present results evaluated with a spherical-shell model for the nucleus. Due to strong cancellations only terms with $|\kappa| \leq 5$ are included in their work. With this approximation we get perfect agreement with their results. In Table I we also present values for U using a uniform nuclear-charge distribution with the same $R_{\text{rms}}=5.751$ fm as for the nuclear shell model. One can see that the effect of the nuclear model is very small. To see the effect of the nuclear radius we also present values with $R_{\text{rms}}=5.860$ fm taken from Zumbro *et al.* [23]. This also gives small changes.

Compared with the calculation by Soff and Mohr we have been able to improve the accuracy significantly. The

main reason for this is our numerical stability that allows us to include partial waves up to $|\kappa| = 15$. Therefore we can also accurately estimate the small contribution from the κ tail. Our results indicate that the κ contributions fall off as κ^{-4} and the κ sum thus converges faster than for the self-energy for which the terms fall off as l^{-3} [9]. Our very accurate κ -extrapolated values are presented in Table II. A comparison with the uranium values in Table I reveals that for the $1s$ and $2s$ states the $|\kappa| > 5$ tail is small and almost cancels the nuclear-radius effect in Table I. However, for the $2p$ states the relative importance of the κ tail is much larger.

In Table III we compare the WK and the Uehling contributions to the vacuum polarization for hydrogenlike levels in selected atoms from Kr to Fm and also for a gedanken superheavy atom with $Z = 170$. Since there is an extra $(Z\alpha)^2$ in the scaling law for the WK term compared to the Uehling term, the WK term becomes more important for higher Z . For the $2s_{1/2}$ state in U it accounts for about 5% of the vacuum polarization and increases to about 10% for the same state with $Z=170$. For the $2p_{3/2}$ state the WK term is more important and becomes almost equal to the Uehling term for $Z = 170$.

To examine the electron-screening effects on the vac-

TABLE IV. Electron screening effects on the vacuum polarization for lithiumlike uranium using a uniform charge density with $R_{\text{rms}} = 5.860$ for the nucleus (eV).

Model potential		$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
Bare nucleus	Ue	-16.4610	-2.9055	-0.1266
	WK	0.8214	0.2057	0.0226
Direct screening	Ue nucleus	-15.7722	-2.6370	-0.1158
	electron core	0.0407	0.0238	0.0067
	WK nucleus	0.7892	0.1876	0.0208
	electron core	-0.0043	-0.0019	-0.0004
	Ue plus WK sum	-14.9466	-2.4276	-0.0887
	Ue plus WK $\Delta\epsilon$	-14.9846	-2.4317	-0.0887
Coulomb exchange	Ue plus WK $\Delta\epsilon$	-14.9532	-2.4511	-0.0898
Breit exchange added	Ue plus WK $\Delta\epsilon$	-14.9318	-2.4271	-0.0890

uum polarization we consider in Table IV the $n = 2$ states in lithiumlike uranium. In the first two lines we repeat the bare-nucleus values from Table III. In lines 3 and 5 we use the same nuclear Uehling and WK vacuum-polarization potentials as in the first two lines but take the expectation values with states screened by two direct interactions with $1s$ [direct part of Fig. 3(e)]. Considering the $2s$ state this screening changes the Uehling contribution by 0.689 eV and the WK contribution by -0.032 eV. Taking into account the $1s^2$ charge density when evaluating the vacuum polarization [direct part of diagram 3(f)] gives much smaller contributions, 0.041 eV for the Uehling term (almost canceling the screening of the WK term) and -0.004 for the WK term. Summing all contributions we get the values labeled “Ue plus WK sum” in this table.

To get the effect of the vacuum-polarization potential self-consistently (not only to first order) we include this potential when generating the orbitals and let it affect the eigenvalues. The change induced in the eigenvalue, $\Delta\epsilon$, then includes the higher-order vacuum-polarization diagram [Fig. 3(i)]. This “self-consistency” effect amounts to -0.038 eV for the $2s$ state. By letting the $n = 2$ states also be affected by the exchange Coulomb and Breit interaction with the $1s^2$ core we get slightly different changes $\Delta\epsilon$ induced by including the full vacuum-polarization potential as presented in the last two lines in Table IV. From these values we can, e.g., deduce a 0.031-eV effect from the Coulomb exchange and 0.021 eV from Breit exchange on the $2s$ state [exchange part of Fig. 3(e)].

In Table V we summarize the vacuum-polarization effects on the $2p_{1/2}-2s_{1/2}$ transition in lithiumlike uranium and compare with results by Blundell [5]. The agreement is perfect for results including direct screening by the $1s^2$ core. However, the contribution from the exchange screening by the core differs significantly. This effect is calculated quite differently in our work, where we let the exchange interaction affect the orbitals self-consistently, while Blundell calculates the first-order perturbation with the restriction that the perturbation is orthogonal to the $1s$ orbital. The discrepancy is resolved to a large extent, however, if we also take into account

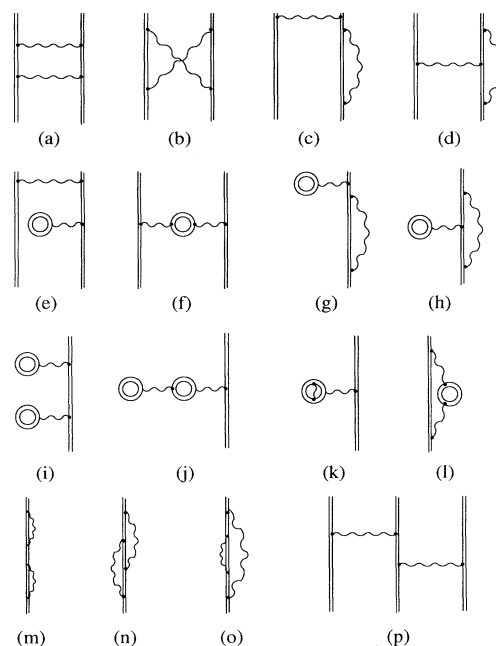


FIG. 3. Two-photon effects.

the change in the $1s^2$ vacuum-polarization effect in the $2p_{1/2}-2s_{1/2}$ transition. Including the direct screening of the core by the valence electron we get again results in perfect agreement with Blundell, while our core results for the exchange screening by the valence electron differ. We note, however, that the sum of the core and valence exchange screening effects agrees better between the two different calculations.

The previously discussed self-consistency effect is not included in the result by Blundell given in Table V. Adding this effect to his results reduces the difference between our final vacuum-polarization results to about 0.01 eV.

A more systematic way of evaluating the effect of the vacuum-polarization potential would be to include this

TABLE V. Vacuum-polarization effects on the $2p_{1/2}-2s_{1/2}$ transition in Li-like U (eV).

		This work	Blundell [5]
Valence			
Direct screening	Uehling (Ue)	13.118	13.12
	Wichmann-Kroll (WK)	-0.599	-0.60
	Ue plus WK sum	12.519	12.52
	Self-consistency effect	0.034	
	Ue plus WK $\Delta\epsilon$	12.553	
Exchange screening effect		-0.048	-0.08
	Coulomb exchange added	Ue plus WK $\Delta\epsilon$	12.502
	Breit exchange added	Ue plus WK $\Delta\epsilon$	12.505
Core			
Direct screening		-0.082	-0.08
Exchange screening effect		0.163	0.21
Total vacuum polarization		12.586	12.56

TABLE VI. A comparison with the experimental $2p_{1/2}$ - $2s_{1/2}$ transition energy in lithium-like uranium (eV).

	This work	Blundell [5]
Vacuum polarization (VP)	12.586	12.56
Self-energy (SE)	-54.32 ^a	-54.24
Combined SE and VP	-0.19 ^b	
Nuclear polarization and recoil	0.10 ^c	0.10
Relativistic MBPT	322.33 ^d	322.41
Total	280.51	280.83
Experiment	280.59(9) ^e	280.59(9) ^e

^aReference. [9].

^bThis work. See also Ref. [24].

^cWith -0.08(8) eV for nuclear recoil [4] and 0.18(5) eV for nuclear polarization [25].

^dReference [26]. The difference 0.04 eV to the value given in [9] is due to a previous double counting of the mass polarization effect.

^eSchweppe *et al.* [18].

potential from the beginning in the relativistic many-body perturbation theory calculation. This would give both the valence and core effects self-consistently.

In order to compare with the experimental $2p_{1/2}$ - $2s_{1/2}$ transition energy we give in Table VI previously calculated effects, the screened self-energy [Figs. 1(a) and 3(c)], the nuclear polarization and recoil and the result of relativistic many-body calculations. We have also calculated the effect of including the vacuum-polarization potential in the orbitals when evaluating the self-energy. This corresponds to Figs. 3(g) and 3(h) and gives a -0.19 eV contribution to the transition energy. This is the largest contribution to the difference between our final transition energy and that given by Blundell. Adding this effect to the result by Blundell changes also his value to fall inside the experimental error bars. This almost perfect agreement between theory and experiment can

be assumed to be partly fortuitous since one can expect, e.g., the two-photon self-energy diagrams 3(m)-3(o), not calculated so far, to be more important than the calculated combined self-energy vacuum-polarization effect. In conclusion one can state that all diagrams with two virtual photons need to be calculated to achieve a reliable theoretical value with an uncertainty comparable to the experimental one.

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