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Calculation of the Lamb shift in neutral alkali metals

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The one-loop Lamb shift is calculated for the ground state of the neutral alkali metals lithium through francium. The method used is Furry representation QED, defined in terms of a variety of local potentials. The method is exact in binding corrections, but is potential dependent. Significant differences with known Lamb shift results for lithium are found, and it is shown that large corrections result from a partial set of screening corrections. Comparison with other calculations is made.

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I. INTRODUCTION

The problem of how to evaluate energy shifts from radiative corrections in neutral atoms is usually overshadowed by the fact that the precision available from modern many-body methods [1] has not yet reached the level of these small corrections. The exceptions are hydrogen, helium, and lithium, where the wave functions are either known analytically or else have been determined with high accuracy with variational methods. However, variational methods rapidly become difficult to apply as one treats atoms further up the Periodic Table. As progress is made in the accurate solution of the Schrödinger equation, and the part per million level is reached, discrepancies with measured energies attributable to radiative corrections will begin to appear, and methods to accurately calculate the Lamb shift in heavier neutral atoms will have to be developed.

There has been considerable progress recently in the related problem of calculating the spectra of highly charged ions [2,3]. Here the structure problem is made tractable by the rapid convergence of the 1/Z expansion, and in addition the radiative corrections are enhanced by a factor of Z^4, so the accurate evaluation of these corrections is essential to understanding the spectra. In a recent paper [2] we have shown that the inclusion of a set of one- and two-photon diagrams allows a solution of the problem for lithiumlike bismuth so accurate that even the two-loop Lamb shift [4] can be discerned.

While the rapid convergence of the perturbation series for highly charged ions is not present for neutral systems, it is known that the properties of alkali metals can be calculated with better than 10% precision in low-order many-body perturbation theory (MBPT) [5]. While this is not adequate for binding energies, which require all-orders methods such as coupled cluster or configuration interaction (CI) [1], a 10% calculation of the Lamb shift *is* adequate for this already very small effect in heavy atoms. We do not, however, claim this accuracy for the calculations presented here, which, with the exception of lithium, are lowest-order results. We will discuss the prospects for obtaining higher accuracy through a combination of MBPT and quantum electrodynamics (QED) in the final section.

In the hydrogenic case, the one-loop Lamb shift of a state v with principal quantum number n can be written in terms of two functions of $Z\alpha$, one accounting for self-energy,

$$\Delta E_v(\mathrm{SE}) = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}F_v(Z\alpha)m_ec^2, \tag{1}$$

and the other for vacuum polarization,

$$\Delta E_v(\mathrm{VP}) = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}H_v(Z\alpha)m_ec^2. \tag{2}$$

We will follow this notation in the nonhydrogenic cases considered here, and tabulate the functions F and H for the valence shell states $ns_{1/2}$, $n=2$–7 for the neutral alkali metals. No expansions in $Z\alpha$ will be made, but the results will depend on the local potential. In the following, natural units with $\hbar=c=1$ will be used.

II. CHOICE OF POTENTIALS

In this paper we use five local potentials, defined in terms of the charge density of the valence state,

$$\rho_v(r) = g_v^2(r) + f_v^2(r) \tag{3}$$

and the charge density of the core,

$$\rho_c(r) = \sum_a (2j_a+1)[g_a^2(r) + f_a^2(r)]. \tag{4}$$

Here $g(r)$ and $f(r)$ are the upper and lower components of Dirac wave functions, determined self-consistently in the local potential $U(r)$, which is in turn defined in terms of an effective charge $Z_{eff}(r)$ through

$$U(r) = -\frac{Z_{eff}(r)\alpha}{r}. \tag{5}$$

The core-Hartree potential used here has an effective charge defined through

TABLE I. Valence removal energies in atomic units of the alkali metals in different potentials.

Atom	Expt.	CH	$x_\alpha=0$	$x_\alpha=1/3$	$x_\alpha=2/3$	$x_\alpha=1$
Li $2s_{1/2}$	−0.198 14	−0.183 097	−0.177 895	−0.185 737	−0.193 504	−0.201 951
Na $3s_{1/2}$	−0.188 86	−0.173 341	−0.167 970	−0.172 243	−0.178 764	−0.189 192
K $4s_{1/2}$	−0.159 52	−0.139 522	−0.133 925	−0.137 752	−0.144 032	−0.154 929
Rb $5s_{1/2}$	−0.153 51	−0.131 786	−0.125 609	−0.129 382	−0.135 854	−0.147 618
Cs $6s_{1/2}$	−0.143 10	−0.120 056	−0.113 986	−0.117 668	−0.124 015	−0.135 835
Fr $7s_{1/2}$	−0.149 67	−0.122 284	−0.114 174	−0.118 154	−0.125 431	−0.139 670

$$Z_{eff}^{CH}(r)=Z_{nuc}(r)-r\int dr'\frac{1}{r_>}\rho_c(r'), \tag{6}$$

and the other potentials have the effective charge, derived from local density theory [6],

$$Z_{eff}^{LD}(r)=Z_{nuc}(r)-r\int dr'\frac{1}{r_>}\rho_t(r') + x_\alpha\left[\frac{81}{32\pi^2}r\rho_t(r)\right]^{1/3}, \tag{7}$$

where $\rho_t(r)=\rho_v(r)+\rho_c(r)$ is the total charge density. We will use effective potentials with $x_\alpha=0$, 1/3, 2/3 and 1. In particular, $x_\alpha=0$ is the Dirac-Hartree (DH) potential, $x_\alpha=2/3$ is the Kohn-Sham (KS) potential, and $x_\alpha=1$ is the Dirac-Slater (DS) potential.

The physically natural large r limit $Z_{eff}(r)\to 1$ is built into the definition of the core-Hartree potential, but has to be enforced for the other four x_α potentials using the Latter correction [7]. It has been our experience that an optimal choice is the Kohn-Sham potential with $x_\alpha=2/3$ [8], but that the core-Hartree potential is also favored because it can be shown that it accounts exactly for the screening of valence electron radiative corrections when exchange diagrams are neglected [9]. None of them, however, account for the important effect of the valence electron on radiative corrections in the core, which will be treated in Sec. V. In Table I we collect the valence removal energies for the alkali metals considered here for the five potentials, along with the experimental values.

III. VACUUM POLARIZATION

For neutral atoms the effect of vacuum polarization is dominated by the Uehling potential,

$$\Delta E_v(VP)=\int d^3r\,\overline{\psi}_v(\vec r)\gamma_0 U_{\rm Ueh}(r)\psi_v(\vec r), \tag{8}$$

where

$$U_{\rm Ueh}(r)=\frac{\alpha^2}{4\pi^2}\int_0^1 dy\frac{y^2(1-y^2/3)}{1-y^2}\times\int d^3x\frac{e^{-2m|\vec x-\vec r|/\sqrt{1-y^2}}}{|x-\vec r|}\nabla_x^2\left[\frac{Z_{eff}(x)}{x}\right]. \tag{9}$$

When $Z_{eff}(x)$ is spherically symmetric, this simplifies, after a change of variable, to

$$U_{\rm Ueh}(r)=\frac{\alpha^2}{12\pi m r}\int_0^1 dz\sqrt{1-z^2}(2+z^2)\times\left\{\int_0^r dx Z_{eff}''(x)\left[e^{-2m(r-x)/z}-e^{-2m(r+x)/z}\right]+\int_r^\infty dx Z_{eff}''(x)\left[e^{-2m(x-r)/z}-e^{-2m(r+x)/z}\right]\right\}. \tag{10}$$

Series expansions tabulated by Fullerton and Rinker [10] allow the accurate evaluation of the Uehling potential. We note that for light atoms where the Uehling potential acts very much like a δ function, a very fine radial grid is needed. In Table II we present vacuum polarization results for the various alkali metals for the five potentials chosen for this paper.

It is of interest at this point to compare our results for lithium with the much more accurate approach available for nonrelativistic atoms with known wave functions. If one makes the approximation of neglecting binding corrections of order $Z\alpha$, the Lamb shift can be represented as the expec-

TABLE II. The vacuum-polarization function $H(Z\alpha)$ for the alkali metals in different potentials.

Atom	CH	$x_\alpha=0$	$x_\alpha=1/3$	$x_\alpha=2/3$	$x_\alpha=1$
Li $2s_{1/2}$	−0.050 443	−0.053 423	−0.050 598	−0.048 959	−0.051 143
Na $3s_{1/2}$	−0.010 265	−0.009 129	−0.008 996	−0.009 800	−0.011 973
K $4s_{1/2}$	−0.005 846	−0.004 918	−0.004 923	−0.005 622	−0.007 435
Rb $5s_{1/2}$	−0.002 817	−0.002 249	−0.002 328	−0.002 786	−0.003 890
Cs $6s_{1/2}$	−0.002 144	−0.001 675	−0.001 752	−0.002 152	−0.003 118
Fr $7s_{1/2}$	−0.002 194	−0.001 556	−0.001 716	−0.002 240	−0.003 422

tation value of a relatively simple operator. As mentioned above, the Uehling potential is proportional to a kind of representation of a δ function, specifically

$$\delta^3(r)=\frac{15m^2}{4\pi r}\int_0^1 dy\frac{y^2(1-y^2/3)}{1-y^2}e^{-2mr/\sqrt{1-y^2}}, \tag{11}$$

in terms of which the associated energy shift is the expectation value of the operator

$$\Sigma_{VP}=-\frac{4Z\alpha^2}{15m^2}\sum_{i=1}^{3}\delta^3(r_i), \tag{12}$$

with $Z=3$. The expectation value of the δ functions is known with high accuracy for the ground state of lithium [11,12],

$$\langle\delta^3(r_1)+\delta^3(r_2)+\delta^3(r_3)\rangle_{2s_{1/2}}=13.842\ \ 609(m\alpha)^3. \tag{13}$$

To get ionization energies, we subtract from the above the analogous term for Li$^+$,

$$\langle\delta^3(r_1)+\delta^3(r_2)\rangle=13.702\,935(m\alpha)^3, \tag{14}$$

to get the variational value for vacuum polarization in neutral lithium of

$$H(Z\alpha)_{Z=3}=-0.034\,671. \tag{15}$$

Comparison with the lithium results in Table II shows that the lowest-order approach significantly overstates the magnitude of vacuum polarization. This is primarily due to the approximate character of the wave function, although we note that even if exact wave functions were used, small disagreements would be expected because the present approach includes binding corrections. We will show below that the inclusion of a partial set of first-order screening effects leads to large corrections that understate the magnitude.

IV. SELF-ENERGY

The self-energy is significantly more difficult to calculate than vacuum polarization. The renormalized energy shift can be written as

$$\Delta E_v(\mathrm{SE})=\Sigma_{vv}(\epsilon_v)$$
$$\equiv\int d^3r\int d^3r'\,\overline{\psi_v}(\vec{r}\,')\Sigma(\vec{r},\vec{r}\,',\epsilon_v)\psi_v(\vec{r}), \tag{16}$$

where

$$\Sigma(\vec{r},\vec{r}\,',E)\equiv-ie^2\int\frac{d^nk}{(2\pi)^n}\frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}}{k^2}\gamma_\mu S_F(\vec{r},\vec{r}\,',E-k_0)\gamma^\mu$$
$$-\delta m^{(2)}\delta(\vec{r}-\vec{r}\,'). \tag{17}$$

Here the integration over the photon momentum k is carried out in $n=4-\epsilon$ dimensions so as to regularize ultraviolet divergences. The self-mass counterterm $\delta m^{(2)}$ is

$$\delta m^{(2)}=\frac{m\alpha}{\pi}\left(\frac{3C}{2\epsilon}+1\right), \tag{18}$$

with

$$C=(4\pi)^{\epsilon/2}\Gamma(1+\epsilon/2). \tag{19}$$

As described in more detail in Ref. [13], we use an approach in which the electron propagator in the external field, S_F, is rearranged in terms of the free propagator S_0 as

$$S_F(\vec{r},\vec{r}\,',E)=\Big[S_F(\vec{r},\vec{r}\,',E)-S_0(\vec{r},\vec{r}\,',E)$$
$$-\int d^3z S_0(\vec{r},\vec{z},E)V(z)S_0(\vec{z},\vec{r}\,',E)\Big]$$
$$+S_0(\vec{r},\vec{r}\,',E)$$
$$+\int d^3z S_0(\vec{r},\vec{z},E)V(z)S_0(\vec{z},\vec{r}\,',E). \tag{20}$$

The terms inside the square brackets are ultraviolet divigent individually but combine to give an ultraviolet finite contribution to the self-energy. We note that the combined term is, in a schematic notation, equivalent to the ‘‘many-potential’’ term $S_0VS_FVS_0$ used by other groups, for example by Blundell and Snyderman [14]. Here, these three terms are evaluated separately in coordinate space with partial wave expansions. In each case, a Wick rotation with $k_0\rightarrow i\omega$ is made. The d^3k integration and the angular integrations in d^3r and d^3r' are then carried out analytically, leaving a three-dimensional integral in $d\omega dr dr'$ that is evaluated numerically. The Wick rotation in the S_F term also passes bound-state poles. Details of these pole terms are given in Ref. [13].

The last two terms in Eq. (20) give rise to ultraviolet divergences. These divergences cancel with the $\delta m^{(2)}$ term, leaving an ultraviolet finite result that is evaluated in momentum space. The two terms involved here are S_0 and S_0VS_0. They are referred to as the zero-potential (0-pot) and one-potential (1-pot) terms, respectively, and are given by

$$\Delta E_{0-\mathrm{pot}}=-\frac{\alpha}{\pi}\int d^3p\,\overline{\psi_v}(\vec{p})(\not{p}-m)\psi_v(\vec{p})$$
$$-\frac{\alpha}{2\pi}\int d^3p\int_0^1 dx\,\frac{1-\epsilon_v^2+\vec{p}^{\,2}/m^2}{1-\epsilon_v^2(1-x)+(1-x)\vec{p}^{\,2}/m^2}$$
$$\times\overline{\psi_v}(\vec{p})[2m-\not{p}(1-x/2)]\psi_v(\vec{p}) \tag{21}$$

and

TABLE III. The self-energy function $F(Z\alpha)$ for the alkali metals in different potentials.

Atom	CH	$x_\alpha=0$	$x_\alpha=1/3$	$x_\alpha=2/3$	$x_\alpha=1$
Li $2s_{1/2}$	1.481	1.558	1.490	1.440	1.506
Na $3s_{1/2}$	0.190 8	0.169 3	0.167 4	0.181 4	0.223 3
K $4s_{1/2}$	0.085 60	0.072 02	0.072 05	0.082 86	0.109 66
Rb $5s_{1/2}$	0.028 60	0.022 82	0.023 59	0.028 34	0.039 59
Cs $6s_{1/2}$	0.016 16	0.012 63	0.013 21	0.016 21	0.023 49
Fr $7s_{1/2}$	0.009 646	0.006 837	0.007 543	0.009 839	0.015 02

$$\Delta E_{1-\text{pot}}=\frac{\alpha^2}{8\pi^3}\int_0^1 \rho d\rho\int_0^1 dx\int \frac{d^3p d^3p' Z_{eff}(|\vec{p}-\vec{p}\,'|)}{|\vec{p}-\vec{p}\,'|^2}\times\left[2\bar{\psi}_v(\vec{p})\gamma_0\psi_v(\vec{p}\,')\ln\frac{\Delta}{m^2}+\frac{N}{\Delta}\right], \tag{22}$$

where $Z_{eff}(|\vec{p}-\vec{p}\,'|)/2\pi^2|\vec{p}-\vec{p}\,'|^2$ is the Fourier transform of $Z_{eff}(r)/r$. Expressions for Δ and N in the above can be found in Ref. [13].

Because we use Feynman gauge, a high degree of cancellation between different contributions is encountered even for the more tractable case of highly charged ions. For neutral atoms this cancellation is much more severe, and requires the use of very fine grids to control numerical error. Care is required in the integration over ω, which becomes unstable as $\omega\rightarrow 0$. Finally the $1/l^3$ convergence of the partial wave expansion does not set in until rather large values of l. Here, 50 partial waves are calculated, and residual high-l contributions are obtained by extrapolations. We present results for the ground-state self-energy of the alkali metals in Table III, with an estimated error of 1 in the fourth significant digit.

It is again of interest to compare the results for lithium with those coming from variational wave functions. Comparison for the self-energy is, however, less straightforward than for vacuum polarization. The difficulty is that our approach, while nonperturbative in the sense that no approximations on the electron propagator are made, nevertheless treats the electron as moving in a central potential. A good choice of potential will account for a great deal of its interactions with other electrons, but ultimately the effect of those interactions will have to be taken into account through perturbation theory or more powerful methods, as will be discussed in Sec. V. The variational approach, however, while relying on nonrelativistic approximations, is exact in its treatment of the electron-electron interaction. We note in particular the fact that terms of the same order of α as the self-energy also arise in many-electron atoms from diagrams involving the exchange of two photons, which form part, but not all, of the term denoted $\Delta E_{L,2}$ in Ref. [12]. Thus even an exact self-energy calculation would not be expected to agree with the result

$$F(Z\alpha)_{Z=3}=0.895 \tag{23}$$

found in Ref. [12]. However, the contribution of $\Delta E_{L,2}$ to $F(Z\alpha)$ is only -0.050, so clearly, as with vacuum polarization, the significant overstatement of our approach is primarily due to the mean field approximation. We now turn to a calculation of leading corrections to our lowest-order results for lithium.

V. FIRST-ORDER CORRECTIONS FOR LITHIUM

Figure 1 shows Feynman diagrams of first-order screening corrections to self-energy and vacuum polarization. The complete calculation of these corrections, first carried out for highly charged lithiumlike ions in Refs. [2] and [3], is quite complex. However, a numerically dominant part of the calculation is relatively straightforward to implement. It comes from Figs. 1(b), 1(c), 1(f), and 1(g) which involve screening corrections to bound-state wave functions. In this section we include these "side diagram" corrections for lithium. The formula for the shift in the self-energy is simply

$$\Delta E=\Sigma_{v\tilde{v}}(\epsilon_v)+\Sigma_{\tilde{v}v}(\epsilon_v)+\sum_a\,[\Sigma_{a\tilde{a}}(\epsilon_a)+\Sigma_{\tilde{a}a}(\epsilon_a)], \tag{24}$$

where

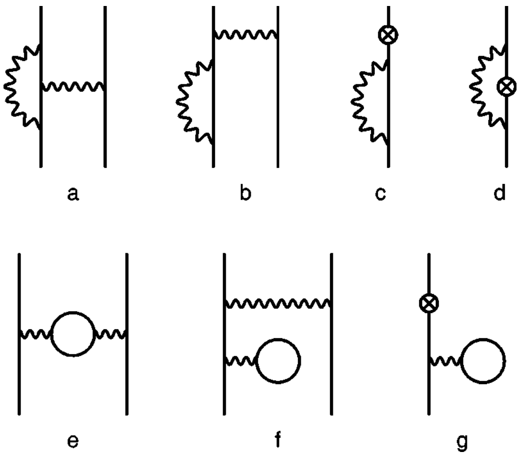

FIG. 1. Feynman diagrams of the first-order screening corrections to self-energy and vacuum polarization. Small circles with a cross at the center represent interactions with the counterpotential.

TABLE IV. Perturbed orbital corrections to the vacuum-polarization function $H(Z\alpha)$ and the self-energy function $F(Z\alpha)$ for the $2s_{1/2}$ state of lithium in different potentials.

Term	CH	$x_\alpha = 0$	$x_\alpha = 1/3$	$x_\alpha = 2/3$	$x_\alpha = 1$
$H(Z\alpha)$	-0.0504	-0.0534	-0.0506	-0.0490	-0.0511
$\tilde{v}$	0.0197	0.0295	0.0202	0.0135	0.0153
$\tilde{a}$	0.0109	0.0136	0.0104	0.0084	0.0076
Sum	-0.0198	-0.0103	-0.0200	-0.0271	-0.0282
$F(Z\alpha)$	1.481	1.558	1.490	1.440	1.506
$\tilde{v}$	-0.592	-0.836	-0.586	-0.389	-0.412
$\tilde{a}$	-0.309	-0.372	-0.292	-0.236	-0.211
Sum	0.580	0.350	0.612	0.815	0.883

$$\begin{aligned}\psi_{\tilde{v}}(\vec{y}) \equiv \alpha \sum_{m\neq v,a} \int \frac{d^3z\,d^3w}{|\vec{z}-\vec{w}|} \frac{\psi_m(\vec{y})}{\epsilon_v-\epsilon_m} &\times [\overline{\psi_m}(\vec{z})\gamma_\mu \psi_v(\vec{z})\overline{\psi_a}(\vec{w})\gamma^\mu \psi_a(\vec{w}) \\ &- e^{i\Delta E|\vec{z}-\vec{w}|}\overline{\psi_m}(\vec{z})\gamma_\mu \psi_a(\vec{z})\overline{\psi_a}(\vec{w})\gamma^\mu \psi_v(\vec{w})] \\ &- \sum_{m\neq v} \int d^3z \frac{\psi_m(\vec{y})}{\epsilon_v-\epsilon_m}\psi_m^\dagger(\vec{z})U(z)\psi_v(\vec{z}) \qquad (25)\end{aligned}$$

is a valence orbital perturbed either by the exchange of a photon with the core electrons or else by a counterpotential $U(z)=(Z_{nuc}-Z_{eff})\alpha/z$, and

$$\begin{aligned}\psi_{\tilde{a}}(\vec{y}) \equiv \alpha \sum_{m\neq a} \int \frac{d^3z\,d^3w}{|\vec{z}-\vec{w}|} \frac{\psi_m(\vec{y})}{\epsilon_a-\epsilon_m} &\times [\overline{\psi_m}(\vec{z})\gamma_\mu \psi_a(\vec{z})\overline{\psi_v}(\vec{w})\gamma^\mu \psi_v(\vec{w}) \\ &- e^{i\Delta E|\vec{z}-\vec{w}|}\overline{\psi_m}(\vec{z})\gamma_\mu \psi_v(\vec{z})\overline{\psi_v}(\vec{w})\gamma^\mu \psi_a(\vec{w})] \qquad (26)\end{aligned}$$

is a core orbital perturbed by the exchange of a photon with the valence electron. In both cases, ΔE is the exchange energy given by $|\epsilon_v-\epsilon_a|$. The shift in the vacuum-polarization energy is given by a formula similar to Eq. (24), but with the self-energy operator Σ replaced by the Uehling potential operator U_{Ueh}.

In Table IV we present the perturbed valence- and core-orbital corrections for the different potentials considered in this paper to the vacuum polarization and self-energy of the $2s$ state of lithium. In both cases the corrections are quite large. For vacuum polarization, they act to bring the lowest-order results, which cluster about 50% in magnitude above the variational results, to a range of 20% to 40% below in magnitude, excluding for the moment the $x_\alpha=0$ potential. For the self-energy, again excluding that potential, the lowest-order results are 50% to 60% higher, and after first-order corrections, 10% to 30% smaller. The excluded $x_\alpha=0$ case has much larger corrections which are likely due to poor convergence of the $1/Z$ expansion. This can also be seen when MBPT is applied to the calculation of the valence removal energy through second order: the CH and $x_\alpha=0$, 1/3, 2/3, and 1 energies differ from experiment by -2.5%, -5.7%, -1.7%, -0.1%, and 0.6%, respectively. Given that the CH and $x_\alpha=0$ potentials have no exchange terms, this indicates the importance of including exchange effects in setting up model potentials for MBPT and QED calculations of neutral alkali metals.

VI. COMPARISON WITH OTHER CALCULATIONS AND DISCUSSION

Calculations similar to those presented in this paper have been carried out by Labzowsky *et al.* using a different computational method [15]. While local density potentials are also used in that work, their x_α parameters are determined by fitting to Dirac-Fock energies and to experiment, and an exact comparison with their results cannot be made. However, we find good qualitative agreement. For example, they find a total Lamb shift for cesium ranging from 0.0018 eV to 0.0033 eV, compared to our range of 0.0016 eV to 0.0029 eV. In the case of francium their values range between 0.0046 eV and 0.0076 eV, compared to our 0.0030 eV to 0.0065 eV.

We also note work in cesium [16] and francium [17] by the Novosibirsk group, in which the Lamb shift is estimated through arguments about the wave function at the origin, which is calculated with methods that sum infinite classes of diagrams. For cesium they find 0.0023 eV, which is consistent with the above ranges, but for francium they find 0.0096 eV, which is somewhat larger than the above results. However, given the large screening corrections found in lithium discussed above, it is possible that a more complete calculation would lead to better agreement. It is of interest that their best value for the ionization energy of francium, using the highly accurate many-body methods developed by that group, is -0.14928 a.u., off by 0.00039 a.u. (0.01 eV) from experiment. If their many-body method is indeed accurate to five figures, then the Lamb shift may actually have been seen in this heavy alkali metal.

The main result of the present paper is to demonstrate that the high-accuracy techniques that we have developed for the evaluation of radiative corrections, which are usually applied to highly charged ions [2,13], can be extended to treat neutral atoms. An advantage of such techniques is the fact that they make no approximations to the electron propagator in the self-energy case, which leads to the automatic accounting of all binding corrections, a vital attribute for highly charged ions because $Z\alpha$ is not small. It may also be necessary to include these binding corrections for neutral atoms like cesium and francium. However, before this can be verified, a more accurate determination of the Lamb shift is necessary. At present, while our propagators are exact, they are also defined in terms of a potential, and that potential is at best only an approximation to the actual environment in which the electron propagates. This accounts for the significant variation of our results as the potential is changed, and also for the disagreement with the known results for lithium.

A systematic way to undo this approximation is MPBT, or its *S*-matrix generalization. As mentioned in the Introduction, the latter approach [2,3] works very well for the treatment of radiative corrections in highly charged ions because of the rapid convergence of the $1/Z$ expansion. As our results for lithium make clear, the rapid convergence of the $1/Z$ series is no longer present in neutral atoms, and a merging of many-body techniques [1] with QED will have to be explored. Inasmuch as the entire Uehling potential and a large part of the self-energy involve the expectation value of δ functions, it seems likely that at least this part of the problem for lithium could be accurately treated with CI techniques [18]. These same techniques may be applicable to heavier alkali metals. However, a simpler approach, which we are at present investigating, is to generalize the second-order MBPT corrections that are known to provide a 10% level of convergence for matrix elements such as hyperfine splitting and oscillator strengths [5] to the Lamb shift.

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