Vacuum polarization calculations for hydrogenlike and alkalilike ions

J. Sapirstein

Department of Physics, University of Notre Dame, Notre Dame, IN 46556

K. T. Cheng

University of California, Lawrence Livermore National Laboratory, Livermore, CA 94550

(Dated: October 26, 2018)

Abstract

Complete vacuum polarization calculations incorporating finite nuclear size are presented for hydrogenic ions with principal quantum numbers \( n = 1 - 5 \). Lithiumlike, sodiumlike, and copperlike ions are also treated starting with Kohn-Sham potentials, and including first-order screening corrections. In both cases dominant Uehling terms are calculated with high accuracy, and smaller Wichmann-Kroll terms are obtained using numerical electron Green’s functions.

PACS numbers: 31.30.-i, 31.30.Jv, 12.20.Ds
I. INTRODUCTION

The most important radiative correction to the spectra of highly charged ions is the Lamb shift, which at the one-loop level consists of two contributions, the self-energy and vacuum polarization. The effect of the latter is dominated by the Uehling term, which was introduced even before the development of the modern form of Quantum Electrodynamics (QED). However, while relatively small, extra effects known as Wichmann-Kroll terms need to be considered when theory is confronted by experimental data on highly-charged ions of ever-increasing accuracy. An important advance in the field was made by Gyulassy, who pointed out that by arranging the calculation so that electron propagator terms with positive and negative values of the angular momentum quantum number $\kappa$ are taken together, a single subtraction of the Uehling term leads to a finite expression for the Wichmann-Kroll term free of the spurious constants that can arise when formally infinite integrals are manipulated. He presented values only for $|\kappa| = 1$, but Soff and Mohr then treated higher $\kappa$ values and showed that the partial wave series converges very rapidly.

The results of Soff and Mohr covered $n = 1$ and $n = 2$ states, and included finite nuclear size through a shell model, which allowed the use of analytic Green’s functions. However, many-electron ions are best described with non-Coulomb potentials that incorporate electron screening, and in this case one is forced to use numerical Green’s functions. We have used these functions extensively in treating the self-energy, and one purpose of this paper is to extend their use to the evaluation of the Wichmann-Kroll terms in a variety of atomic systems.

Other work in the field includes a basis set based approach by Persson et al. that can also be applied to non-Coulomb potentials. Ref. in particular calculates the Wichmann-Kroll effect for lithiumlike uranium, which will also be treated here. We note the work of Beier et al. for hydrogenic ions, which is of particularly high accuracy. Finally, a calculation of vacuum polarization effects on lithiumlike ions, very similar in its treatment of screening to what will be presented here, can be found in Ref.

In the next section, we briefly describe our treatment of the dominant Uehling term. In the following section, formulas for the Wichmann-Kroll term are given, along with a discussion of numerical issues. Screening terms are then defined, and results are given in a set of tables. A brief discussion of the accuracy of our results for lithiumlike, sodiumlike,
and copperlike uranium completes the paper.

II. FORMALISM

We work in Furry representation QED [9], with a lowest-order Hamiltonian given by

\[ H_0 = \int d^3x \psi(x)^\dagger \left[ -i\vec{\alpha} \cdot \vec{\nabla} + \beta m - \frac{Z_{\text{eff}}(r)\alpha}{r} \right] \psi(x), \]

where \( r = |\vec{x}| \). Natural units in which \( \hbar = c = 1 \) are used here. In the usual Furry representation, \( Z_{\text{eff}}(r) = Z_{\text{nuc}}(r) \) describes the Coulomb field of the nucleus, which will be modeled here with a Fermi distribution. However, when describing many-electron atoms and ions in a QED framework, it is often convenient to incorporate some screening through the use of non-Coulomb potentials. Here we work with three effective charges, designed to incorporate screening effects in lithiumlike, sodiumlike, and copperlike ions. They represent Kohn-Sham potentials, defined through

\[ Z_{\text{eff}}(r) = Z_{\text{nuc}}(r) - r \int dr' \frac{1}{r>} \rho_t(r') + \frac{2}{3} \left[ \frac{81}{32\pi^2} r \rho_t(r) \right]^{1/3}, \]

where

\[ \rho_t(r) = g_v^2(r) + f_v^2(r) + \sum_a (2j_a + 1) \left[ g_a^2(r) + f_a^2(r) \right] \]

is the electronic charge density such that \( \int \rho_t(r) dr = N \), the total number of electrons. Here \( g(r) \) and \( f(r) \) are the upper and lower components of Dirac wave functions determined self-consistently, and the indices \( v \) and \( a \) refer to valence and core electrons, respectively. For lithiumlike ions, \( v = 2s \) and \( a = 1s_{1/2} \) state. For sodiumlike ions, \( v = 3s \) and \( a \) ranges over the \( 2s_{1/2}, 2p_{1/2}, \) and \( 2p_{3/2} \) states also. Finally for copperlike ions, \( v = 4s \), and \( a \) includes the additional \( 3s_{1/2}, 3p_{1/2}, 3p_{3/2}, 3d_{3/2}, \) and \( 3d_{5/2} \) core states.

The basic expression for vacuum polarization is given by

\[ E^{\text{VP}} = -i\alpha \int \frac{dk_0}{2\pi} \int d^3x d^3y \bar{\psi}_v(\vec{x}) \gamma_0 \psi_v(\vec{x}) \frac{1}{|\vec{x} - \vec{y}|} \text{Tr} \left[ \gamma_0 S_F(\vec{y}; \vec{y}; k_0) \right], \]

where the bound electron propagator \( S_F \) satisfies the equation

\[ \left[ E + i\vec{\alpha} \cdot \vec{\nabla} - \beta m + \frac{Z_{\text{eff}}(x)\alpha}{x} \right] S_F(x, y; E) = \delta^3(\vec{x} - \vec{y}) \gamma_0. \]

We will also need the free electron propagator \( S_0(x, y; E) \), which satisfies

\[ \left[ E + i\vec{\alpha} \cdot \vec{\nabla} - \beta m \right] S_0(x, y; E) = \delta^3(\vec{x} - \vec{y}) \gamma_0, \]
and is solved by
\[ S_0(\vec{x}, \vec{y}; E) = \int \frac{d^3p}{(2\pi)^3} \frac{e^{i\vec{p} \cdot (\vec{x} - \vec{y})}}{E\gamma_0 - \vec{p} \cdot \vec{\gamma} - m}. \] (7)

The bound propagator \( S_F \) can be expanded in terms of the free propagator \( S_0 \) through
\[ S_F(\vec{x}, \vec{z}; E) = S_0(\vec{x}, \vec{z}; E) - \int d^3y S_0(\vec{x}, \vec{y}; E) \frac{Z_{\text{eff}}(y)\alpha_{\vec{y}}}{y} \gamma_0 S_F(\vec{y}, \vec{z}; E). \] (8)

### A. Uehling Term

When the above expansion of the propagator is used in Eq. (4), the first term on the right-hand side makes no contribution because of Furry’s theorem [10], which states that there is an exact cancellation between loop diagrams with an odd number of external photons when the momentum in the loop is reversed, which follows from a charge conjugation argument. When we set up the numerical calculation of the Wichmann-Kroll terms below using a partial wave expansion of the electron propagator, we will again discuss the vanishing of this term.

The Uehling approximation to vacuum polarization comes from replacing the last bound propagator \( S_F \) in Eq. (8) with a free propagator \( S_0 \), which leads to the ultraviolet divergent energy shift
\[ E_{\text{Ueh}}^{\text{VP}} = \frac{i\alpha}{2\pi} \int dk_0 \int d^3x d^3y d^3z \bar{\psi}_v(\vec{x}) \gamma_0 \psi_v(\vec{x}) \frac{1}{|\vec{x} - \vec{y}|} \times \text{Tr} \left[ \gamma_0 S_0(\vec{y}, \vec{z}; k_0) \frac{Z_{\text{eff}}(z)\alpha_{\vec{z}}}{z} \gamma_0 S_0(\vec{z}, \vec{y}; k_0) \right]. \] (9)

It is useful at this point to define the vacuum-polarization tensor in \( n = 4 - \epsilon \) dimensions,
\[ \Pi_{\mu\nu}(q) = -ie^2 \int \frac{d^n k}{(2\pi)^n} \text{Tr} \left[ \gamma^\mu \frac{1}{\vec{q} + \vec{k} - m} \gamma^\nu \frac{1}{\vec{k} - m} \right], \] (10)
which is ultraviolet finite for positive \( \epsilon \). An advantage of this so-called dimensional regularization is that an automatically gauge-invariant form results after combining denominators with a Feynman parameter \( u \) and carrying out the \( d^n k \) integration,
\[ \Pi_{\mu\nu}(q) = \left( q^2 g_{\mu\nu} - q_\mu q_\nu \right) \left\{ Z_3^{(2)} - \frac{2\alpha}{\pi} \int_0^1 du u (1 - u) \ln \left[ 1 - u (1 - u) q^2 / m^2 \right] \right\}. \] (11)

The constant \( Z_3^{(2)} \), which diverges as \( 1/\epsilon \), is removed by the renormalization procedure, leaving a finite expression. In the case of vacuum polarization the relevant 4-vector \( q \) has a vanishing time component, and \( E_{\text{Ueh}}^{\text{VP}} \) depends only the \( \mu = \nu = 0 \) component,
\[ \Pi_{00}(q) = \frac{2\alpha}{\pi} \bar{q}^2 \int_0^1 du u (1 - u) \ln \left[ 1 + u (1 - u) \bar{q}^2 / m^2 \right]. \] (12)
If we now use the representation of the free propagator given in Eq. (7) for the Uehling energy \( E_{\text{Ueh}}^{\text{VP}} \) shown in Eq. (10), an expression involving the vacuum polarization tensor results, allowing us to write

\[
E_{\text{Ueh}}^{\text{VP}} = -\frac{\alpha}{2\pi^2} \int d^3x \int d^3y \int d^3z \frac{1}{|\vec{r} - \vec{y}|} \psi_v^\dagger(\vec{r}) \psi_v(\vec{r}) \frac{Z_{\text{eff}}(z)\alpha}{z} \times \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q} \cdot (\vec{r} - \vec{y})} \int_0^1 du \frac{(1 - u)^2}{m^2 + (1 - u)q^2/m^2} \ln [1 + u(1 - u)q^2/m^2].
\]  

Carrying out the \( d^3y \) integration gives

\[
E_{\text{Ueh}}^{\text{VP}} = -\frac{2\alpha}{\pi} \int d^3x \int d^3z \frac{\psi_v^\dagger(\vec{r}) \psi_v(\vec{r}) Z_{\text{eff}}(z)\alpha}{z} \times \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q} \cdot (\vec{r} - \vec{y})} \int_0^1 du \frac{(1 - u)^2}{m^2 + (1 - u)q^2/m^2} \ln [1 + u(1 - u)q^2/m^2].
\]  

A partial integration with respect to \( u \) gives a factor \( q^2 \) that can be written as \(-\nabla_z^2\) operating on the exponential. Two additional partial integrations with respect to \( \nabla_z \) then leads to

\[
E_{\text{Ueh}}^{\text{VP}} = -\frac{\alpha}{\pi} \int d^3x \psi_v^\dagger(\vec{r}) \psi_v(\vec{r}) \nabla_z^2 \left[ \frac{Z_{\text{eff}}(z)\alpha}{z} \right] \times \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q} \cdot (\vec{r} - \vec{y})} \int_0^1 du \frac{(1 - u)^2}{m^2 + (1 - u)q^2/m^2} \frac{1}{3} \frac{1}{m^2 + (1 - u)q^2/m^2}.
\]

which results in

\[
E_{\text{Ueh}}^{\text{VP}} = -\frac{\alpha}{4\pi^2} \int d^3x \psi_v^\dagger(\vec{r}) \psi_v(\vec{r}) \int d^3y \nabla_y^2 \left[ \frac{Z_{\text{eff}}(y)\alpha}{y} \right] \int_0^1 du \frac{(1 - u)^2}{1 - u} \frac{1 - 2u}{3} e^{\frac{m|\vec{r} - \vec{y}|}{2}} \frac{1}{|\vec{r} - \vec{y}|}. \]

This is equivalent to an alternative form sometimes presented for the Uehling term,

\[
E_{\text{Ueh}}^{\text{VP}} = \frac{\alpha}{4\pi^2} \int d^3x \psi_v^\dagger(\vec{r}) \psi_v(\vec{r}) \int d^3y \nabla_y^2 \left[ \frac{Z_{\text{eff}}(y)\alpha}{y} \right] \int_0^1 dv \frac{v^2}{1 - v^2} \frac{e^{\frac{m|\vec{r} - \vec{y}|}{2}}}{|\vec{r} - \vec{y}|},
\]

as can be seen by setting \( u = (1 - v)/2 \) in the region \( u = 0 \) to \( 1/2 \) and \( u = (1 + v)/2 \) in the region \( u = 1/2 \) to 1. When the effective charge is spherically symmetric, as will be assumed for all cases considered here, the alternative form can be rewritten, after carrying out the angle integration in the \( d^3y \) integration and making the final change of variable \( v = \sqrt{1 - 1/t^2} \),

\[
E_{\text{Ueh}}^{\text{VP}} = \frac{\alpha^2}{6\pi m} \int d^3x \psi_v^\dagger(\vec{r}) \psi_v(\vec{r}) \frac{1}{x} \int_0^\infty dy Z_{\text{eff}}''(y) \times \int_1^\infty dt \sqrt{t^2 - 1} \left[ \frac{1}{2t^4} + \frac{1}{t^2} \right] e^{-2m|x-y|t} - e^{-2m(x+y)t}.
\]
The $t$ integration has been treated by Fullerton and Rinker [12], who give numerical fitting formulas that allow fast and accurate evaluation of its value, after which a single numerical $y$ integration gives the Uehling potential $U_V(x)$ as defined by

$$E_{\text{Ueh}}^\text{VP} \equiv \int d^3 x \psi_v^\dagger(\vec{x})U_V(x)\psi_v(\vec{x}) \equiv (U_V)_{vv},$$  \hspace{1cm} (19)

such that the Uehling energy is given by the expectation value of this potential. Before presenting results for the contribution of the Uehling terms to vacuum polarization, we turn to a description of the calculation of Wichmann-Kroll terms.

B. Wichmann-Kroll terms

With the Uehling term accounted for, the remaining part of the vacuum polarization is given by the Wichmann-Kroll term,

$$E_{\text{WK}}^\text{VP} = -\frac{i\alpha}{2\pi} \int dk_0 \int d^3 x \, d^3 y \, \psi_v^\dagger(\vec{x})\psi_v(\vec{y}) \frac{1}{|\vec{x} - \vec{y}|} \text{Tr}\left\{\gamma_0 \left[ S_F(\vec{y}, \vec{y}; k_0) - S_0(\vec{y}, \vec{y}; k_0) + \int d^3 z \, S_0(\vec{y}, \vec{z}; k_0) \frac{Z_{\text{eff}}(z)\alpha}{z} \gamma_0 S_0(\vec{z}, \vec{y}; k_0) \right]\right\}. \hspace{1cm} (20)$$

While this combination is ultraviolet finite by power counting, a spurious, non-gauge invariant finite term can show up if sufficient care is not taken. As was shown by Gyulassy [3], this problem can be avoided when the propagators are represented with a partial wave expansion by an appropriate grouping of that expansion. The calculation is carried out as follows. We first make a Wick rotation $k_0 \to i\omega$. Unlike the case of the self-energy, no poles are passed in this process. The next step is to replace the electron propagators with the partial wave expansion

$$S_F(\vec{x}, \vec{y}; E) = \sum_{\kappa, \mu} \left[ \theta(x - y) w_{\kappa\mu}^E(\vec{x}) \bar{u}_{\kappa\mu}^E(\vec{y}) + \theta(y - x) u_{\kappa\mu}^E(\vec{x}) \bar{\omega}_{\kappa\mu}^E(\vec{y}) \right]. \hspace{1cm} (21)$$

Here, $\theta(x)$ is the step function such that $\theta(x) = 1$ if $x > 0$ and $\theta(x) = 0$ if $x < 0$, and $w_{\kappa\mu}^E$ and $u_{\kappa\mu}^E$ are the solutions of the Dirac equation regular at infinity and the origin, respectively. They are represented as

$$u_{\kappa\mu}^E(\vec{r}) = \frac{1}{r} \begin{pmatrix} i \, g_0^0(E, r) \, \chi_{\kappa\mu}(\Omega) \\ f_0^0(E, r) \, \chi_{-\kappa\mu}(\Omega) \end{pmatrix},$$  \hspace{1cm} (22)
and
\[ w^{E}_{\kappa\mu}(\vec{r}) = \frac{1}{r} \left( \begin{array}{c} i g^{\infty}_{\kappa}(E, r) \chi_{\kappa\mu}(\Omega) \\ f^{\infty}_{\kappa}(E, r) \chi_{-\kappa\mu}(\Omega) \end{array} \right). \] (23)

The unsubtracted vacuum polarization is, in terms of this expansion of the electron propagator,
\[ E^{\text{VP}} = \frac{\alpha}{2\pi} \int_{-\infty}^{\infty} d\omega \int \frac{d^3x \, d^3y}{|\vec{x} - \vec{y}|} \psi^{\dagger}_{\nu}(\vec{x})\psi_{\nu}(\vec{x}) \frac{1}{y^2} \sum_{\kappa\mu} \text{Tr} \left[ g_{\kappa}^{\infty}(\i\omega, \vec{y}) \overline{\psi}_{\kappa\mu}(\vec{y}) \right] \]
\[ = \frac{\alpha}{2\pi} \int_{-\infty}^{\infty} d\omega \int \frac{d^3x \, d^3y}{|\vec{x} - \vec{y}|} \psi^{\dagger}_{\nu}(\vec{x})\psi_{\nu}(\vec{x}) \frac{1}{y^2} \sum_{\kappa\mu} \left\{ g^{\infty}_{\kappa}(\i\omega, \vec{y}) g_{\kappa}^{0}(\i\omega, \vec{y}) \text{Tr} \left[ \chi_{\kappa\mu}(\Omega_y) \chi^{\dagger}_{\kappa\mu}(\Omega_y) \right] \right. \]
\[ + f^{\infty}_{\kappa}(\i\omega, y) f_{\kappa}^{0}(\i\omega, y) \text{Tr} \left[ \chi_{-\kappa\mu}(\Omega_y) \chi^{\dagger}_{-\kappa\mu}(\Omega_y) \right] \} \]. (24)

If we then use the identity
\[ \text{Tr} \left[ \sum_{\mu} \chi_{\kappa\mu}(\Omega) \chi^{\dagger}_{\kappa\mu}(\Omega) \right] = \frac{\kappa}{2\pi} \] (25)
we have the compact expression
\[ E^{\text{VP}} = \frac{\alpha}{4\pi^2} \sum_{\kappa} |\kappa| \int_{-\infty}^{\infty} d\omega \int \frac{d^3x \, d^3y}{|\vec{x} - \vec{y}|} \psi^{\dagger}_{\nu}(\vec{x})\psi_{\nu}(\vec{x}) \frac{1}{y^2} \left[ g^{\infty}_{\kappa}(\i\omega, \vec{y}) g_{\kappa}^{0}(\i\omega, \vec{y}) + f^{\infty}_{\kappa}(\i\omega, y) f_{\kappa}^{0}(\i\omega, y) \right]. \] (26)

Before continuing to the subtraction of the Uehling term, we discuss the subtraction of the free propagator term, which vanishes by Furry’s theorem [10]. In terms of the partial wave expansion of the free propagator term, which is given by the same expression as above but with the bound radial Green’s functions \( g_{\kappa}^{0,\infty} \) and \( f_{\kappa}^{0,\infty} \) replaced by the corresponding free-electron functions, the manifestation of this cancellation is particularly simple, as each positive value of \( \kappa \) gives a contribution canceled by the corresponding negative value. This was shown analytically by Gyulassy [3], but here, since we treat both the bound and free propagators with the same numerical methods, we use it as a check on the accuracy of our Green’s functions. In Table II we present partial wave results of the free-propagator term \( E^{\text{VP}}(S_0) \) for low values of \( \kappa \) for the finite nuclear size 1s ground state of hydrogenlike mercury (\( Z = 80 \)). The cancellation of this term between the positive and negative \( \kappa \) partial waves is obvious. Only six digits past the decimal point are shown, but the actual cancellation is even finer, which is one of the numerical tests used in this work. Also shown in the same table are values of the bound propagator term \( E^{\text{VP}} \) which can be seen to scale roughly with \( |\kappa| \), which is how a quadratic ultraviolet divergence is manifested in a partial wave expansion.

We next turn to the unrenormalized Uehling term, which must be evaluated with high accuracy, as it cancels out many digits of the unrenormalized vacuum polarization. While it
can be formed analytically, we have found that numerical methods actually work somewhat better, and continue to use them. A short calculation gives the Uehling term as

\[ E_{\text{Ueh}}^{\text{VP}} = -\frac{2\alpha}{\pi} \Re \int_{0}^{\infty} d\omega \int_{0}^{\infty} dr \left[ g_\nu(r)^2 + f_\nu(r)^2 \right] \int_{0}^{\infty} dr' \frac{1}{r'} \int_{0}^{\infty} dx \frac{Z_{\text{eff}}(x) \alpha}{x} \sum |\kappa| \times \left\{ \theta(r' - x) \left[ g_\nu^0(\omega, x)^2 + f_\nu^0(\omega, x)^2 \right] \left[ g_\kappa^\infty(\omega, r')^2 + f_\kappa^\infty(\omega, r')^2 \right] \\
+ \theta(x - r') \left[ g_\kappa^\infty(\omega, x)^2 + f_\kappa^\infty(\omega, x)^2 \right] \left[ g_\nu^0(\omega, r')^2 + f_\nu^0(\omega, r')^2 \right] \right\}. \quad (27) \]

To carry out the evaluation of the partial wave expansion form of the Uehling term with sufficient accuracy requires a great deal of care. Matters are facilitated by using an extremely fine radial grid of up to 50,000 points. This is particularly helpful in controlling the accuracy of the \( \omega \) integration where the virtual infinity of the calculation can exceed \( 1 \times 10^6 \, mc^2 \) and numerical instabilities at the highest \( \omega \) values can lead to unphysical oscillations in the renormalized effective charge density at very small and very large radial points. These same problems play a much smaller role in self-energy calculations, where the bound state wave function provides suppression at these regions; here, however, the wave function does not provide any suppression.

The second test of the numerics of our approach has to do with the integral over the effective charge density \( \rho(r) \), defined through

\[ E_{\text{WK}}^{\text{VP}} = \int_{0}^{\infty} dr \rho(r) \phi(r), \quad (28) \]

where

\[ \phi(r) = \int_{0}^{\infty} dr' \frac{1}{r'} \left[ g_\nu(r')^2 + f_\nu(r')^2 \right]. \quad (29) \]

Without the screening potential \( \phi(r) \) from the bound electron \( \nu \), the effective charge density \( \rho(r) \) should integrate to zero, as there should not be any change in the net charge. Contributions to this integral from the unrenormalized vacuum polarization and Uehling terms cancel to a level that is typically of order \( 10^{-8} \) or better. If this cancellation is not this precise, we have found that our answers become unstable and go into disagreement with previous calculations.

Partial wave results of the unrenormalized Uehling term for the 1s state of Hg\(^{79+}\) are shown also in Table I. It can be seen that they are independent of the sign of \( \kappa \) and show the same rate of increase with \( |\kappa| \) as the bound propagator term \( E_{\text{VP}}^{\text{VP}} \). The quadratic ultraviolet divergence in these terms cancels, however, and their sum gives the finite Wichmann-Kroll term which can be seen to converge very rapidly with \( |\kappa| \).
We now present results for the hydrogenic vacuum polarization including finite nuclear
size for states of principal quantum number $n = 1 - 5$, excluding $d$ and higher angular
momentum states which have very small contributions. We model the nuclear charge distri-
bution with the Fermi distributions described in Ref. [14], with the exception of the cases
$Z = 90$ and $Z = 92$, where we use $c = 7.0589$ and $c = 7.13753$, respectively, which were
derived from Ref. [19, 20]. It is convenient to pull out the overall $Z$ and $n$ behavior by
working in terms of the function $F_n(Z\alpha)$ defined through

$$E_{\text{VP}} = \frac{\alpha}{\pi} \left(\frac{Z\alpha}{n^3}\right)^4 F_n(Z\alpha) mc^2.$$  

(30)

Results for $ns$, $np_{1/2}$ and $np_{3/2}$ states are given in Tables II – IV. Where comparison is
possible, we find our results to be in good agreement with previous calculations cited in the
introduction.

C. Screening Corrections

We now turn to the evaluation of vacuum polarization in many-electron ions with an
alkalilike electronic configuration. Formulas for the Uehling and Wichmann-Kroll terms
given above are valid for any effective charge $Z_{\text{eff}}(r)$, so while it would be possible to always
start with a Coulomb potential and calculate screening effects starting from that point, we
choose here to incorporate the dominant effect of screening for the lithium, sodium, and
copper isoelectronic sequences by using the Kohn-Sham potentials defined in Eq. (2). While
this is adequate for the Wichmann-Kroll terms, we account for screening more fully for the
Uehling terms in this section. The theory for lithiumlike ions was set out in some detail in
[13], so we simply briefly generalize it here to the sodiumlike and copperlike sequences.

There are four sources of screening for the Uehling term: valence perturbed orbital terms,
core perturbed orbital terms, insertions of the Uehling term in one-photon exchange, and
derivative terms. Representative Feynman diagrams for the first three sources are shown in
Figs. Ia – IIc; though the derivative terms do not have a standard diagrammatic representa-
tion. Beginning with the insertion of the Uehling term in one-photon exchange, we note
that the first-order energy of an alkalilike ion is given by

$$E^{(1)} = \sum_a \left[ g_{vava}(0) - g_{vaav}(\delta E_{va}) \right] - U_{vv},$$  

(31)
where $\delta E_{va} = \epsilon_v - \epsilon_a$, $U(r) = [Z_{\text{nuc}}(r) - Z_{\text{eff}}(r)]/r$ is the counter potential, and

$$g_{ijkl}(E) = \alpha \int d^3x d^3y \frac{e^{iE|x-y|}}{|x-y|} \bar{\psi}_i(x) \gamma^\mu \psi_k(x) \bar{\psi}_j(y) \gamma^\nu \psi_l(y).$$  \tag{32}$$

The insertion effect shown in Fig. 1c can be accounted for by replacing the $g$ factors in the above, which involve the exchange of a massless photon, with a weighted integration over $g$ factors involving the exchange of a massive photon. The explicit form is

$$E_{\text{Ex}}^{\text{VP}} = \frac{\alpha}{\pi} \int_0^1 du \frac{u^2(1 - u^2/3)}{1 - u^2} \sum_a \left[ g_{ava}(i\xi) - g_{vaav}(i\sqrt{\xi^2 - \delta E_{va}^2}) \right],$$  \tag{33}$$

where $\xi = \sqrt{4m^2/(1 - u^2)}$. We compared our results for this term with results for lithiumlike uranium given in Ref. \[8\], and obtained exact agreement for the $2p_{1/2}$ and $2p_{3/2}$ states but a slightly different result (0.001 eV) for the $2s_{1/2}$ state, which we attribute to different treatment of the nucleus.

The next contributions to screening are the “perturbed orbital” (PO) terms shown in Figs. 1a and 1b. They are given by

$$E_{\text{PO}}^{\text{VP}} = (U_V)_{v\bar{v}} + (U_V)_{\bar{v}v} + \sum_a \left[ (U_V)_{a\bar{a}} + (U_V)_{\bar{a}a} \right],$$  \tag{34}$$

where $U_V$ is the Uehling potential defined in Eq. (19),

$$\tilde{\psi}_v(\bar{y}) \equiv \alpha \sum_{m \neq v,a} \int \frac{d^3z d^3w}{|z-w|} \psi_m(\bar{y}) \left[ \bar{\psi}_m(z) \gamma_\mu \tilde{\psi}_v(z) \bar{\psi}_a(w) \gamma^\mu \psi_a(w) \\
- e^{i\delta E_{va}|z-w|} \bar{\psi}_m(z) \gamma_\mu \psi_a(z) \bar{\psi}_a(w) \gamma^\mu \psi_v(w) \right] \\
- \sum_{m \neq \bar{v}} \int d^3z \frac{\psi_m(\bar{y})}{\epsilon_v - \epsilon_m} \psi_m^\dagger(z) U(z) \psi_v(z),$$  \tag{35}$$

is a valence orbital perturbed either by the exchange of a photon with the core electrons or else by the counter potential $U(z)$, and

$$\tilde{\psi}_\bar{a}(\bar{y}) \equiv \alpha \sum_{m \neq \bar{a}} \int \frac{d^3z d^3w}{|z-w|} \psi_m(\bar{y}) \left[ \bar{\psi}_m(z) \gamma_\mu \tilde{\psi}_\bar{a}(z) \bar{\psi}_v(w) \gamma^\mu \psi_v(w) \\
- e^{i\delta E_{va}|z-w|} \bar{\psi}_m(z) \gamma_\mu \psi_v(z) \bar{\psi}_v(w) \gamma^\mu \psi_a(w) \right]$$  \tag{36}$$

is a core orbital perturbed by the exchange of a photon with the valence electron.

Finally, the “derivative” terms, which arise from the energy dependence of one-photon exchange, are given by

$$E_{\text{der}}^{\text{VP}} = - \sum_a (U_{vv} - U_{aa}) g_{ava}^f (\delta E_{av}).$$  \tag{37}$$
We have precise agreement with the Coulomb potential results for lithiumlike uranium presented in Ref. \cite{8}, where this contribution is denoted by $E_b$.

In Tables \textbf{V} - \textbf{VII} we present vacuum polarization results for the three alkalilike isoelectronic sequences mentioned above. We choose to use atomic units in this case, and results of the screening calculations just described are presented, along with those of the Uehling and Wichmann-Kroll terms. It is interesting to note that while the higher-order screening corrections are typically smaller in size than the lowest-order Uehling energies, such is not the case for the $np_{3/2}$ states, where the screening corrections are consistently larger than, or at least comparable to, the corresponding Uehling energies.

\section{III. CONCLUSIONS}

The calculations presented here are intended to play a role in precision spectroscopy of highly charged ions, so it is important to be quantitative about the accuracy. We choose to do this in the context of ions of uranium, which are of interest because these ions have the highest nuclear charge that has precision spectroscopy available, and relativistic and QED effects are highly enhanced at high $Z$. The earliest precise measurement, on lithiumlike uranium \cite{15}, had a precision of 0.1 eV. This experiment measured the $2s_{1/2} - 2p_{1/2}$ transition, and subsequently the $2s_{1/2} - 2p_{3/2}$ transition was measured with an accuracy of 0.27 eV in Ref. \cite{21}. More recently, the $3s - 3p_{3/2}$ transition in sodiumlike uranium has been measured \cite{16}, and the experimental precision has reached 0.02 eV. Finally, the $4s - 4p_{3/2}$ transition in copperlike uranium has been measured to the remarkable precision of 0.0019 eV \cite{17}.

These high precision measurements pose a considerable challenge to the theory of many-electron ions. While correlation calculations based on Dirac-Fock or model potentials converge quite rapidly at this high $Z$ and are presently sufficiently accurate, the proper incorporation of negative-energy state and retardation effects is best done in a field-theoretic context, with the relativistic many-body treatment of correlation replaced with the evaluation of Feynman diagrams involving the exchange of two photons between electrons. This procedure has been carried out for lithiumlike ions \cite{8,18}. After this has been done, one needs to carry out radiative correction calculations in the many-electron environment, which requires both precise one-loop calculations and associated screening corrections. One purpose of the present paper has been to carry out the vacuum polarization part of this program.
with accuracy at least at the level of the experimental uncertainties, and we now discuss to what extent we have succeeded in this attempt.

We begin by discussing lithiumlike uranium, where the overall contribution of vacuum polarization to the $2s_{1/2}$ energy is -14.742 eV. While the numerical determination of the Uehling contribution to this of -15.831 eV is extremely accurate, care must be taken with nuclear size dependence. Varying the $c$ parameter used here, 7.13753 fm, by one percent leads to changes of 0.008 eV, and because the uncertainty quoted by Zumbro et al. [20] for the $c$ parameter is 0.0012 fm (0.02 %), this part of the calculation needs no improvement. If experiment continues to improve, however, a more detailed study of the effect of different distributions of charge and higher multipoles may be necessary.

Turning to the Wichmann-Kroll calculation, which contributes 0.789 eV, the main uncertainty here is the cutting off of the partial wave series at $\kappa = 5$. For the case of the $n = 2$ states of lithiumlike uranium, we extended the sum to $\kappa = 10$, and found a change of only 0.001 eV. In view of the rapid convergence of the partial wave series for this term, stopping the calculation at $\kappa = 5$ should be quite adequate.

Finally, a more delicate issue involves screening. Here we made one approximation that can be important, namely, treating the vacuum polarization contribution to exchange photons in Uehling approximation. Ref. [8] explicitly calculated the residual Wichmann-Kroll term using a Coulomb potential, and found a 0.0005 eV contribution to the $2s$ energy, so our approximation is valid. However, higher-order screening graphs have not been treated here, and we therefore estimate the size of their contributions by comparing the results of different model potentials. We use a core-Hartree potential, defined with an effective charge

$$Z_{\text{eff}}(r) = Z_{\text{nuc}}(r) - r \int dr' \frac{1}{r'} \rho_c(r'), \quad (38)$$

where $\rho_c(r) = \sum_a (2j_a + 1)[g_a^2(r) + f_a^2(r)]$ is the total charge density of the core electrons. In Table VIII we compare Kohn-Sham (KS) and core-Hartree (CH) results for all three states. Considering the $2s$ state, we see that while a 0.096 eV change is present in the Uehling potential, inclusion of screening reduces this to a 0.016 eV difference, far smaller than the experimental error. The $2p$ states are seen to be under even better control. We consider that our results for vacuum polarization are accurate to under 0.02 eV for lithiumlike uranium.

While the experimental accuracy of sodiumlike uranium is higher than lithiumlike uranium, the higher principal quantum number reduces the size of vacuum polarization, so
that it need be known with less precision. Arguments similar to those given for lithiumlike uranium can be used to show that the Uehling and Wichmann-Kroll terms are sufficiently well determined. A comparison of the KS and CH results is given again in Table VIII. It can be seen that the 3s Uehling energy changes by 0.054 eV, but inclusion of screening reduces this to 0.001 eV. We estimate the accuracy of our result here to be 0.003 eV, which is due mainly to the potential dependence of the Wichmann-Kroll term and is again well under the experimental error.

Finally, copperlike uranium presents the greatest challenge to theory, both because of the complexity of the ion and the very high experimental precision that has been reached. We again compare KS and CH results in Table VIII and see that 4s Uehling energy changes by 0.031 eV, an order of magnitude larger than the experimental error. Inclusion of first-order screening reduces this to 0.002 eV, same as the experimental error. We note that the 4p_{1/2} energy shifts by about the same amount, so the potential dependence of the 4s_{1/2} – 4p_{1/2} transition energy is much less than the experimental error, but the shift of the 4p_{3/2} level is smaller, though it still reduces the potential dependence of the 4s_{1/2} – 4p_{3/2} transition energy. The shift of the Wichmann-Kroll terms is seen to be significant on the scale of the experimental error, but cancels when transitions are considered. Were we to include screening corrections to the Wichmann-Kroll term, we expect the results of the two potentials would give closer answers for the individual states. Thus for copperlike uranium, the vacuum polarization results presented here should be regarded as having an accuracy comparable to experiment for transitions, but further work is needed for ionization energies.

While the vacuum polarization calculations presented here are adequate at present, further reduction of experimental error will require a more accurate treatment of screening. The treatment given here is equivalent to first-order many body perturbation theory (MBPT), though it is done in a field theoretic manner. Further accuracy should be obtainable by inclusion of second-order MBPT, which is a straightforward though lengthy procedure.

The next step is to treat the self-energy diagram including screening corrections. This has been carried out for lithiumlike ions [8, 18], and the theoretical interest for this isoelectronic sequence has shifted to the proper inclusion of the two-loop Lamb shift, which has recently been calculated for the ground state of hydrogenic ions [22]. While considerable work remains to extend these calculations to the sodium and copper isoelectronic sequences, the prospect of treating these truly many-electron systems in a purely QED manner is quite promising.
Acknowledgments

The work of J.S. was supported in part by NSF Grant No. PHY-0097641. The work of K.T.C. was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48. We acknowledge useful conversations with P.J. Mohr.

[1] E.A. Uehling, Phys. Rev. 48, 55 (1935); R. Serber, ibid 48, 49 (1935).
[2] E.H. Wichmann and N.M. Kroll, Phys. Rev. 101, 843 (1956).
[3] M. Gyulassy, Nucl. Phys. A244, 497 (1975).
[4] G. Soff and P.J. Mohr, Phys. Rev. A 38, 5066 (1988).
[5] K.T. Cheng, W.R. Johnson, and J. Sapirstein, Phys. Rev. A 47, 1817 (1993).
[6] H. Persson, I. Lindgren, S. Salomonson, and P. Sunnergren, Phys. Rev. A 48, 2772 (1983).
[7] T. Beier, G. Plunien, M. Greiner and G. Soff, J. Phys. B 30, 2761 (1997).
[8] A.N. Artemyev, T. Beier, G. Plunien, V.M. Shabaev, G. Soff, and V.A. Yerokhin, Phys. Rev. A 60, 45 (1999).
[9] W.H. Furry, Phys. Rev. 81, 115 (1951).
[10] W.H. Furry, Phys. Rev. 51, 125 (1937).
[11] J. Sapirstein and K.T. Cheng, Phys. Rev. A 66, 042501 (2002).
[12] L.W. Fullerton and G.A. Rinker, Phys. Rev. A 13, 1283 (1976).
[13] J. Sapirstein and K.T. Cheng, Phys. Rev. A 66, 042501 (2002).
[14] W.R. Johnson and G. Soff, At. Data Nucl. Data Tables 33, 405 (1985).
[15] J. Schwepppe, A. Belkacem, L. Blumenfeld, N. Claytor, B. Feinberg, H. Gould, V.E. Kostroun, L. Levy, S. Misawa, J.R. Mowat, and M.H. Prior, Phys. Rev. Lett. 66, 1434 (1991).
[16] P. Beiersdorfer, E. Träbert, H. Chen, M.H. Chen, M.J. May, and A.L. Osterheld, Phys. Rev. A (in press) (2003).
[17] S.B. Utter, P. Beiersdorfer, E. Träbert, and E.J. Clothiaux, Phys. Rev. A 67, 032502 (2003).
[18] J. Sapirstein and K.T. Cheng, Phys. Rev. A 64, 022502 (2001).
[19] J. D. Zumbro, R. A. Naumann, M. V. Hoehn, W. Reuter, E. B. Shera, C. E. Bemis, Jr., and Y. Tanaka, Phys. Lett. 167B, 383 (1986).
[20] J.D. Zumbro, E.B. Shera, Y. Tanaka, C.E. Bemis, Jr., R.A. Nauman, M.V. Hoehn, W. Reuter, and R.M. Steffen, Phys. Rev. Lett. 53, 1888 (1984).

[21] P. Beiersdorfer, D. Knapp, R.E. Marrs, S.R. Elliot, and M.H. Chen, Phys. Rev. Lett. 71, 3939 (1993).

[22] V.A. Yerokhin, V. Shabaev, and P. Indelicato, preprint hep-ph/0302268 (2003).

FIG. 1: Feynman diagrams for the screening correction to vacuum polarization.
TABLE I: Behavior of the unrenormalized vacuum polarization for the 1s ground state of hydrogenlike mercury (Z = 80). W-K is the finite Wichmann-Kroll term given by the sum of the first three terms. Units: a.u.

| κ   | $E^{VP}$    | $E^{VP}(S_0)$ | Uehling      | W-K         |
|-----|-------------|---------------|--------------|-------------|
| -1  | -263.566739 | -33.856852    | 229.754601   |             |
| 1   | -195.878973 | 33.856852     | 229.754601   |             |
| Sum | -459.445712 | 0.000000      | 459.509201   | 0.063489    |
| -2  | -515.532936 | -54.346160    | 461.190811   |             |
| 2   | -406.842658 | 54.346160     | 461.190811   |             |
| Sum | -922.375594 | 0.000000      | 922.381621   | 0.006027    |
| -3  | -761.361202 | -68.805626    | 692.556408   |             |
| 3   | -623.750313 | 68.805626     | 692.556408   |             |
| Sum | -1385.111515| 0.000000      | 1385.112815  | 0.001300    |
| -4  | -1003.705497| -79.878165    | 923.827583   |             |
| 4   | -843.949263 | 79.878165     | 923.827583   |             |
| Sum | -1847.654760| 0.000000      | 1847.655166  | 0.000406    |
| -5  | -1243.815854| -88.801356    | 1155.014595  |             |
| 5   | -1066.213175| 88.801356     | 1155.014595  |             |
| Sum | -2310.029029| 0.000000      | 2310.029189  | 0.000160    |
TABLE II: Finite nuclear size Coulomb results for \( ns \)-state vacuum polarization in terms of the function \( F(Z\alpha) \).

| Z  | Contribution | 1s\(_{1/2}\) | 2s\(_{1/2}\) | 3s\(_{1/2}\) | 4s\(_{1/2}\) | 5s\(_{1/2}\) |
|----|--------------|-------------|-------------|-------------|-------------|-------------|
| 30 | Uehling      | -0.2386     | -0.2468     | -0.2470     | -0.2466     | -0.2462     |
|    | W-K          | 0.0020      | 0.0020      | 0.0020      | 0.0021      | 0.0021      |
|    | Sum          | -0.2366     | -0.2448     | -0.2450     | -0.2445     | -0.2441     |
| 40 | Uehling      | -0.2418     | -0.2569     | -0.2572     | -0.2565     | -0.2557     |
|    | W-K          | 0.0033      | 0.0035      | 0.0035      | 0.0035      | 0.0035      |
|    | Sum          | -0.2385     | -0.2534     | -0.2537     | -0.2530     | -0.2522     |
| 50 | Uehling      | -0.2507     | -0.2757     | -0.2762     | -0.2749     | -0.2736     |
|    | W-K          | 0.0051      | 0.0054      | 0.0054      | 0.0054      | 0.0053      |
|    | Sum          | -0.2456     | -0.2703     | -0.2708     | -0.2695     | -0.2683     |
| 60 | Uehling      | -0.2661     | -0.3055     | -0.3061     | -0.3039     | -0.3018     |
|    | W-K          | 0.0073      | 0.0081      | 0.0081      | 0.0080      | 0.0080      |
|    | Sum          | -0.2588     | -0.2974     | -0.2980     | -0.2959     | -0.2938     |
| 70 | Uehling      | -0.2896     | -0.3503     | -0.3511     | -0.3475     | -0.3440     |
|    | W-K          | 0.0102      | 0.0118      | 0.0118      | 0.0116      | 0.0115      |
|    | Sum          | -0.2794     | -0.3385     | -0.3393     | -0.3359     | -0.3325     |
| 80 | Uehling      | -0.3244     | -0.4176     | -0.4184     | -0.4122     | -0.4066     |
|    | W-K          | 0.0141      | 0.0172      | 0.0171      | 0.0168      | 0.0165      |
|    | Sum          | -0.3103     | -0.4004     | -0.4013     | -0.3954     | -0.3901     |
| 82 | Uehling      | -0.3332     | -0.4348     | -0.4355     | -0.4286     | -0.4224     |
|    | W-K          | 0.0150      | 0.0185      | 0.0184      | 0.0181      | 0.0178      |
|    | Sum          | -0.3182     | -0.4163     | -0.4171     | -0.4105     | -0.4046     |
| 90 | Uehling      | -0.3753     | -0.5198     | -0.5199     | -0.5093     | -0.4999     |
|    | W-K          | 0.0194      | 0.0252      | 0.0249      | 0.0243      | 0.0238      |
|    | Sum          | -0.3559     | -0.4946     | -0.4950     | -0.4850     | -0.4761     |
| 92 | Uehling      | -0.3882     | -0.5462     | -0.5461     | -0.5342     | -0.5238     |
|    | W-K          | 0.0206      | 0.0272      | 0.0269      | 0.0262      | 0.0257      |
|    | Sum          | -0.3676     | -0.5190     | -0.5192     | -0.5080     | -0.4981     |
| 100| Uehling      | -0.4524     | -0.6821     | -0.6800     | -0.6609     | -0.6445     |
|    | W-K          | 0.0270      | 0.0378      | 0.0372      | 0.0360      | 0.0350      |
|    | Sum          | -0.4254     | -0.6443     | -0.6428     | -0.6249     | -0.6095     |
TABLE III: Finite nuclear size Coulomb results for \( np_{1/2} \)-state vacuum polarization in terms of the function \( F(Z\alpha) \).

| Z   | Contribution | \(2p_{1/2} \) | \(3p_{1/2} \) | \(4p_{1/2} \) | \(5p_{1/2} \) |
|-----|--------------|---------------|---------------|---------------|---------------|
| 30  | Uehling      | -0.0033       | -0.0039       | -0.0041       | -0.0042       |
|     | W-K          | 0.0001        | 0.0001        | 0.0001        | 0.0001        |
|     | Sum          | -0.0032       | -0.0038       | -0.0040       | -0.0041       |
| 40  | Uehling      | -0.0063       | -0.0075       | -0.0079       | -0.0080       |
|     | W-K          | 0.0001        | 0.0002        | 0.0002        | 0.0002        |
|     | Sum          | -0.0062       | -0.0073       | -0.0077       | -0.0078       |
| 50  | Uehling      | -0.0111       | -0.0132       | -0.0138       | -0.0141       |
|     | W-K          | 0.0003        | 0.0004        | 0.0004        | 0.0004        |
|     | Sum          | -0.0108       | -0.0128       | -0.0134       | -0.0137       |
| 60  | Uehling      | -0.0187       | -0.0221       | -0.0231       | -0.0235       |
|     | W-K          | 0.0007        | 0.0009        | 0.0009        | 0.0009        |
|     | Sum          | -0.0180       | -0.0212       | -0.0222       | -0.0226       |
| 70  | Uehling      | -0.0309       | -0.0364       | -0.0379       | -0.0383       |
|     | W-K          | 0.0015        | 0.0018        | 0.0018        | 0.0018        |
|     | Sum          | -0.0294       | -0.0346       | -0.0361       | -0.0365       |
| 80  | Uehling      | -0.0511       | -0.0600       | -0.0621       | -0.0625       |
|     | W-K          | 0.0030        | 0.0035        | 0.0036        | 0.0036        |
|     | Sum          | -0.0481       | -0.0565       | -0.0585       | -0.0589       |
| 82  | Uehling      | -0.0567       | -0.0665       | -0.0686       | -0.0690       |
|     | W-K          | 0.0034        | 0.0040        | 0.0041        | 0.0041        |
|     | Sum          | -0.0533       | -0.0625       | -0.0645       | -0.0649       |
| 90  | Uehling      | -0.0864       | -0.1008       | -0.1034       | -0.1035       |
|     | W-K          | 0.0059        | 0.0068        | 0.0069        | 0.0069        |
|     | Sum          | -0.0805       | -0.0940       | -0.0965       | -0.0966       |
| 92  | Uehling      | -0.0964       | -0.1123       | -0.1149       | -0.1149       |
|     | W-K          | 0.0068        | 0.0077        | 0.0078        | 0.0078        |
|     | Sum          | -0.0896       | -0.1046       | -0.1071       | -0.1071       |
| 100 | Uehling      | -0.1524       | -0.1759       | -0.1785       | -0.1772       |
|     | W-K          | 0.0118        | 0.0132        | 0.0133        | 0.0132        |
|     | Sum          | -0.1406       | -0.1627       | -0.1652       | -0.1640       |
TABLE IV: Finite nuclear size Coulomb results for $np_{3/2}$-state vacuum polarization in terms of the function $F(Z\alpha)$.

| Z  | Contribution | $2p_{3/2}$ | $3p_{3/2}$ | $4p_{3/2}$ | $5p_{3/2}$ |
|----|--------------|------------|------------|------------|------------|
| 30 | Uehling      | -0.0005    | -0.0006    | -0.0007    | -0.0007    |
|    | W-K          | 0.0000     | 0.0001     | 0.0001     | 0.0001     |
|    | Sum          | -0.0005    | -0.0005    | -0.0006    | -0.0006    |
| 40 | Uehling      | -0.0009    | -0.0011    | -0.0012    | -0.0012    |
|    | W-K          | 0.0000     | 0.0001     | 0.0001     | 0.0001     |
|    | Sum          | -0.0009    | -0.0010    | -0.0011    | -0.0011    |
| 50 | Uehling      | -0.0013    | -0.0016    | -0.0017    | -0.0018    |
|    | W-K          | 0.0001     | 0.0001     | 0.0001     | 0.0001     |
|    | Sum          | -0.0012    | -0.0015    | -0.0016    | -0.0017    |
| 60 | Uehling      | -0.0019    | -0.0023    | -0.0025    | -0.0025    |
|    | W-K          | 0.0002     | 0.0002     | 0.0002     | 0.0002     |
|    | Sum          | -0.0017    | -0.0021    | -0.0023    | -0.0023    |
| 70 | Uehling      | -0.0025    | -0.0031    | -0.0033    | -0.0034    |
|    | W-K          | 0.0003     | 0.0003     | 0.0004     | 0.0004     |
|    | Sum          | -0.0022    | -0.0028    | -0.0029    | -0.0030    |
| 80 | Uehling      | -0.0032    | -0.0040    | -0.0043    | -0.0044    |
|    | W-K          | 0.0004     | 0.0005     | 0.0006     | 0.0006     |
|    | Sum          | -0.0028    | -0.0035    | -0.0037    | -0.0038    |
| 82 | Uehling      | -0.0034    | -0.0043    | -0.0046    | -0.0047    |
|    | W-K          | 0.0005     | 0.0006     | 0.0006     | 0.0006     |
|    | Sum          | -0.0029    | -0.0037    | -0.0040    | -0.0041    |
| 90 | Uehling      | -0.0040    | -0.0052    | -0.0055    | -0.0057    |
|    | W-K          | 0.0007     | 0.0008     | 0.0009     | 0.0009     |
|    | Sum          | -0.0033    | -0.0044    | -0.0046    | -0.0048    |
| 92 | Uehling      | -0.0042    | -0.0054    | -0.0058    | -0.0060    |
|    | W-K          | 0.0007     | 0.0009     | 0.0010     | 0.0010     |
|    | Sum          | -0.0035    | -0.0045    | -0.0048    | -0.0050    |
| 100| Uehling      | -0.0050    | -0.0065    | -0.0070    | -0.0072    |
|    | W-K          | 0.0010     | 0.0013     | 0.0013     | 0.0014     |
|    | Sum          | -0.0040    | -0.0052    | -0.0057    | -0.0058    |
| Z  | Contribution | $2s_{1/2}$   | $2p_{1/2}$   | $2p_{3/2}$   |
|----|--------------|--------------|--------------|--------------|
| 30 | Uehling      | -0.00278     | -0.00003     | 0.00000      |
|    | W-K          | 0.00000      | 0.00000      | 0.00000      |
|    | Screening    | 0.00010      | 0.00010      | 0.00009      |
|    | Sum          | -0.00268     | 0.00007      | 0.00009      |
| 40 | Uehling      | -0.00939     | -0.00019     | -0.00000     |
|    | W-K          | 0.00013      | 0.00001      | 0.00000      |
|    | Screening    | 0.00006      | 0.00025      | 0.00021      |
|    | Sum          | -0.00900     | 0.00006      | 0.00021      |
| 50 | Uehling      | -0.02498     | -0.00090     | -0.00008     |
|    | W-K          | 0.00050      | 0.00003      | 0.00001      |
|    | Screening    | 0.00060      | 0.00057      | 0.00044      |
|    | Sum          | -0.02388     | -0.00300     | 0.00037      |
| 60 | Uehling      | -0.05795     | -0.00327     | -0.00027     |
|    | W-K          | 0.00155      | 0.00013      | 0.00003      |
|    | Screening    | 0.00126      | 0.00119      | 0.00080      |
|    | Sum          | -0.05514     | -0.00195     | 0.00055      |
| 70 | Uehling      | -0.12395     | -0.01025     | -0.00074     |
|    | W-K          | 0.00420      | 0.00051      | 0.00093      |
|    | Screening    | 0.00252      | 0.00239      | 0.00134      |
|    | Sum          | -0.11722     | -0.00735     | 0.00070      |
| 80 | Uehling      | -0.25327     | -0.02940     | -0.00170     |
|    | W-K          | 0.01044      | 0.00174      | 0.00025      |
|    | Screening    | 0.00494      | 0.00482      | 0.00215      |
|    | Sum          | -0.23790     | -0.02284     | 0.00071      |
| 83 | Uehling      | -0.31231     | -0.03991     | -0.00213     |
|    | W-K          | 0.01356      | 0.00249      | 0.00034      |
|    | Screening    | 0.00603      | 0.00597      | 0.00246      |
|    | Sum          | -0.29271     | -0.03145     | 0.00067      |
| 90 | Uehling      | -0.50673     | -0.08045     | -0.00352     |
|    | W-K          | 0.02455      | 0.00555      | 0.00063      |
|    | Screening    | 0.00962      | 0.00996      | 0.00333      |
|    | Sum          | -0.47256     | -0.06495     | 0.00044      |
| 92 | Uehling      | -0.58176     | -0.09815     | -0.00404     |
|    | W-K          | 0.02900      | 0.00695      | 0.00075      |
|    | Screening    | 0.01101      | 0.01157      | 0.00362      |
|    | Sum          | -0.54175     | -0.07963     | 0.00033      |
| 100| Uehling      | -1.01615     | -0.21776     | -0.00677     |
|    | W-K          | 0.05627      | 0.01692      | 0.00143      |
|    | Screening    | 0.01911      | 0.02165      | 0.00500      |
|    | Sum          | -0.94078     | -0.17919     | -0.00034     |
TABLE VI: Kohn-Sham results for vacuum polarization in the sodium isoelectronic sequence: units a.u..

| Z  | Contribution | $3s_{1/2}$   | $3p_{1/2}$   | $3p_{3/2}$   |
|----|--------------|---------------|---------------|---------------|
| 30 | Uehling      | -0.00054      | -0.00000      | 0.00000       |
|    | W-K          | 0.00000       | 0.00000       | 0.00000       |
|    | Screening    | 0.00001       | 0.00004       | 0.00004       |
|    | Sum          | -0.00053      | 0.00004       | 0.00004       |
| 40 | Uehling      | -0.00206      | -0.00004      | 0.00000       |
|    | W-K          | 0.00003       | 0.00000       | 0.00000       |
|    | Screening    | 0.00014       | 0.00013       | 0.00012       |
|    | Sum          | -0.00190      | 0.00009       | 0.00012       |
| 50 | Uehling      | -0.00586      | -0.00022      | -0.00001      |
|    | W-K          | 0.00011       | 0.00001       | 0.00000       |
|    | Screening    | 0.00032       | 0.00030       | 0.00026       |
|    | Sum          | -0.00542      | 0.00008       | 0.00025       |
| 60 | Uehling      | -0.01418      | -0.00087      | -0.00006      |
|    | W-K          | 0.00038       | 0.00004       | 0.00001       |
|    | Screening    | 0.00068       | 0.00064       | 0.00052       |
|    | Sum          | -0.01312      | -0.00020      | 0.00045       |
| 70 | Uehling      | -0.03120      | -0.00284      | -0.00019      |
|    | W-K          | 0.00105       | 0.00014       | 0.00003       |
|    | Screening    | 0.00137       | 0.00131       | 0.00096       |
|    | Sum          | -0.02880      | -0.00142      | 0.00076       |
| 80 | Uehling      | -0.06505      | -0.00839      | -0.00047      |
|    | W-K          | 0.00266       | 0.00049       | 0.00008       |
|    | Screening    | 0.00268       | 0.00264       | 0.00172       |
|    | Sum          | -0.05974      | -0.00532      | 0.00124       |
| 83 | Uehling      | -0.08060      | -0.01146      | -0.00060      |
|    | W-K          | 0.00348       | 0.00071       | 0.00010       |
|    | Screening    | 0.00328       | 0.00326       | 0.00204       |
|    | Sum          | -0.07389      | -0.00757      | 0.00143       |
| 90 | Uehling      | -0.13199      | -0.02338      | -0.00103      |
|    | W-K          | 0.00634       | 0.00158       | 0.00019       |
|    | Screening    | 0.00525       | 0.00536       | 0.00302       |
|    | Sum          | -0.12048      | -0.01654      | 0.00199       |
| 92 | Uehling      | -0.15186      | -0.02858      | -0.00120      |
|    | W-K          | 0.00750       | 0.00199       | 0.00023       |
|    | Screening    | 0.00602       | 0.00620       | 0.00337       |
|    | Sum          | -0.13844      | -0.02053      | 0.00220       |
| 100| Uehling      | -0.26701      | -0.06381      | -0.00209      |
|    | W-K          | 0.01463       | 0.00484       | 0.00045       |
|    | Screening    | 0.01051       | 0.01132       | 0.00530       |
|    | Sum          | -0.24205      | -0.04785      | 0.00329       |
Kohn-Sham results for vacuum polarization in the copper isoelectronic sequence:
units a.u..

| Z  | Contribution | $4s_{1/2}$   | $4p_{1/2}$   | $4p_{3/2}$   |
|----|--------------|--------------|--------------|--------------|
| 60 | Uehling      | -0.00351     | -0.00021     | -0.00001     |
|    | W-K          | 0.00009      | 0.00000      | 0.00000      |
|    | Screening    | 0.00031      | 0.00025      | 0.00021      |
|    | Sum          | -0.00311     | 0.00004      | 0.00019      |
| 70 | Uehling      | -0.00851     | -0.00076     | -0.00005     |
|    | W-K          | 0.00029      | 0.00004      | 0.00001      |
|    | Screening    | 0.00064      | 0.00054      | 0.00041      |
|    | Sum          | -0.00758     | -0.00019     | 0.00037      |
| 80 | Uehling      | -0.01890     | -0.00243     | -0.00013     |
|    | W-K          | 0.00077      | 0.00014      | 0.00002      |
|    | Screening    | 0.00128      | 0.00113      | 0.00080      |
|    | Sum          | -0.01686     | -0.00117     | 0.00067      |
| 83 | Uehling      | -0.02377     | -0.00337     | -0.00017     |
|    | W-K          | 0.00103      | 0.00021      | 0.00003      |
|    | Screening    | 0.00157      | 0.00141      | 0.00096      |
|    | Sum          | -0.02119     | -0.00178     | 0.00079      |
| 90 | Uehling      | -0.04006     | -0.00711     | -0.00031     |
|    | W-K          | 0.00192      | 0.00048      | 0.00006      |
|    | Screening    | 0.00251      | 0.00234      | 0.00148      |
|    | Sum          | -0.03565     | -0.00433     | 0.00117      |
| 92 | Uehling      | -0.04641     | -0.00877     | -0.00037     |
|    | W-K          | 0.00229      | 0.00061      | 0.00007      |
|    | Screening    | 0.00287      | 0.00271      | 0.00167      |
|    | Sum          | -0.04128     | -0.00549     | 0.00131      |
| 100| Uehling      | -0.08348     | -0.02009     | -0.00067     |
|    | W-K          | 0.00457      | 0.00152      | 0.00015      |
|    | Screening    | 0.00495      | 0.00495      | 0.00272      |
|    | Sum          | -0.07402     | -0.01369     | 0.00209      |
TABLE VIII: Comparing Kohn-Sham (KS) with core-Hartree (CH) results for lithiumlike, sodiumlike and copperlike uranium: units eV.

| Ion  | State  | Potential | Uehling | W-K  | Screening | Sum   |
|------|--------|-----------|---------|------|-----------|-------|
| Li-like | 2s\(_{1/2}\) | KS        | -15.831 | 0.789 | 0.300     | -14.742 |
|       |        | CH        | -15.735 | 0.784 | 0.220     | -14.731 |
|       | 2p\(_{1/2}\) | KS        | -2.671  | 0.189 | 0.315     | -2.167  |
|       |        | CH        | -2.614  | 0.185 | 0.259     | -2.170  |
|       | 2p\(_{3/2}\) | KS        | -0.110  | 0.020 | 0.099     | 0.009   |
|       |        | CH        | -0.109  | 0.020 | 0.097     | 0.008   |
| Na-like | 3s\(_{1/2}\) | KS        | -4.132  | 0.204 | 0.164     | -3.764  |
|       |        | CH        | -4.078  | 0.201 | 0.109     | -3.768  |
|       | 3p\(_{1/2}\) | KS        | -0.778  | 0.054 | 0.169     | -0.555  |
|       |        | CH        | -0.755  | 0.052 | 0.141     | -0.562  |
|       | 3p\(_{3/2}\) | KS        | -0.033  | 0.006 | 0.092     | 0.065   |
|       |        | CH        | -0.025  | 0.006 | 0.085     | 0.066   |
| Cu-like | 4s\(_{1/2}\) | KS        | -1.263  | 0.063 | 0.077     | -1.123  |
|       |        | CH        | -1.232  | 0.061 | 0.044     | -1.127  |
|       | 4p\(_{1/2}\) | KS        | -0.239  | 0.017 | 0.073     | -0.149  |
|       |        | CH        | -0.229  | 0.017 | 0.061     | -0.151  |
|       | 4p\(_{3/2}\) | KS        | -0.010  | 0.002 | 0.044     | 0.036   |
|       |        | CH        | -0.010  | 0.002 | 0.043     | 0.035   |