

Vacuum polarization in a strong external field

Gerhard Soff and Peter J. Mohr

*Institute for Theoretical Physics, University of California, Santa Barbara, California 93106;
Gesellschaft für Schwerionenforschung (GSI), Planckstrasse 1, Postfach 110 552, D-6100 Darmstadt, Federal Republic of Germany;
and National Bureau of Standards, Gaithersburg, Maryland 20899*

(Received 17 March 1988)

Vacuum polarization in the field of a high- Z finite-size nucleus is examined, and the polarization charge density in coordinate space of order $\alpha(Z\alpha)^n$ with $n \geq 3$ is calculated. Energy-level shifts of K - and L -shell electrons in hydrogenlike systems are given.

I. INTRODUCTION

Vacuum polarization corrections to energy eigenvalues of bound leptons have been examined extensively in the past.¹⁻²³ For bound electrons, the dominant contribution of the quantum electrodynamic (QED) effects is the self-energy correction. Modern calculations of this correction²²⁻³³ include Feynman diagrams to all orders in the coupling constant of the external field. However, the corresponding influence of vacuum polarization effects on electron levels in atoms has not been completely calculated. The purpose of the present work is to carry out a complete calculation of the vacuum polarization of order α in order to provide improved electron binding-energy values and to investigate more closely radiative corrections for strongly bound electrons in superheavy systems. In view of the current level of interest³⁴⁻⁴¹ (see also Refs. 22 and 23, and references therein) in experimental tests of QED on K - and L -shell electrons in high- Z hydrogenlike ions, more accurate theoretical predictions are desirable. In addition, we consider the vacuum polarization charge density in a superheavy system with a critical nuclear charge number $Z_{cr}=170$, at which the energy eigenvalue of the strongest bound $1s_{1/2}$ state nearly reaches the lower continuum, i.e., $E_{1s} = -mc^2$.

The dominant vacuum polarization correction arises from the Uehling potential (Refs. 1, 2, 4, 5, 11, 12, and 21-23) which is linear in the external field and of order $\alpha(Z\alpha)$. The Uehling potential and the associated energy shift of bound electrons in the field of a finite-size nucleus can easily be calculated. We restrict the following discussion to the vacuum polarization potential of order $\alpha(Z\alpha)^n$ with $n \geq 3$.

An evaluation of the higher-order, $\alpha(Z\alpha)^n$ with $n \geq 3$, vacuum polarization charge density induced by a high- Z nucleus of finite extent has been made by Gyulassy.⁶⁻⁸ In that work, the Wichmann-Kroll nonperturbative formalism,³ based on explicit solutions of the Dirac equation in the external potential, was applied. Energy shifts for muonic lead and superheavy electronic atoms were computed. As a major approximation, only the terms with $|\kappa| = 1$ in the partial wave decomposition of the Green function were taken into account, where κ denotes the Dirac angular-momentum quantum number.

The calculations of Gyulassy⁸ were repeated by Negha-

bian²⁰ who employed the same truncation of the partial-wave decomposition of the Green function. With the aid of the Poisson equation for the vacuum polarization charge density, he derived the momentum-space expression for the vacuum polarization potential. The computed energy shifts are in excellent agreement with those of Gyulassy.

Higher-order vacuum polarization corrections have also been evaluated for the heavy muonic atom spectrum^{5,8-11,13-19} that provides an ideal testing ground for the short-range aspect of this correction. In this case, experimental data are in good agreement with theoretical results. Various approximations were made in some of these calculations, e.g., (a) the assumption of a pointlike nucleus, (b) the neglect of the electron rest mass in the determination of the Green function, (c) the restriction to radial distances much less than the electron Compton wavelength in the evaluation of the vacuum polarization potential.

For pointlike nuclei, an explicit expression for the vacuum polarization potential of order $\alpha(Z\alpha)^3$ was derived by Blomqvist.⁵ For low- Z atoms the present calculation should reproduce the results of Blomqvist.

This paper is organized as follows. In Sec. II we briefly review the theoretical basis for the vacuum polarization charge density in a strong external potential. Section III provides an analytic evaluation of the Uehling contribution. For the external potential of a homogeneously charged spherical shell, the integrand of the Uehling term can be expressed completely in analytical form for arbitrary angular momentum in the partial-wave decomposition of the free Green function. The evaluation of the Dirac Green function for the potential of a spherical shell is described in Sec. IV. Numerical results for the vacuum polarization charge density and the corresponding energy shifts of bound electrons in hydrogenlike systems with various values of Z in the range 30-100, and in the superheavy system with $Z = 170$ are summarized in Sec. V.

II. VACUUM POLARIZATION CHARGE DENSITY

From bound-state QED (Ref. 42) the energy shift corresponding to the vacuum polarization is given by ($\hbar=c=m=1$)

$$\Delta E = 4\pi i \alpha \int d(t_2 - t_1) \int d\mathbf{x}_2 \int d\mathbf{x}_1 \bar{\phi}_n(\mathbf{x}_2) \gamma^\mu \phi_n(\mathbf{x}_2) D_F(x_2 - x_1) \text{Tr}[\gamma_\mu S_F(x_1, x_1)], \quad (1)$$

where the photon propagator is

$$D_F(x_2 - x_1) = \frac{-i}{(2\pi)^4} \int d^4 k \frac{e^{-ik(x_2 - x_1)}}{k^2 + i\epsilon} \quad (2)$$

and the Feynman propagator for the electrons is

$$S_F(x_2, x_1) = \begin{cases} \sum_{n^+} \phi_n(x_2) \bar{\phi}_n(x_1), & t_2 > t_1 \\ -\sum_{n^-} \phi_n(x_2) \bar{\phi}_n(x_1), & t_2 < t_1. \end{cases} \quad (3)$$

In Eq. (3) the sum runs over positive-energy (n^+) and

negative-energy (n^-) states separately. The electron propagator may be represented by the alternative expression

$$S_F(x_2, x_1) = \frac{1}{2\pi i} \int_{C_F} dz \sum_n \frac{\phi_n(\mathbf{x}_2) \bar{\phi}_n(\mathbf{x}_1)}{E_n - z} e^{-iz(t_2 - t_1)} \\ = \frac{1}{2\pi i} \int_{C_F} dz \mathcal{G}(\mathbf{x}_2, \mathbf{x}_1, z) \gamma^0 e^{-iz(t_2 - t_1)}. \quad (4)$$

Only the term with $\mu=0$ contributes in (1), so we have for the energy shift

$$\Delta E = 4\pi i \alpha \int d(t_2 - t_1) \int d\mathbf{x}_2 \int d\mathbf{x}_1 \phi_n^\dagger(\mathbf{x}_2) \phi_n(\mathbf{x}_2) D_F(x_2 - x_1) \text{Tr}[\gamma_0 S_F(x_1, x_1)]. \quad (5)$$

The level shift can be written in terms of an effective potential as

$$\Delta E = \int d\mathbf{x}_2 \phi_n^\dagger(\mathbf{x}_2) \phi_n(\mathbf{x}_2) U(\mathbf{x}_2), \quad (6)$$

where

$$U(\mathbf{x}_2) = 4\pi i \alpha \int d(t_2 - t_1) \int d\mathbf{x}_1 D_F(x_2 - x_1) \text{Tr}[\gamma_0 S_F(x_1, x_1)] \\ = \frac{-2i\alpha}{(2\pi)^4} \int d(t_2 - t_1) \int d\mathbf{x}_1 \int d^4 k \frac{1}{k_0^2 - \mathbf{k}^2 + i\epsilon} e^{-ik_0(t_2 - t_1)} e^{i\mathbf{k} \cdot (\mathbf{x}_2 - \mathbf{x}_1)} \int_{C_F} dz \text{Tr} \mathcal{G}(\mathbf{x}_1, \mathbf{x}_1, z). \quad (7)$$

Integration over the four-vector k yields

$$U(\mathbf{x}_2) = \frac{i\alpha}{2\pi} \int d\mathbf{x}_1 \frac{1}{|\mathbf{x}_2 - \mathbf{x}_1|} \int_{C_F} dz \text{Tr} \mathcal{G}(\mathbf{x}_1, \mathbf{x}_1, z). \quad (8)$$

The corresponding vacuum polarization charge density ρ is identified by writing

$$U(\mathbf{x}_2) = -e \int d\mathbf{x}_1 \frac{\rho(\mathbf{x}_1)}{|\mathbf{x}_2 - \mathbf{x}_1|}, \quad (9)$$

so that we have

$$\rho(\mathbf{x}) = \frac{e}{2\pi i} \int_{C_F} dz \text{Tr} \mathcal{G}(\mathbf{x}, \mathbf{x}, z) \quad (10)$$

for the charge density

This is a formal expression that contains the infinite unrenormalized charge. Expansion of the total vacuum polarization in powers of the coupling constant $Z\alpha$ of the external field³ isolates the divergences in the Uehling term that is of order $\alpha(Z\alpha)$. Terms with an even number of interactions with the external field vanish. The higher-order terms [$\alpha(Z\alpha)^n$ with $n \geq 3$] are finite, but there is a spurious contribution from the term of order $\alpha(Z\alpha)^3$. A regularization procedure for the total vacuum

polarization charge density is thus to subtract the Uehling contribution which can be renormalized separately and subtract the spurious piece of the third-order term.

The Uehling term is

$$\rho^{(1)}(\mathbf{x}) = \frac{e}{2\pi i} \int_{C_F} dz \text{Tr} \mathcal{G}^{(1)}(\mathbf{x}, \mathbf{x}, z), \quad (11)$$

where

$$\mathcal{G}^{(1)}(\mathbf{x}, \mathbf{x}, z) = - \int d\mathbf{y} \mathcal{F}(\mathbf{x}, \mathbf{y}, z) V(\mathbf{y}) \mathcal{F}(\mathbf{y}, \mathbf{x}, z). \quad (12)$$

\mathcal{F} is the free Green function, which is the limit of \mathcal{G} as $Z\alpha \rightarrow 0$. The charge density that is third order in the external potential corresponds to a Feynman diagram with a free electron-positron loop with four vertices. It is well known that this diagram contains a spurious gauge noninvariant piece that must be removed in order to obtain a correct physical result. This term has been discussed by Wichmann and Kroll,³ by Gyulassy,⁸ and by Borie and Rinker¹¹ in the context of vacuum polarization. The third-order charge density is given by

$$\rho^{(3)}(\mathbf{x}) = \frac{e}{2\pi i} \int_{C_F} dz \text{Tr} \mathcal{G}^{(3)}(\mathbf{x}, \mathbf{x}, z), \quad (13)$$

where

$$\mathcal{G}^{(3)}(\mathbf{x}, \mathbf{x}, z) = - \int d\mathbf{y}_1 \int d\mathbf{y}_2 \int d\mathbf{y}_3 \mathcal{F}(\mathbf{x}, \mathbf{y}_1, z) V(\mathbf{y}_1) \mathcal{F}(\mathbf{y}_1, \mathbf{y}_2, z) V(\mathbf{y}_2) \mathcal{F}(\mathbf{y}_2, \mathbf{y}_3, z) V(\mathbf{y}_3) \mathcal{F}(\mathbf{y}_3, \mathbf{x}, z). \quad (14)$$

The gauge-invariant physical result for the vacuum polarization charge density is obtained by subtracting from the third-order term the same expression with the electron mass replaced with a large mass M , denoted $\rho_M^{(3)}(\mathbf{x})$, and taking the limit as M becomes infinite. The limit is independent of M and is given by

$$\tilde{\rho}^{(3)}(\mathbf{x}) = \lim_{M \rightarrow \infty} \rho_M^{(3)}(\mathbf{x}) = \frac{e}{2\pi i} \int_{C_F} dz \operatorname{Tr} \tilde{\mathcal{G}}^{(3)}(\mathbf{x}, \mathbf{x}, z), \quad (15)$$

where

$$\tilde{\mathcal{G}}^{(3)}(\mathbf{x}, \mathbf{x}, z) = -V^3(\mathbf{x}) \int d\mathbf{y}_1 \int d\mathbf{y}_2 \int d\mathbf{y}_3 \mathcal{F}(\mathbf{x}, \mathbf{y}_1, z) \mathcal{F}(\mathbf{y}_1, \mathbf{y}_2, z) \mathcal{F}(\mathbf{y}_2, \mathbf{y}_3, z) \mathcal{F}(\mathbf{y}_3, \mathbf{x}, z) \quad (16)$$

for an arbitrary potential V . We have

$$\tilde{\mathcal{G}}^{(3)}(\mathbf{x}, \mathbf{x}, z) = -\frac{1}{6} V^3(\mathbf{x}) \lim_{\mathbf{x}' \rightarrow \mathbf{x}} \frac{d^3}{dz^3} \mathcal{F}(\mathbf{x}, \mathbf{x}', z). \quad (17)$$

A Wick rotation of the contour C_F , together with the explicit expression for $\mathcal{F}(\mathbf{x}, \mathbf{x}', z)$, yields

$$\tilde{\rho}^{(3)}(\mathbf{x}) = -\frac{e}{3\pi^2} V^3(\mathbf{x}). \quad (18)$$

The physical higher-order charge density is thus given by

$$\rho^{(3+)}(\mathbf{x}) = \rho(\mathbf{x}) - \rho^{(1)}(\mathbf{x}) - \tilde{\rho}^{(3)}(\mathbf{x}). \quad (19)$$

Expansion of the Green function in (10) in eigenfunctions of angular momentum yields^{3,8,26,27}

$$\rho(x) = \frac{e}{2\pi i} \int_{C_F} dz \sum_{\kappa=\pm 1}^{\pm\infty} \frac{|\kappa|}{2\pi} \sum_{n=1}^2 \mathcal{G}_\kappa^{nn}(x, x, z) \quad (20)$$

for the radial vacuum polarization charge density. In Eq. (20), x denotes the radial coordinate. If we assume that there are no bound-state poles on the negative real axis

between $z = -m$ and 0 we can rotate the Feynman contour to the imaginary z axis and change the variable of integration to u , where $z = iu$, to obtain

$$\rho(x) = \frac{e}{2\pi^2} \int_0^\infty du \sum_{\kappa=\pm 1}^{\pm\infty} |\kappa| \sum_{n=1}^2 \operatorname{Re}[\mathcal{G}_\kappa^{nn}(x, x, iu)]. \quad (21)$$

The Uehling term is

$$\rho^{(1)}(x) = \frac{e}{2\pi^2} \int_0^\infty du \sum_{\kappa=\pm 1}^{\pm\infty} |\kappa| \sum_{n=1}^2 \operatorname{Re}[\mathcal{G}_\kappa^{(1)nn}(x, x, iu)], \quad (22)$$

with

$$\mathcal{G}_\kappa^{(1)nn}(x, x, iu) = -\sum_{m=1}^2 \int_0^\infty dy y^2 \mathcal{F}_\kappa^{nm}(x, y, iu) \times V(y) \mathcal{F}_\kappa^{mn}(y, x, iu), \quad (23)$$

where \mathcal{F}_κ^{nm} denotes the free radial Green function.²⁶ This leads to

$$\rho^{(1)}(x) = -\frac{e}{2\pi^2} \int_0^\infty du \sum_{\kappa=\pm 1}^{\pm\infty} |\kappa| \operatorname{Re} \left[\int_0^\infty dy y^2 \sum_{n,m=1}^2 [\mathcal{F}_\kappa^{nm}(x, y, iu)]^2 V(y) \right]. \quad (24)$$

The expansion of the spurious piece of the third-order term is given by

$$\tilde{\rho}^{(3)}(x) = -\frac{e}{12\pi^2} V^3(x) \int_0^\infty du \frac{d^3}{du^3} \sum_{\kappa=\pm 1}^{\pm\infty} |\kappa| \sum_{n=1}^2 \operatorname{Re}[i \mathcal{F}_\kappa^{nn}(x, x, iu)], \quad (25)$$

where the limit $\mathbf{x}' \rightarrow \mathbf{x}$ has been taken in the individual terms in the summation over κ . Substitution of these expressions into Eq. (19) yields an expression for the higher-order charge density $\rho^{(3+)}(x)$ in terms of summations over the angular momentum quantum number κ . In this calculation, the sums are truncated after summing terms with $|\kappa| \leq K$ in order to obtain an approximation to the higher-order charge density with the remainder denoted by R_K . If the summation over κ in the expression for $\tilde{\rho}^{(3)}(x)$ is restricted to a finite number of terms, then the contribution from these terms vanishes. This is readily seen by explicitly carrying out the integration over u in each term. We thus obtain the complete expression for the higher-order charge density as

$$\begin{aligned} \rho^{(3+)}(x) &= \rho(x) - \rho^{(1)}(x) - \tilde{\rho}^{(3)}(x) \\ &= \frac{e}{2\pi^2} \int_0^\infty du \left[\sum_{\kappa=\pm 1}^{\pm K} |\kappa| \operatorname{Re} \left[\sum_{n=1}^2 \mathcal{G}_\kappa^{nn}(x, x, iu) + \int_0^\infty dy y^2 V(y) \sum_{n,m=1}^2 [\mathcal{F}_\kappa^{nm}(x, y, iu)]^2 \right] \right] \\ &\quad + \frac{e}{2\pi} \sum_{-m < E < 0} |\kappa| [f_1^2(x) + f_2^2(x)] + R_K. \end{aligned} \quad (26)$$

This equation includes terms from any bound-state poles on the negative real z axis in (20). These terms would be picked up as residues in the rotation of the contour of integration leading to (26). Such terms only appear for superheavy systems where the binding energy of the elec-

tron exceeds the electron rest mass. In Eq. (26) $f_1(x)$ and $f_2(x)$ denote components of the radial Dirac wave function, normalized according to

$$\int_0^\infty dx x^2 [f_1^2(x) + f_2^2(x)] = 1. \quad (27)$$

III. EVALUATION OF THE UEHLING TERM

For the simple potential of a homogeneously charged spherical shell the Uehling contribution can be expressed analytically for arbitrary angular momentum. The Uehling contribution to the vacuum polarization charge density is given by

$$\rho^{(1)}(x) = \int_0^\infty du \sum_{k=1}^\infty S_k^{(1)}(x, u). \quad (28)$$

Here we define

$$S_k^{(1)}(x, u) = -\frac{e}{2\pi^2} \sum_{\kappa=\pm k} |\kappa| \operatorname{Re} \left[\int_0^\infty dy y^2 V(y) (\mathcal{F}_\kappa^{11} \mathcal{F}_\kappa^{11} + \mathcal{F}_\kappa^{12} \mathcal{F}_\kappa^{12} + \mathcal{F}_\kappa^{21} \mathcal{F}_\kappa^{21} + \mathcal{F}_\kappa^{22} \mathcal{F}_\kappa^{22}) \right]. \quad (29)$$

The quantity $S_k^{(1)}(x, u)$ may be calculated analytically as indicated in this section. For $y > x$ the components of the free Green function are²⁶

$$\begin{aligned} \mathcal{F}_\kappa^{11}(x, y, iu) &= -(iu + 1) c j_{|\kappa+1/2|-1/2}(icx) \\ &\quad \times h_{|\kappa+1/2|-1/2}^{(1)}(icy), \\ \mathcal{F}_\kappa^{12}(x, y, iu) &= -ic^2 \frac{\kappa}{|\kappa|} j_{|\kappa+1/2|-1/2}(icx) \\ &\quad \times h_{|\kappa-1/2|-1/2}^{(1)}(icy), \\ \mathcal{F}_\kappa^{21}(x, y, iu) &= -ic^2 \frac{\kappa}{|\kappa|} j_{|\kappa-1/2|-1/2}(icx) \\ &\quad \times h_{|\kappa+1/2|-1/2}^{(1)}(icy), \\ \mathcal{F}_\kappa^{22}(x, y, iu) &= -(iu - 1) c j_{|\kappa-1/2|-1/2}(icx) \\ &\quad \times h_{|\kappa-1/2|-1/2}^{(1)}(icy), \end{aligned} \quad (30)$$

with

$$c = (1 + u^2)^{1/2}. \quad (31)$$

$j_l(z)$ and $h_l^{(1)}(z)$ denote the spherical Bessel function and spherical Hankel function of the first kind, respectively. For $y < x$ we simply employ²⁶

$$\begin{aligned} \mathcal{F}_\kappa^{11}(x, y, iu) &= \mathcal{F}_\kappa^{11}(y, x, iu), \\ \mathcal{F}_\kappa^{12}(x, y, iu) &= \mathcal{F}_\kappa^{21}(y, x, iu), \\ \mathcal{F}_\kappa^{21}(x, y, iu) &= \mathcal{F}_\kappa^{12}(y, x, iu), \\ \mathcal{F}_\kappa^{22}(x, y, iu) &= \mathcal{F}_\kappa^{22}(y, x, iu). \end{aligned} \quad (32)$$

In this paper we consider the spherical-shell distribution as a model for the nuclear charge density

$$\rho_n(x) = \frac{Ze}{4\pi R^2} \delta(R - x), \quad (33)$$

where R denotes the nuclear radius. The corresponding potential is

$$V(x) = -\frac{Z\alpha}{R} \Theta(R - x) - \frac{Z\alpha}{x} \Theta(x - R). \quad (34)$$

We let $A(y)$ represent the integrand in (29) such that

$$S_k^{(1)}(x, u) = -\frac{e}{2\pi^2} \operatorname{Re} \left[\int_0^\infty A(y) dy \right], \quad (35)$$

and divide the integration domain into three parts

$$\begin{aligned} S_k^{(1)}(x, u) &= -\frac{e}{2\pi^2} \operatorname{Re} \left[\int_0^{a_1} A(y) dy + \int_{a_1}^{a_2} A(y) dy \right. \\ &\quad \left. + \int_{a_2}^\infty A(y) dy \right] \\ &= T_1 + T_2 + T_3, \end{aligned} \quad (36)$$

with

$$a_1 = \min(x, R), \quad a_2 = \max(x, R). \quad (37)$$

It is useful to define the functions

$$\begin{aligned} \mathcal{J}_{1,n}(a) &= \int_0^a y j_n^2(icy) dy, \\ \mathcal{J}_{2,n}(a) &= \int_0^a y^2 j_n^2(icy) dy, \\ \mathcal{H}_{1,n}(a) &= \int_a^\infty y h_n^{(1)2}(icy) dy, \\ \mathcal{H}_{2,n}(a) &= \int_a^\infty y^2 h_n^{(1)2}(icy) dy. \end{aligned} \quad (38)$$

With $l = |\kappa|$, we have

$$T_1 = \frac{e}{\pi^2} \frac{Z\alpha}{R} l \{ (1 - u^2) c^2 [h_l^{(1)2}(icx) \mathcal{J}_{2,l}(a_1) + h_m^{(1)2}(icx) \mathcal{J}_{2,m}(a_1)] - c^4 [h_m^{(1)2}(icx) \mathcal{J}_{2,l}(a_1) + h_l^{(1)2}(icx) \mathcal{J}_{2,m}(a_1)] \}, \quad (39)$$

with

$$m = l - 1. \quad (40)$$

For T_3 we have

$$T_3 = \frac{e}{\pi^2} Z\alpha l \{ (1 - u^2) c^2 [j_l^2(icx) \mathcal{H}_{1,l}(a_2) + j_m^2(icx) \mathcal{H}_{1,m}(a_2)] - c^4 [j_l^2(icx) \mathcal{H}_{1,m}(a_2) + j_m^2(icx) \mathcal{H}_{1,l}(a_2)] \}. \quad (41)$$

For the determination of T_2 we have to distinguish the two cases $x > R$ and $x \leq R$. In the first case ($x > R$) the expression reads

$$T_2 = \frac{e}{\pi^2} Z \alpha l \{ (1-u^2)c^2 \{ h_l^{(1)2}(icx) [\mathcal{J}_{1,l}(a_2) - \mathcal{J}_{1,l}(a_1)] + h_m^{(1)2}(icx) [\mathcal{J}_{1,m}(a_2) - \mathcal{J}_{1,m}(a_1)] \} - c^4 \{ h_m^{(1)2}(icx) [\mathcal{J}_{1,l}(a_2) - \mathcal{J}_{1,l}(a_1)] + h_l^{(1)2}(icx) [\mathcal{J}_{1,m}(a_2) - \mathcal{J}_{1,m}(a_1)] \} \} , \tag{42}$$

while in the second case ($x \leq R$) it yields

$$T_2 = \frac{e}{\pi^2} \frac{Z \alpha}{R} l \{ (1-u^2)c^2 \{ j_l^2(icx) [\mathcal{H}_{2,l}(a_1) - \mathcal{H}_{2,l}(a_2)] + j_m^2(icx) [\mathcal{H}_{2,m}(a_1) - \mathcal{H}_{2,m}(a_2)] \} - c^4 \{ j_l^2(icx) [\mathcal{H}_{2,m}(a_1) - \mathcal{H}_{2,m}(a_2)] + j_m^2(icx) [\mathcal{H}_{2,l}(a_1) - \mathcal{H}_{2,l}(a_2)] \} \} . \tag{43}$$

The remaining task is to evaluate the integrals $\mathcal{J}_{1,n}(a)$, $\mathcal{J}_{2,n}(a)$, $\mathcal{H}_{1,n}(a)$, and $\mathcal{H}_{2,n}(a)$. For this purpose we employ the relationships⁴³

$$j_n^2(icy) = (-1)^n \frac{\pi}{2cy} I_{n+1/2}^2(cy) , \tag{44}$$

$$h_n^{(1)2}(icy) = (-1)^n \frac{2}{\pi cy} K_{n+1/2}^2(cy) , \tag{45}$$

where $I_\nu(z)$ and $K_\nu(z)$ denote modified Bessel functions. The functions $\mathcal{J}_{2,n}(a)$ and $\mathcal{H}_{2,n}(a)$ are readily determined^{44,45}

$$\mathcal{J}_{2,n}(a) = (-1)^n \frac{\pi}{4c} a^2 [I_{n+1/2}^2(ca) - I_{n-1/2}(ca) I_{n+3/2}(ca)] , \tag{46}$$

$$\mathcal{H}_{2,n}(a) = (-1)^{n+1} \frac{1}{\pi c} a^2 [K_{n+1/2}^2(ca) - K_{n-1/2}(ca) K_{n+3/2}(ca)] . \tag{47}$$

For the special case $n=0$ we employ⁴³ $K_{1/2}(z) = K_{-1/2}(z)$ as well as the explicit representation

$$\mathcal{J}_{2,0}(a) = \frac{1}{2c^3} [\sinh(ca) \cosh(ca) - ca] . \tag{48}$$

For the computation of $\mathcal{H}_{1,n}(a)$ we utilize the series representation⁴³

$$h_n^{(1)2}(icy) = (-1)^n 4e^{-2cy} \left[\sum_{k=0}^n (n + \frac{1}{2}, k) (2cy)^{-k-1} \right]^2 , \tag{49}$$

with Hankel's symbol

$$(n, k) = \frac{\Gamma(\frac{1}{2} + n + k)}{k! \Gamma(\frac{1}{2} + n - k)} . \tag{50}$$

With⁴³

$$\int_a^\infty \frac{e^{-y}}{y^n} dy = \frac{E_n(a)}{a^{n-1}} , \tag{51}$$

where $E_n(z)$ denotes the exponential integral, $H_{1,n}(a)$ is easily determined by a termwise integration. The remaining quantity $\mathcal{J}_{1,n}(a)$ may be evaluated applying a similar procedure. Again we start from a series representation⁴⁴

$$I_{n+1/2}(cy) = \frac{1}{\sqrt{2\pi cy}} \left[e^{cy} \sum_{s=0}^n \frac{(-1)^s (n+s)!}{s!(n-s)!(2cy)^s} + (-1)^{n+1} e^{-cy} \sum_{s=0}^n \frac{(n+s)!}{s!(n-s)!(2cy)^s} \right] . \tag{52}$$

Substitution of this series into the expression for $\mathcal{J}_{1,n}(a_2) - \mathcal{J}_{1,n}(a_1)$ leads to a finite sum of integrals. For ca_1 not too small, the integrals are numerically evaluated by means of the asymptotic expansion generated by repeated integration by parts

$$\begin{aligned} \int_{a_1}^{a_2} \frac{ce^{cy}}{(cy)^n} dy &= \frac{e^{cy}}{(cy)^n} \Big|_{a_1}^{a_2} + n \int_{a_1}^{a_2} \frac{ce^{cy}}{(cy)^{n+1}} dy \\ &= e^{cy} \left[\sum_{m=n}^{M-1} \frac{(m-1)!}{(n-1)!} \frac{1}{(cy)^m} \Big|_{a_1}^{a_2} + O((ca_1)^{-M}) \right] . \end{aligned} \tag{53}$$

However, for small arguments ca_2 and ca_1 it is more efficient to start from the Taylor expansion⁴⁶ of the modified Bessel function

$$I_{n+1/2}(cy) = \sum_{s=0}^\infty \frac{1}{s! \Gamma(s+n+3/2)} \left(\frac{cy}{2} \right)^{2s+n+1/2} , \tag{54}$$

which leads to

$$\mathcal{J}_{1,n}(a_2) - \mathcal{J}_{1,n}(a_1) = (-1)^n \frac{\pi}{2c} \int_{a_1}^{a_2} \left[\frac{cy}{2} \right]^{2n+1} \left[\sum_{s=0}^{\infty} \frac{1}{s! \Gamma(s+n+3/2)} \left[\frac{cy}{2} \right]^{2s} \right]^2 dy. \quad (55)$$

A termwise integration completes the determination of the Uehling term.

IV. DETERMINATION OF THE DIRAC GREEN FUNCTION

According to Wichmann and Kroll³ the radial Green function may be represented by solutions of the radial Dirac equation. For $y > x$ we have

$$\begin{aligned} \mathcal{G}_{\kappa}^{11}(x, y, z) &= g_o(x)g_i(y)/W, \\ \mathcal{G}_{\kappa}^{12}(x, y, z) &= g_o(x)f_i(y)/W, \\ \mathcal{G}_{\kappa}^{21}(x, y, z) &= f_o(x)g_i(y)/W, \\ \mathcal{G}_{\kappa}^{22}(x, y, z) &= f_o(x)f_i(y)/W, \end{aligned} \quad (56)$$

and for $x > y$

$$\begin{aligned} \mathcal{M}_1 &= \frac{1+z}{r^{3/2}} \left[(s-\nu)M_{\nu-1/2,s}(2cr) - \left[\kappa - \frac{\gamma}{c} \right] M_{\nu+1/2,s}(2cr) \right], \\ \mathcal{M}_2 &= \frac{c}{r^{3/2}} \left[(s-\nu)M_{\nu-1/2,s}(2cr) + \left[\kappa - \frac{\gamma}{c} \right] M_{\nu+1/2,s}(2cr) \right], \\ \mathcal{W}_1 &= \frac{1+z}{r^{3/2}} \left[\left[\kappa + \frac{\gamma}{c} \right] W_{\nu-1/2,s}(2cr) + W_{\nu+1/2,s}(2cr) \right], \\ \mathcal{W}_2 &= \frac{c}{r^{3/2}} \left[\left[\kappa + \frac{\gamma}{c} \right] W_{\nu-1/2,s}(2cr) - W_{\nu+1/2,s}(2cr) \right], \\ u_1 &= (1+z')j_{|\kappa+1/2|-1/2}(ic'r), \\ u_2 &= ic' \frac{\kappa}{|\kappa|} j_{|\kappa-1/2|-1/2}(ic'r), \\ v_1 &= -c'h_{|\kappa+1/2|-1/2}^{(1)}(ic'r), \\ v_2 &= i(z'-1) \frac{\kappa}{|\kappa|} h_{|\kappa-1/2|-1/2}^{(1)}(ic'r), \end{aligned} \quad (59)$$

with the abbreviations

$$\begin{aligned} \gamma &= Z\alpha, \\ s &= (\kappa^2 - \gamma^2)^{1/2}, \\ c &= (1-z^2)^{1/2}, \quad \text{Re}(c) \geq 0, \\ \nu &= \gamma z / c, \\ z' &= z + \gamma / R, \\ c' &= (1-z'^2)^{1/2}, \quad \text{Re}(c') \geq 0. \end{aligned} \quad (60)$$

$M_{\alpha,\beta}(z)$ and $W_{\alpha,\beta}(z)$ denote the Whittaker functions⁴³

$$\begin{aligned} \mathcal{G}_{\kappa}^{11}(x, y, z) &= g_i(x)g_o(y)/W, \\ \mathcal{G}_{\kappa}^{12}(x, y, z) &= g_i(x)f_o(y)/W, \\ \mathcal{G}_{\kappa}^{21}(x, y, z) &= f_i(x)g_o(y)/W, \\ \mathcal{G}_{\kappa}^{22}(x, y, z) &= f_i(x)f_o(y)/W, \end{aligned} \quad (57)$$

where f and g are the components of the solutions of the radial Dirac equation with the spherically symmetric Coulomb potential, and the subscripts o and i label the solutions regular at the origin and infinity, respectively. W denotes the Wronskian, which is independent of the radial coordinate r

$$W = [f_o(r)g_i(r) - g_o(r)f_i(r)]r^2. \quad (58)$$

For the potential of a homogeneously charged spherical shell, the Green function may also be expressed analytically.⁸ For the sake of completeness we summarize here the essential results. First we define the functions

that are regular at the origin and at infinity, respectively. They are computed according to the prescriptions in Refs. 27 and 43. $j_n(z)$ and $h_n^{(1)}(z)$ are the spherical Bessel function and Hankel function of the first kind, respectively. With these definitions we express the radial functions in Eqs. (56) and (57) as

$$\begin{aligned} g_o(r) &= \Theta(R-r)u_1 + \Theta(r-R)(a\mathcal{M}_1 + b\mathcal{W}_1), \\ f_o(r) &= \Theta(R-r)u_2 + \Theta(r-R)(a\mathcal{M}_2 + b\mathcal{W}_2), \\ g_i(r) &= \Theta(R-r)(cu_1 + dv_1) + \Theta(r-R)\mathcal{W}_1, \\ f_i(r) &= \Theta(R-r)(cu_2 + dv_2) + \Theta(r-R)\mathcal{W}_2. \end{aligned} \quad (61)$$

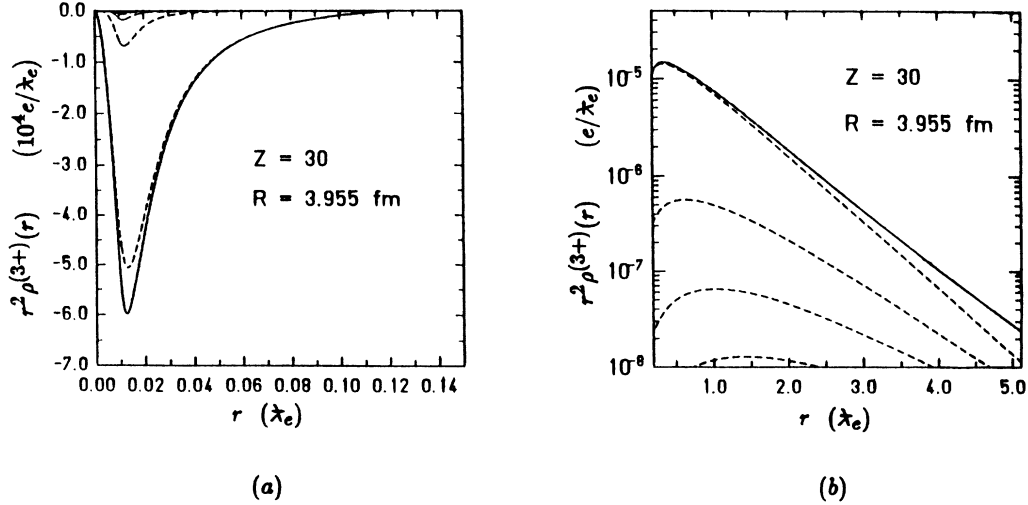


FIG. 1. Higher-order vacuum polarization density $r^2\rho^{(3+)}(r)$ and the individual radial components $r^2\rho_k(r)$ for the system with $Z = 30$ and a nuclear radius of $R = 3.955$ fm plotted as a function of the radial coordinate r . The total density is shown as a solid line, and the individual components are shown as dashed lines where the largest magnitude contribution corresponds to $k = 1$ and the successively smaller magnitude contributions correspond to increasing values of k . In (a) the charge density is negative and a linear scale is employed. In (b) the charge density is positive and a logarithmic scale is employed.

The coefficients $a, b, c,$ and d follow from the condition of continuity at $r = R$:

$$\begin{aligned} a &= (u_2\mathcal{W}_1 - u_1\mathcal{W}_2)/w, \\ b &= (\mathcal{M}_2u_1 - \mathcal{M}_1u_2)/w, \\ c &= (\mathcal{W}_2v_1 - \mathcal{W}_1v_2)/w', \\ d &= (u_2\mathcal{W}_1 - u_1\mathcal{W}_2)/w', \end{aligned} \tag{62}$$

with

$$w = \mathcal{M}_2\mathcal{W}_1 - \mathcal{M}_1\mathcal{W}_2 = 4(1+z) \frac{c^2}{R^2} \frac{\Gamma(2s+1)}{\Gamma(s-\nu)}, \tag{63}$$

$$w' = u_2v_1 - u_1v_2 = R^{-2}. \tag{64}$$

The functions in (62) are evaluated at $r = R$. The Wronskian (58) is given at $r = R$ by

$$W(z) = R^2(u_2\mathcal{W}_1 - u_1\mathcal{W}_2). \tag{65}$$

We checked the Green-function components (56)-(57) for $x = y = r$. A comparison of the Green function determined by the above equations to the Green function determined numerically by solving the radial Dirac equation gives an agreement to at least ten decimal places. In the numerical evaluation of the analytic expressions for the Green function it is convenient to isolate all exponen-

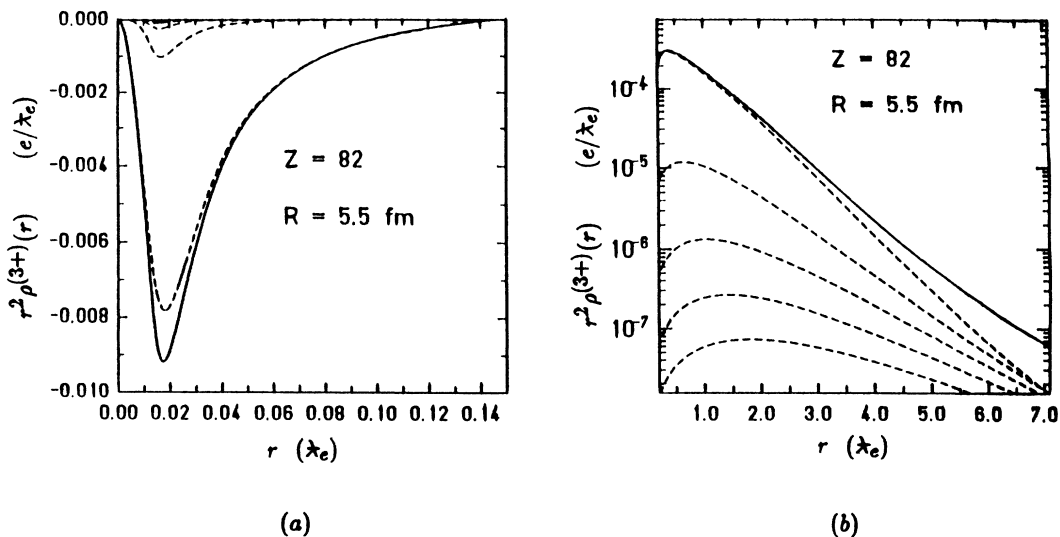


FIG. 2. The same as in Fig. 1 for $Z = 82$ with a nuclear radius $R = 5.5$ fm.

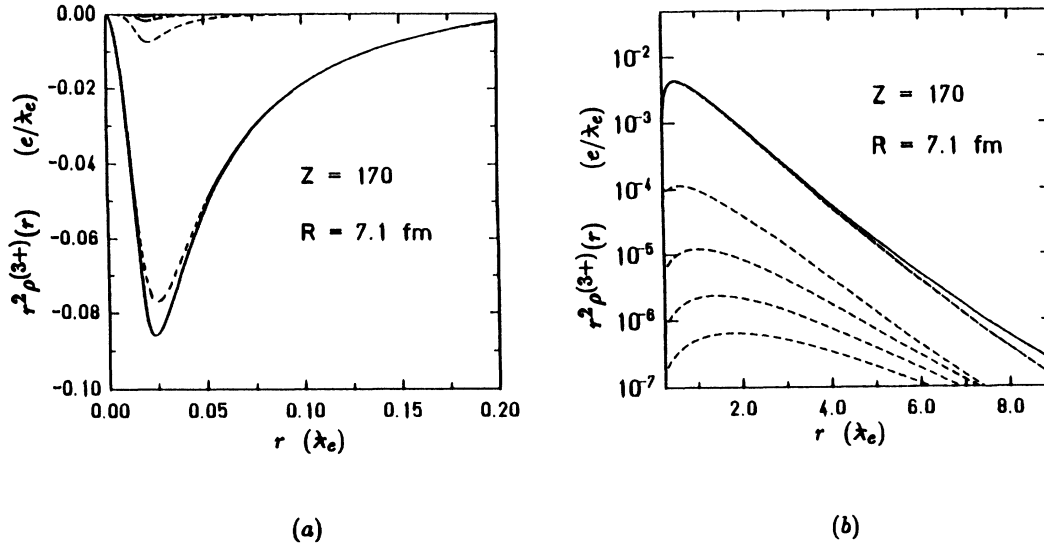


FIG. 3. The same as in Fig. 1 for the almost critical system $Z = 170$ with a nuclear radius $R = 7.1$ fm.

tial factors and treat them separately. In particular, the relationship⁴³

$$j_n(iz) = \left(\frac{iz}{2} \right)^n \frac{\sqrt{\pi}}{2\Gamma(\frac{3}{2} + n)} e^z {}_1F_1(n+1, 2n+2; -2z) \quad (66)$$

is useful for this purpose.

V. NUMERICAL EVALUATION OF THE VACUUM POLARIZATION CHARGE DENSITY AND CONCLUSION

We write the higher-order vacuum polarization charge density as

$$\rho^{(3+)}(r) = \sum_{k=1}^K \rho_k(r) + R_K, \quad (67)$$

where

$$\rho_k(r) = \int_0^\infty du S_k(r, u). \quad (68)$$

The function $S_k(r, u)$ is the integrand of the integral over u in (26) summed over $\kappa = \pm k$. For the nuclear charge number $Z = 170$ the energy eigenvalue of the $1s_{1/2}$, as well as of the $2p_{1/2}$ state are below $E = 0$. The corresponding radial bound-state wave functions $f_1(r)$ and $f_2(r)$ in (26) are easily determined with the methods described in Ref. 47.

The integrand $S_k(r, u)$ was evaluated numerically by the techniques described in the preceding sections. For $ru \gg 1$ we found numerically that

$$S_k(r, u) \simeq a(r)u^{-b}, \quad (69)$$

TABLE I. Wichmann-Kroll contributions to the Lamb shift of K - and L -shell electrons in various hydrogenlike systems. For the nuclear charge distribution we assumed a spherical shell with a radius R .

System	R (fm)	$H_{3+}(Z\alpha)$			
		$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
^{30}Zn	3.955	0.0020	0.0020	0.0000	0.0000
^{36}Kr	4.230	0.0027	0.0028	0.0001	0.0000
^{40}Zr	4.273	0.0033	0.0035	0.0001	0.0000
^{45}Rh	4.502	0.0041	0.0044	0.0002	0.0001
^{50}Sn	4.655	0.0051	0.0054	0.0003	0.0001
^{54}Xe	4.826	0.0059	0.0064	0.0004	0.0001
^{60}Nd	4.915	0.0073	0.0081	0.0007	0.0002
^{64}Gd	5.089	0.0084	0.0094	0.0010	0.0002
^{70}Yb	5.237	0.0102	0.0118	0.0015	0.0003
^{74}W	5.359	0.0116	0.0137	0.0020	0.0003
^{79}Au	5.437	0.0136	0.0166	0.0028	0.0004
^{82}Pb	5.500	0.0150	0.0185	0.0035	0.0005
^{86}Rn	5.632	0.0170	0.0216	0.0045	0.0006
^{92}U	5.751	0.0207	0.0272	0.0068	0.0007
^{96}Cm	5.816	0.0236	0.0320	0.0089	0.0009
^{100}Fm	5.886	0.0269	0.0377	0.0118	0.0010
$Z = 170$	7.100	0.518	0.764	3.75	0.017

with $b \approx 5$. Thus the integral over u converges rapidly as a function of an upper cutoff u_m . This integral was evaluated by Gaussian quadrature⁴³ with two numbers of grid points, which provides a reliable error control. For $k = 1$ the limit on the error was 10^{-6} . The integration over u was extended to a limit u_m that was large enough that $S_k(r, u)$ approached its asymptotic form for $u \approx u_m$. The remainder from the region u_m to infinity was estimated by evaluating the asymptotic form of $S_k(r, u)$ analytically. To check the accuracy of the resulting value for $\rho_k(r)$, we recalculated the numerical integration with an upper limit $2u_m$. If the two values for $\rho_1(r)$ agreed within a relative error of 10^{-5} , we accepted the value; otherwise, the numerical integration was continued to larger u_m .

An additional accuracy test of the computed vacuum polarization charge density follows from the requirement that for each value of k the total induced vacuum polarization charge should vanish,

$$Q_k = 4\pi \int_0^\infty dr r^2 \rho_k(r) = 0. \quad (70)$$

As a typical example, for lead ($Z = 82$, $R = 5.5$ fm) we found by Gaussian quadrature $Q_1 \approx -3 \times 10^{-8}e$, which should be compared with the total induced negative charge $Q_1^- \approx -4 \times 10^{-3}e$. Of course, we have $Q_k^- + Q_k^+ = Q_k$. The sum over the angular momentum components yields the total vacuum polarization charge density of order $\alpha(Z\alpha)^n$ with $n \geq 3$. The comparison of the total induced positive and negative charge provides a reliable error estimate. The relative accuracies Δ that were achieved amount to $\Delta = 4 \times 10^{-5}$, 3×10^{-6} , and 1.5×10^{-6} for $Z = 30, 82$, and 170 , respectively.

The computed vacuum polarization charge density is shown in Figs. 1–3 for $Z = 30, 82$, and 170 . The nuclear radii are indicated, and the various contributions for $k = 1–5$ are shown separately. Part (a) shows $r^2\rho_k(r)$ on a linear scale in the range where the charge density is negative. The large distance behavior of $r^2\rho_k(r)$ is shown in Figs. 1–3(b) on a logarithmic scale. Here the radial charge density is positive and decreases rapidly as the radial coordinate increases. The contribution to the vacuum polarization charge density from $k = 1$ dominates by about an order of magnitude. A rapid convergence in the summation over k is evident. For large distances ($2 \leq r \leq 7$), $r^2\rho_k(r)$ decreases with different rates for the various k components. In the asymptotic region ($r \rightarrow \infty$) the high- k components become increasingly important.

Figure 3 shows the results for the almost critical system $Z = 170$ with an assumed nuclear radius of $R = 7.1$ fm. The binding energies of the most strongly bound electron states are $E_{1s} = -1020.895$ keV and $E_{2p_{1/2}} = -569.837$ keV, respectively. Again the $k = 1$ contribution dominates completely. In summary, we remark that the approximation in Refs. 8 and 20, in which only the term with $k = 1$ in the calculation of the vacuum polarization charge density was considered, is justified.

To determine the vacuum polarization potential from the charge density, we employ the Poisson equation, which yields

$$U(r) = -4\pi\alpha \left[\frac{1}{r} \int_0^r \rho(r') r'^2 dr' + \int_r^\infty \rho(r') r' dr' \right]. \quad (71)$$

In the range $0 \leq r \leq 500R$ the vacuum polarization charge density was computed at 152 grid points. Next we performed a B -spline interpolation⁴⁸ of $r^2\rho^{(3+)}(r)$ using two different orders of the B spline to monitor the accuracy of the interpolation. For $r > 500R$ the total radial densities $r^2\rho^{(3+)}(r)$ were assumed to decrease as an inverse power of r . In the angular momentum summation, we included all terms up to $k = 5$. Due to rather strong cancellations between the various terms in Eq. (26) higher angular momentum components were not incorporated in the present treatment. To do so would require a relative accuracy of better than 10^{-12} in the numerical evaluation of the Green function and the Uehling term. The energy shift in bound-state electron follows from

$$\Delta E = \int_0^\infty [f_1^2(r) + f_2^2(r)] U(r) r^2 dr. \quad (72)$$

The vacuum polarization potential as well as the corresponding energy shifts were computed by Gaussian quadrature.

The effect of the higher-order vacuum polarization on a K -shell electron in lead ($Z = 82$) amounts to $\Delta E_{1s} \approx 2.3$ eV, whereas for the superheavy system $Z = 170$, we found $\Delta E_{1s} \approx 1.46$ keV. The corresponding numbers for the $2s$ and the $2p_{1/2}$ states are $\Delta E_{2s}(Z = 82) \approx 0.35$ eV, $\Delta E_{2p_{1/2}}(Z = 82) \approx 0.07$ eV and $\Delta E_{2s}(Z = 170) \approx 0.269$ keV, $\Delta E_{2p_{1/2}}(Z = 170) \approx 1.32$ keV, respectively. The numbers for lead are in fair agreement with earlier calculations in Ref. 23 in which the vacuum polarization of order $\alpha(Z\alpha)^3$ was computed for pointlike nuclei and additionally the contributions of order $\alpha(Z\alpha)^5$ and $\alpha(Z\alpha)^7$ were estimated. For fermium we get a noticeable energy shift of about 9 eV for the K_α line.

The energy shifts of K - and L -shell electrons in various hydrogen systems due to the vacuum polarization of order $\alpha(Z\alpha)^n$ with $n \geq 3$ may be deduced from Table I. The energy correction ΔE is expressed in terms of the function $H_{3+}(Z\alpha)$ with

$$\Delta E = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n^3} H_{3+}(Z\alpha) mc^2, \quad (73)$$

where n denotes the principle quantum number of the electron state. In Table I we give the dimensionless quantities $H_{3+}(Z\alpha)$ corresponding to the level shifts from $\rho^{(3+)}(r)$. The uncertainty is expected to be smaller than 1 in the last figure quoted.

In conclusion, we have computed the vacuum polarization charge density of order $\alpha(Z\alpha)^n$ with $n \geq 3$ for various hydrogenlike systems of known elements as well as for the nearly critical system $Z = 170$. Employing this computer code, more accurate numbers for the electron Lamb-shift effects in hydrogenlike atoms can be provided. In addition, we remark that the higher-order vacuum polarization correction, which is repulsive, does not appear to prevent the diving of the $1s_{1/2}$ state into the negative-energy continuum for nuclear charge numbers $Z \gtrsim 170$.

ACKNOWLEDGMENTS

G. S. is grateful for helpful suggestions and support by Professor W. Greiner, Professor P. Kienle, and Dr. Y.-K.

Kim. This research was supported in part by the National Science Foundation under Grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration.

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