Simplified partial wave expansion of the Lamb shift

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A method for calculating the self-energy part of the Lamb shift is revisited. When the electron propagator in an external field is represented as an expansion in partial waves, the original method converges relatively slowly, requiring the calculation of dozens of partial waves. Here we show an improved method in which accurate results can be obtained using a much smaller number of partial waves. The method is illustrated for the ground states of hydrogenlike and lithiumlike boron and the possibility of high accuracy calculations on lower Z hydrogenic ions is discussed.

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I. INTRODUCTION

The small $2s - 2p_{1/2}$ splitting in the spectrum of hydrogen measured by Lamb and Retherford [1] played a seminal role in the development of quantum electrodynamics (QED) [2]. The effect is generally referred to as the Lamb shift and requires the evaluation of two types of radiative corrections—vacuum polarization (VP) and the electron self-energy (SE). The first calculations exact to all orders in $Z\alpha$, where Z is the nuclear charge and α the fine-structure constant,

$$\alpha \equiv \frac{e^2}{4\pi\epsilon_0\hbar c} = 1/137.035\,999\,084(21), \tag{1}$$

were carried out for VP by Wichmann and Kroll [3]. Meanwhile, evaluations of SE assumed $Z\alpha$ was a small quantity and could not be applied to cases when Z was large. However, the possibility of extending the work of Wichmann and Kroll to SE was realized, and not long after their work the first all-order SE calculations were presented by Desiderio and Johnson [4] and by Mohr [5]. While both use partial wave expansions to represent the photon and electron propagators, they differ in an important way in how the sum over all partial waves is carried out.

As will be seen in this paper, evaluation of the self-energy term always involves multiple integrals over position r, a single integral over an energy ω, and an infinite sum over the partial wave ℓ. Mohr used a point-Coulomb potential, and the fact that the electron propagator in this case can be expressed in terms of Whittaker functions allowed him to sum the partial waves to convergence for any value of coordinate and energy, even though, for some values of the integrand, large sums were required. This is the most accurate approach and we will refer to it as the Mohr method in the following.

The work of Desiderio and Johnson (DJ), based on the method of Brown *et al.* [6], was able to represent the electron propagator in a general spherically symmetric potential, but because it used numerically generated Green's functions it was limited by how high a partial wave the numerical method could handle. In this case the coordinate and energy integral was carried out for as many partial waves as this limitation made possible, after which an extrapolation to higher values was made for better convergence.

The work to be described here is a modification of a method we developed in collaboration with Johnson [7]. It is based on Ref. [4], using a modification suggested by Snyderman [8] and implemented by Blundell and Snyderman [9]. Because, as will be described below, an expansion of the propagator in terms of an external potential is used, we call it the potential-expansion method as suggested by Yerokhin, Pachucki, and Shabaev [10]. In that paper, references to a number of different approaches can be found, but the potential-expansion method closest to ours is given in [11]. As mentioned above, potential-expansion methods differ from the Mohr method in that they carry out coordinate and energy integrations partial wave by partial wave, afterward carrying out the final partial wave summation. As in practice only a finite number of partial waves can be included, an extrapolation of the partial wave expansion to infinity must be made and there is a significant numerical uncertainty associated with this procedure. In the following we will refer to our original potential-expansion calculation as the DJA method. The purpose of the present paper is to describe the DJB method, a modification that improves the behavior of the partial wave series.

The most accurate calculations of the self-energy have been obtained for point-Coulomb cases using the Mohr method [12]. We illustrate the strikingly high accuracy the method can attain with the self-energy of the ground state of hydrogenlike boron which is given by the dimensionless function $F_a(Z\alpha)$ for a bound state a as

$$E_{SE}(a, Z) = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n_a^3} F_a(Z\alpha)\, mc^2, \tag{2}$$

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with

$$F_{1s}(5\alpha) = 6.251\,627\,078\,(1). \tag{3}$$

We will use this particular self-energy in the following to illustrate details of the DJA and DJB methods and refer to it as the test case. All self-energy results shown in this work will also be given in terms of the dimensionless function $F_a(Z\alpha)$.

In Ref. [10], it was pointed out that the potential-expansion method described in Ref. [11] could be improved by using generalizations of identities used in the Mohr method. These identities involve commuting (C) the potential (P) and the free-electron propagator (P) and we will refer to them as CPP identities. They can be used to create approximations to terms of arbitrary order in the potential expansion. These terms can be numerically evaluated very precisely, but can also be expressed as partial wave expansions. In the latter form, it is shown in Ref. [10] that, when combined with the partial waves computed in Ref. [11], a much more tractable expansion results. It is the purpose of this paper to describe how using a CPP identity allows us to create a similarly improved partial wave expansion. Even with these improvements, the potential-expansion method cannot reach the very high accuracy of Ref. [12], though in the treatment of the hydrogen isoelectronic sequence given in Ref. [13], we note that the self-energy results presented are quite precise.

The plan of this paper is as follows. After the potential-expansion method is described in Sec. II, Sec. III describes the DJA method and the behavior of the first 30 partial waves for the test case is shown. In Sec. IV, the DJB method is set up and the improvement of the partial wave expansion shown for the test case. In Sec. V, the DJB method is applied to the $2s$ state of lithiumlike boron with a finite-nucleus model potential. Finally, a discussion of how higher accuracy might be reached is given in the Conclusion.

II. FORMALISM AND SUBTRACTION SCHEMES

A central object in the self-energy calculation is the electron propagator, which satisfies the equation

$$(z - H_x)G(z, \mathbf{x}, \mathbf{y}) = \delta^3(\mathbf{x} - \mathbf{y}), \tag{4}$$

with

$$H_x = -i\hbar c\,\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_x + mc^2\beta + V(x) \tag{5}$$

and with the understanding that $m^2 \to m^2 - i\epsilon'$. We adopt the convention for any three-vector that $r \equiv |\mathbf{r}|$, so we are assuming our potential to be spherically symmetric. In that case one can work with angular momentum eigenstates characterized by the quantum numbers κ and μ, where $\kappa = -l - 1$ for $j = l + 1/2$ and $\kappa = l$ for $j = l - 1/2$, and μ is the magnetic quantum number ranging from $-|\kappa|$ to $+|\kappa|$. In the following, for simplicity we will assume the potential to be that of a point nucleus of charge Z,

$$V(r) = -\frac{Z\alpha\hbar c}{r}. \tag{6}$$

Generalization to other potentials is straightforward. The Dirac equation

$$H_x\psi_{a\kappa\mu}(\mathbf{x}) = E_a\psi_{a\kappa\mu}(\mathbf{x}) \tag{7}$$

with energy $E_a \equiv mc^2\epsilon_a$ has the solution

$$\psi_{a\kappa\mu}(\mathbf{x}) = \begin{pmatrix} g_a(x)\chi_{\kappa\mu}(\hat{x}) \\ if_a(x)\chi_{-\kappa\mu}(\hat{x}) \end{pmatrix}, \tag{8}$$

where the spherical spinor $\chi_{\kappa\mu}$ is given by

$$\chi_{\kappa\mu}(\hat{x}) = \sum_m C(l, 1/2, j; \mu - m, m, \mu)Y_{l\,\mu-m}(\hat{x})\xi_m, \tag{9}$$

with $C(l, 1/2, j; \mu - m, m, \mu)$ being the Clebsch-Gordan coefficient, $Y_{l\,\mu-m}(\hat{x})$ the spherical harmonics, and ξ_m the two-component spinor:

$$\xi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \xi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{10}$$

A formally exact solution of Eq. (4) is obtained from a summation over all possible κ and μ values,

$$G(z, \mathbf{x}, \mathbf{y}) = \sum_{\kappa\mu}[\theta(x - y)W_{\kappa\mu}(z, \mathbf{x})U^\dagger_{\kappa\mu}(z, \mathbf{y}) + \theta(y - x)U_{\kappa\mu}(z, \mathbf{x})W^\dagger_{\kappa\mu}(z, \mathbf{y})]. \tag{11}$$

Here $U_{\kappa\mu}(z, \mathbf{x})$ and $W_{\kappa\mu}(z, \mathbf{x})$ are bispinors of the form of $\psi_{z\kappa\mu}(\mathbf{x})$ in Eq. (8), with the radial functions being solutions to the Dirac equation regular at the origin and infinity, respectively. Also, $\theta(t) = 0$ or 1 for $t <$ or >0 is the step function.

The one-loop self-energy of an electron state a before regularization and renormalization is

$$E^{(2)}_{SE} = -4\pi i\alpha c^2\int\frac{d^4k}{(2\pi)^4}\iint d^3x\,d^3y\,\frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k_0^2 - \mathbf{k}^2 + i\delta} \times \bar{\psi}_a(\mathbf{x})\gamma_\nu G(E_a - ck_0, \mathbf{x}, \mathbf{y})\gamma_0\gamma^\nu\psi_a(\mathbf{y}). \tag{12}$$

After renormalization, the finite remainder is the self-energy part of the one-loop Lamb shift given by $E_{SE}(a, Z)$ in Eq. (2). It has scaling factors Z^4 and $1/n_a^3$ and is of order $mc^2\alpha^5$.

To evaluate $E^{(2)}_{SE}$ without expanding in $Z\alpha$ requires a treatment of the propagator that allows regularization and removal of ultraviolet infinities, at the same time including the finite parts of the calculation. To do this we expand the propagator around the free propagator $F(z, \mathbf{x}, \mathbf{y})$, which satisfies Eq. (4) when $V(x)$ vanishes. The expansion is

$$G(z, \mathbf{x}, \mathbf{y}) = F(z, \mathbf{x}, \mathbf{y}) + \int d\mathbf{r}_1 F(z, \mathbf{x}, \mathbf{r}_1)V(r_1)F(z, \mathbf{r}_1, \mathbf{y}) + \iint d\mathbf{r}_1 d\mathbf{r}_2 F(z, \mathbf{x}, \mathbf{r}_1)V(r_1)F(z, \mathbf{r}_1, \mathbf{r}_2)V(r_2)F(z, \mathbf{r}_2, \mathbf{y}) + \iiint d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 F(z, \mathbf{x}, \mathbf{r}_1)V(r_1)F(z, \mathbf{r}_1, \mathbf{r}_2)V(r_2)F(z, \mathbf{r}_2, \mathbf{r}_3)V(r_3)F(z, \mathbf{r}_3, \mathbf{y}) + \ldots. \tag{13}$$

If we use the labeling scheme

$$G(z,\mathbf{x},\mathbf{y}) \equiv \sum_{i=0}^{\infty} G_i(z,\mathbf{x},\mathbf{y}), \tag{14}$$

where i refers to the number of potentials $V(r)$ in the expansion terms on the right-hand side of Eq. (13), the self-energy can be similarly expanded,

$$E_{SE}^{(2)} = \sum_{i=0}^{\infty} E_{iP}, \tag{15}$$

which defines the potential-expansion method. All ultraviolet infinities are associated with the first two terms in the expansion, E_{0P}, referred to as the zero-potential term, and E_{1P}, referred to as the one-potential term. When these are separated from the complete sum, we define the result as the many-potential term,

$$E_{MP} = \sum_{i=2}^{\infty} E_{iP}. \tag{16}$$

In the DJA method, E_{MP} is evaluated in coordinate space and E_{0P} and E_{1P} in momentum space. We now give a brief description of the calculation, with emphasis on E_{0P}, modifications of which are used in the DJB method.

III. DJA METHOD

To evaluate the zero- and one-potential terms we first define the momentum space wave function,

$$\psi_a(\mathbf{p}) \equiv \int d^3x\, e^{-i\mathbf{x}\cdot\mathbf{p}/\hbar}\, \psi_a(x). \tag{17}$$

The Dirac equation in momentum space is

$$(\not{p} - mc)\,\psi_a(\mathbf{p}) = -4\pi Z\alpha \int \frac{d\mathbf{p}_1}{(2\pi)^3}\,\frac{\gamma_0\,\psi_a(\mathbf{p}_1)}{|\mathbf{p}-\mathbf{p}_1|^2}, \tag{18}$$

where we have introduced the four-vector $p = (mc\epsilon, \mathbf{p})$. For the Dirac equation $\epsilon = \epsilon_a$, but when p is present in an electron propagator we leave ϵ as a variable that can be differentiated for later use when we describe the DJB method.

We regulate the ultraviolet infinities in E_{0P} and E_{1P} by changing $d^4k \to d^nk$, with $n = 4 - \delta$. In dimensional regularization we note that the self-mass of a free electron at one-loop order is

$$\delta m^{(2)} = m\,\frac{\alpha}{\pi}\left(\frac{3C}{\delta} + 2\right), \tag{19}$$

with

$$C = (4\pi)^{\delta/2}\,\Gamma(1+\delta/2). \tag{20}$$

Using the representation of the free-electron propagator

$$F(z,\mathbf{x},\mathbf{y}) = \frac{1}{\hbar^3}\int \frac{d^3p}{(2\pi)^3}\,\frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})/\hbar}}{z\gamma_0 - c\,\boldsymbol{\gamma}\cdot\mathbf{p} - mc^2}\,\gamma_0, \tag{21}$$

the zero-potential term can be shown to be

$$E_{0P}(\epsilon) = -\frac{4\pi i\alpha c}{\hbar^3}\int \frac{d\mathbf{p}}{(2\pi)^3}\,\bar{\psi}_a(\mathbf{p})X(p,\epsilon)\psi_a(\mathbf{p}), \tag{22}$$

with

$$X(p,\epsilon) \equiv \int \frac{d^nk}{(2\pi)^n}\,\frac{1}{k^2} \times \gamma_\nu \frac{1}{(mc\epsilon - k_0)\gamma_0 - \boldsymbol{\gamma}\cdot(\mathbf{p}-\mathbf{k}) - mc}\,\gamma^\nu. \tag{23}$$

Standard manipulations give

$$\begin{aligned} X(p,\epsilon) &= \frac{1}{c}\int \frac{d^nk}{(2\pi)^n}\,\frac{\gamma_\nu(\not{p}-\not{k}+mc)\gamma^\nu}{k^2[(p-k)^2-m^2c^2]} \\ &= \frac{1}{c}\int_0^1 dx \int \frac{d^nk}{(2\pi)^n}\,\frac{(2-n)(\not{p}-\not{k})+n\cdot mc}{[(k-xp)^2+x(1-x)p^2-xm^2c^2]^2} \\ &= \frac{iC(mc)^{-\delta}}{8\pi^2c\delta}\int_0^1 dx\,[\not{p}(1-x)(2-n)+n\cdot mc]\Delta^{-\delta/2}, \end{aligned} \tag{24}$$

with

$$\Delta = x - x(1-x)[\epsilon^2 - \mathbf{p}^2/(mc)^2]. \tag{25}$$

Expanding in δ and discarding terms of order δ and higher leads to

$$X(p,\epsilon) = \frac{i}{8\pi^2}\,m\left(\frac{3C}{\delta}+2\right) - \frac{i}{8\pi^2c}\,(\not{p}-mc)\left(\frac{C}{\delta}+1\right) + \frac{i}{8\pi^2c}\int_0^1 dx\big[\,\not{p}(1-x) - 2mc\,\big]\ln\frac{\Delta}{x^2}. \tag{26}$$

The zero-potential term is then

$$\begin{aligned} E_{0P}(\epsilon) = {}& \frac{\alpha}{2\pi}\,mc^2\left(\frac{3C}{\delta}+2\right)\frac{1}{\hbar^3}\int\frac{d\mathbf{p}}{(2\pi)^3}\,\bar{\psi}_a(\mathbf{p})\psi_a(\mathbf{p}) - \frac{\alpha}{2\pi}\left(\frac{C}{\delta}+1\right)\frac{c}{\hbar^3}\int\frac{d\mathbf{p}}{(2\pi)^3}\bar{\psi}_a(\mathbf{p})(\not{p}-mc)\psi_a(\mathbf{p}) \\ &+ \frac{\alpha}{2\pi}\,\frac{c}{\hbar^3}\int\frac{d\mathbf{p}}{(2\pi)^3}\int_0^1 dx\,\bar{\psi}_a(\mathbf{p})[\not{p}(1-x)-2mc]\psi_a(\mathbf{p})\ln\frac{\Delta}{x^2}. \end{aligned} \tag{27}$$

The first term in the right-hand side is removed by mass renormalization.

Turning to E_{1P}, it is given by

$$E_{1P} = \frac{16\pi^2 icZ\alpha^2}{\hbar^3}\int\frac{d\mathbf{p}_2}{(2\pi)^3}\int\frac{d\mathbf{p}_1}{(2\pi)^3}\,\frac{1}{|\mathbf{p}_2-\mathbf{p}_1|^2}\,\bar{\psi}_a(\mathbf{p}_2)Y(\mathbf{p}_2,\mathbf{p}_1)\psi_a(\mathbf{p}_1), \tag{28}$$

with

$$Y(\mathbf{p}_2,\mathbf{p}_1) \equiv \int\frac{d^nk}{(2\pi)^n}\,\frac{\gamma_\nu(\not{p}_2-\not{k}+mc)\gamma_0(\not{p}_1-\not{k}+mc)\gamma^\nu}{k^2[(k-p_2)^2-(mc)^2][(k-p_1)^2-(mc)^2]}. \tag{29}$$

In the above, $p_1=(mc\epsilon_a,\ \mathbf{p}_1)$ and $p_2=(mc\epsilon_a,\ \mathbf{p}_2)$: there is no need in this case to introduce ϵ and ϵ_a can be used directly. A standard set of manipulations then leads to

$$E_{1P} = \frac{\alpha}{2\pi}\left(\frac{C}{\delta}-\frac{1}{2}\right)\frac{c}{\hbar^3}\int\frac{d\mathbf{p}}{(2\pi)^3}\,\bar{\psi}(\mathbf{p})(\not{p}-mc)\psi(\mathbf{p}) + 2\,\frac{Z\alpha^2c}{\hbar^3}\int\frac{d\mathbf{p}_2}{(2\pi)^3}\int\frac{d\mathbf{p}_1}{(2\pi)^3}\,\frac{\bar{\psi}(\mathbf{p}_2)\gamma_0\psi(\mathbf{p}_1)}{|\mathbf{p}_2-\mathbf{p}_1|^2}\int_0^1\rho\,d\rho\int_0^1 dx\ln\frac{\Delta_1}{\rho}$$
$$+\frac{Z\alpha^2c}{\hbar^3}\int\frac{d\mathbf{p}_2}{(2\pi)^3}\int\frac{d\mathbf{p}_1}{(2\pi)^3}\int_0^1 d\rho\int_0^1 dx\,\frac{1}{\Delta_1}\,\frac{\bar{\psi}(\mathbf{p}_2)N\psi(\mathbf{p}_1)}{|\mathbf{p}_2-\mathbf{p}_1|^2}, \tag{30}$$

where the Dirac equation has been used in the first line and the explicit form of N can be found in Ref. [7]. If we define

$$E_{01P} \equiv E_{0P} + E_{1P}, \tag{31}$$

after mass renormalization, we see it is ultraviolet finite. The counterterms present in the renormalization procedure that would make the individual terms ultraviolet finite cancel because of the Ward identity.

It is difficult to evaluate the finite part of E_{1P} with high precision as it stands. The solution used to improve the numerics is to employ the CPP identity introduced by Mohr [5]. The source of the numerical difficulties is the region where $|\mathbf{p_1}-\mathbf{p_2}|$ is small. If we replace $\mathbf{p_2}$ with $\mathbf{p_1}$ everywhere in the finite terms in E_{1P} except the denominator and the wave function, the Dirac equation, Eq. (18), can be used to carry out the $d\mathbf{p_2}$ integration, resulting in a much simpler integral. By subtracting this term before using the Dirac equation, the extra cancellation that results when $|\mathbf{p_2}-\mathbf{p_1}|^2$ is small allows the integral to be evaluated with the accuracy needed. (This procedure is carried out symmetrically, with $\mathbf{p_1}$ being replaced with $\mathbf{p_2}$ in a second subtraction term.) What we have just described is essentially the procedure introduced by Mohr [5], where the replacement of $\mathbf{p_2}$ with $\mathbf{p_1}$ in the propagator is the result of commuting the propagator through the potential.

The momentum space result for the test case from $0P$ and $1P$ is

$$E_{01P} = -767.728\,102. \tag{32}$$

The accuracy of the numerical integrations, which are done using the program CUHRE from the Cuba package [14], is such that all digits shown are significant. While the accuracy could be improved, there would be no point in doing so because the partial wave expansion involved in E_{MP} leads to much larger numerical uncertainty.

We begin the coordinate space evaluation of E_{MP} by carrying out the d^3k integration in Eq. (12),

$$E_{SE}^{(2)} = i\alpha\hbar c^2\int\frac{dk_0}{2\pi}\iint d^3x\,d^3y\,\frac{e^{ik_0|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|}\,\bar{\psi}_a(\mathbf{x})\gamma_\nu G(E_a-ck_0,\mathbf{x},\mathbf{y})\gamma_0\gamma^\nu\psi_a(\mathbf{y}). \tag{33}$$

We define the order of the partial wave expansion ℓ by introducing the standard expansion of the photon propagator,

$$\frac{e^{ik_0|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|} = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} 4\pi ik_0 j_\ell(k_0r)h_\ell(k_0r')Y_{\ell m}(\hat{x})Y^*_{\ell m}(\hat{y}), \tag{34}$$

with $r=\min(x,y)$ and $r'=\max(x,y)$. We now again use ϵ, understood to be taken to ϵ_a for the DJA method, and find

$$E_{SE}^{(2)}(\epsilon) = i\alpha\hbar c^2\int\frac{dk_0}{2\pi}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}4\pi ik_0\iint d^3x\,d^3y\,j_\ell(k_0r)h_\ell(k_0r')Y_{\ell m}(\hat{x})Y^*_{\ell m}(\hat{y})$$
$$\times\Bigg[\sum_{\kappa\mu}\theta(x-y)\bar{\psi}_a(\mathbf{x})\gamma_\nu U_{\kappa\mu}(\epsilon_a-k_0,\ \mathbf{x})W^\dagger_{\kappa\mu}(\epsilon_a-k_0,\ \mathbf{y})\gamma_0\gamma^\nu\psi_a(\mathbf{y})$$
$$+\theta(y-x)\bar{\psi}_a(\mathbf{x})\gamma_\nu W_{\kappa\mu}(\epsilon_a-k_0,\ \mathbf{x})U^\dagger_{\kappa\mu}(\epsilon_a-k_0,\ \mathbf{y})\gamma_0\gamma^\nu\psi_a(\mathbf{y})\Bigg]. \tag{35}$$

In this form one can analytically carry out the angle integrations along with the sum over m and μ. The resulting Clebsch-Gordon coefficients then limit the sum over κ for a given value of ℓ, and they are understood to be all included for

TABLE I. DJA partial wave contributions to the self-energy of the $Z = 5$ point-Coulomb $1s$ state. E_{MP} = Main − E_{0P} − E_{1P}. Sum_A is the cumulative partial-wave sum of E_{MP}.

ℓ	Main	E_{0P}	Main − E_{0P}	E_{1P}	E_{MP}	Sum_A
0	32953.2587[a]	30259.7520	2693.5067	1937.5587	755.9480	−11.7801[b]
1	34284.1223	33832.2160	451.9063	440.3507	11.5556	−0.2245
2	34159.6544	33932.9018	226.7526	223.8197	2.9329	2.7084
3	33733.5632	33592.7097	140.8535	139.5826	1.2709	3.9792
4	33160.4627	33064.4550	96.0077	95.3232	0.6845	4.6637
5	32510.9396	32442.0604	68.8793	68.4636	0.4157	5.0794
6	31823.0807	31772.0957	50.9849	50.7121	0.2728	5.3522
7	31119.2099	31080.7241	38.4859	38.2968	0.1890	5.5412
8	30413.0504	30383.6582	29.3922	29.2557	0.1365	5.6777
9	29713.2633	29690.6918	22.5715	22.4698	0.1017	5.7794
10	29025.3708	29008.0375	17.3334	17.2556	0.0777	5.8571
11	28352.8744	28339.6399	13.2345	13.1738	0.0607	5.9178
12	27697.9380	27687.9599	9.9781	9.9298	0.0482	5.9661
13	27061.8230	27054.4646	7.3584	7.3194	0.0389	6.0050
14	26445.1730	26439.9441	5.2289	5.1971	0.0318	6.0368
15	25848.2057	25844.7229	3.4828	3.4565	0.0263	6.0631
16	25270.8445	25268.8038	2.0407	2.0187	0.0220	6.0851
17	24712.8100	24711.9676	0.8424	0.8238	0.0185	6.1037
18	24173.6846	24173.8431	−0.1585	−0.1743	0.0158	6.1194
19	23652.9589	23653.9569	−0.9980	−1.0114	0.0135	6.1329
20	23150.0646	23151.7690	−1.7043	−1.7160	0.0116	6.1446
21	22664.3984	22666.6988	−2.3003	−2.3104	0.0101	6.1547
22	22195.3394	22198.1435	−2.8041	−2.8129	0.0088	6.1635
23	21742.2613	21745.4918	−3.2305	−3.2382	0.0077	6.1712
24	21304.5417	21308.1331	−3.5914	−3.5982	0.0068	6.1780
25	20881.5681	20885.4650	−3.8969	−3.9029	0.0060	6.1840
26	20472.7424	20476.8976	−4.1552	−4.1606	0.0053	6.1893
27	20077.4842	20081.8573	−4.3732	−4.3779	0.0048	6.1941
28	19695.2324	19699.7889	−4.5565	−4.5607	0.0043	6.1983
29	19325.4469	19330.1569	−4.7100	−4.7138	0.0038	6.2022
30	18967.6086	18972.4465	−4.8379	−4.8413	0.0034	6.2056
High-ℓ correction from $1/\ell^3$ fit					0.0500	6.2557
High-ℓ correction $\Delta\ell_{2,5}^{-3}$ from Eq. (38)					0.0465	6.2521
Ref. [12]						6.2516

[a]Include contribution from the pole term in Eq. (36).
[b]Include momentum-space contribution from E_{01P} in Eq. (32).

any given partial wave. Evaluation of the integrals over k_0, x, and y can now be carried out if one has the radial functions for the electron Green's function, which are available analytically in terms of Whittaker functions for the point-Coulomb case or numerically for the general case as in the present calculations.

In the DJA method, integrations over $\omega = ck_0$ are carried out for each partial wave ℓ and the resulting partial wave series is summed to give the final results. $E_{SE}^{(2)}$ thus calculated will be referred to as the Main term. To form the ultraviolet convergent many-potential term $E_{MP} = E_{SE}^{(2)} - E_{0P} - E_{1P}$, we begin by subtracting the zero-potential term E_{0P} from the Main term. Computationally, E_{0P} in coordinate space is the same as $E_{SE}^{(2)}$ with the bound-electron Green's function $G(z, \mathbf{x}, \mathbf{y})$ replaced by the free-electron Green's function $F(z, \mathbf{x}, \mathbf{y})$, which can be generated analytically or numerically. Partial waves of the Main and E_{0P} terms up to $\ell = 30$ are shown in the second and third columns of Table I for the test case and their difference is shown in the fourth column. It is clear that there are substantial cancellations between Main and E_{0P}, but Main − E_{0P} is a partial wave expansion that does not converge and the gradual falloff with ℓ eventually goes as $1/\ell$, which corresponds to a logarithmic divergence.

We note that, in evaluating $E_{SE}^{(2)}$, a Wick rotation, $\omega \to i\omega$, is carried out and a deformation of the contour to avoid bound-state poles gives rise to the "Pole terms." Details can be found in Ref. [7]. Pole terms do not involve electron Green's functions and can be calculated very accurately. For the $E_{1s}(5\alpha)$ test case considered here, there is only one $1s$ pole term given by

$$E_{1s}(\text{pole}) = 20\,210.432\,546. \tag{36}$$

This term is combined with the $\ell = 0$ partial wave of the Main term in Table I, as this is the only partial wave affected by the $1s$ pole from symmetry and energy considerations.

To finally form the ultraviolet finite many potential term, we need to compute

$$E_{1P} = i\alpha\hbar c^2 \int \frac{dk_0}{2\pi} \iint d^3x\, d^3y\, \frac{e^{ik_0|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|}\, \bar{\psi}_a(\mathbf{x})\gamma_\nu G_2(E_a - ck_0, \mathbf{x}, \mathbf{y})\gamma_0\gamma^\nu\psi_a(\mathbf{y})$$
$$= i\alpha\hbar c^2 \int \frac{dk_0}{2\pi} \iiint d^3x\, d^3w\, d^3y\, \frac{e^{ik_0|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|}\, \bar{\psi}_a(\mathbf{x})\gamma_\nu F(E_a - ck_0, \mathbf{x}, \mathbf{w})\gamma_0 \frac{\hbar c Z\alpha}{w} F(E_a - ck_0, \mathbf{w}, \mathbf{y})\gamma_0\gamma^\nu\psi_a(\mathbf{y}). \quad (37)$$

The ordering of the magnitudes x, w, and y determines which spherical Bessel functions must be used and requires the evaluation of three different integrals. However, only one more integration variable is present compared to the zero-potential term and no numerical difficulties arise. The result is presented in the fifth column of Table I. Subtractions of E_{1P} from Main $- E_{0P}$ give the E_{MP} term listed in the sixth column. Once again, there are substantial cancellations, but the resulting partial wave series of E_{MP} now converges as $1/\ell^3$.

In the seventh column of Table I, the cumulative partial-wave sums of E_{MP} are shown as Sum_A. By adding E_{01P} in Eq. (32) to the $\ell = 0$ term, Sum_A should converge to the final self-energy result. Indeed, Sum_$A(\ell)$ can be seen to approach the high-precision results of 6.2516... from Ref. [12], with Sum_$A(30) = 6.2056$ converged to the first decimal point for an accuracy of 0.74%. By extrapolating the partial wave series with an $1/\ell^3$ fit, the high-ℓ contribution from $\ell = 31 - \infty$ of 0.0500 can be added to Sum_$A(30)$ for a result of 6.2557 shown in the third row from the bottom in Table I. This improves the convergence by one more decimal point and the accuracy to 0.06%. High-ℓ corrections have also been calculated with an accelerated-convergence method based on a k-point least-square, rational polynomial fit of the form

$$f_{m,k}^{-n}(\ell) \approx 1/[\ell^n(a_0 + a_1/\ell + \cdots + a_m/\ell^m)], \quad (38)$$

where the number of least-square points k must be greater than the order of the rational polynomial m. In fact, the $1/\ell^3$ fit is a special case with $n = 3$, $m = 0$, and $k = 1$. As shown in the second row from the bottom of Table I, the high-ℓ correction $\Delta\ell_{2,5}^{-3}$ of 0.0465 does accelerate the convergence and further improves the self-energy result by another decimal point to 6.2521 for an accuracy of 0.01%.

While the difference between the two high-ℓ extrapolation results reflects the intrinsic uncertainty of these corrections, their contributions can be greatly reduced by extending the calculation to include more partial waves. For higher-Z ions than the $Z = 5$ test case, that is usually not necessary as partial wave series tend to converge much faster. For lower-Z ions, however, partial wave series converge much slower and, unlike the Mohr method that utilizes analytic functions extensively, the numerical approach of the DJA method limits the number of partial waves that can be accurately calculated. A different approach with faster partial wave convergence is needed. For that, we turn to the new DJB method which is based on a variation of the method in Ref. [10].

IV. DJB METHOD

The next logical step in the potential-expansion method would appear to be the evaluation of the two-potential term E_{2P} given by

$$E_{2P} = -4\pi i\alpha c^2 \int \frac{d^4k}{(2\pi)^4} \iint d^3x\, d^3y\, \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k_0^2 - \mathbf{k}^2 + i\delta}\, \bar{\psi}_a(\mathbf{x})\gamma_\nu$$
$$\times \iint d\mathbf{r}_1 d\mathbf{r}_2\, F(E_a - ck_0, \mathbf{x}, \mathbf{r}_1)V(r_1)$$
$$\times\, F(E_a - ck_0, \mathbf{r}_1, \mathbf{r}_2)V(r_2)F(E_a - ck_0, \mathbf{r}_2, \mathbf{y})\gamma^\nu\psi_a(\mathbf{y}). \quad (39)$$

However, after transforming to momentum space and evaluating the d^4k integral with Feynman parameters, one has a multidimensional integral of nominal dimension 9. Evaluating such an integral to high precision would be an extremely challenging proposition even with the subtractions described for E_{1P}. We consider instead an approximation in the modified two-potential term $\tilde{E}_{2P}$ given by

$$\tilde{E}_{2P} \equiv -4\pi i\alpha c^2 \int \frac{d^4k}{(2\pi)^4} \iint d^3x\, d^3y\, \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k_0^2 - \mathbf{k}^2 + i\delta}\, \bar{\psi}_a(\mathbf{x})\gamma_\nu$$
$$\times \iint d\mathbf{r_1} d\mathbf{r_2}\, F(E_a - ck_0, \mathbf{x}, \mathbf{r_1})V(x)$$
$$\times\, F(E_a - ck_0, \mathbf{r_1}, \mathbf{r_2})V(y)F(E_a - ck_0, \mathbf{r_2}, \mathbf{y})\gamma^\nu\psi_a(\mathbf{y}). \quad (40)$$

Because the free-electron propagator $F(z, \mathbf{x}, \mathbf{y})$ emphasizes the region $\mathbf{x} = \mathbf{y}$, the replacement of $V(r_1)$ with $V(x)$ and $V(r_2)$ with $V(y)$ in $\tilde{E}_{2P}$ can be expected to capture a dominant part of the integral. The replacement corresponds to a CPP method, with $V(r_1)$ commuted to the left and $V(r_2)$ commuted to the right.

The DJB method involves replacing the MP term in the DJA method with

$$E_{MP} = (E_{MP} - \tilde{E}_{2P}) + \tilde{E}_{2P} \equiv \tilde{E}_{MP} + \tilde{E}_{2P}. \quad (41)$$

The relative simplicity of $\tilde{E}_{2P}$ comes from the identity

$$\iint d^3u\, d^3w\, F(z, \mathbf{x}, \mathbf{u})F(z, \mathbf{u}, \mathbf{w})F(z, \mathbf{w}, \mathbf{y})$$
$$= \frac{1}{2}\frac{d^2}{dz^2}F(z, \mathbf{x}, \mathbf{y}). \quad (42)$$

This allows the $\mathbf{r_1}$ and $\mathbf{r_2}$ integrations in $\bar{E}_{2P}$ to be carried out and we have

$$\tilde{E}_{2P} = -2\pi i\alpha c^2 \frac{d^2}{dE_a^2} \int \frac{d^4k}{(2\pi)^4} \iint d^3x\, d^3y\, V(x)V(y)$$
$$\times \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k_0^2 - \mathbf{k}^2 + i\delta}\bar{\psi}_a(\mathbf{x})\gamma_\nu F(E_a - ck_0, \mathbf{x}, \mathbf{y})\gamma_0\gamma^\nu\psi_a(\mathbf{y}). \quad (43)$$

In coordinate space form, this is to be subtracted from E_{MP} and to compensate we need to add it back in momentum space form.

To do this, we work with Eq. (27), which we treated as a function of ϵ. $\tilde{E}_{2P}$ involves differentiating with respect to ϵ twice, after which case one can take $\epsilon \to \epsilon_a$. We start by noting

$$\frac{d^2X(p)}{d\epsilon_a^2} = \frac{i}{4\pi^2 m^2 c^5}\int_0^1 dx\, x(1-x) \times\left[\frac{\epsilon_a N_0 - N_1}{\Delta} + \frac{2D_B(\epsilon_a N_0 + N_1)}{\Delta^2}\right], \quad (44)$$

where $N_0 = -\gamma_0(1-x)/c$ and $N_1 = 2mc + \boldsymbol{\gamma}\cdot\mathbf{p}\,(1-x)$. If we define the momentum space function

$$\psi_{a_1}(\mathbf{p}) \equiv \int d^3x\, e^{-i\mathbf{x}\cdot\mathbf{p}/\hbar}\,\frac{Z(x)}{x}\,\psi_a(x), \quad (45)$$

one has

$$\tilde{E}_{2P} = \frac{\alpha}{3\pi m^2 c^3\hbar^3}\int\frac{d\mathbf{p}}{(2\pi)^3}\int_0^1 dx\, x(1-x)\bar{\psi}_{a_1}(\mathbf{p}) \times\left[\frac{\epsilon_a N_0 - N_1}{\Delta} + \frac{2D_B(\epsilon_a N_0 + N_1)}{\Delta^2}\right]\psi_{a_1}(\mathbf{p}), \quad (46)$$

which can be easily evaluated with high accuracy. Its value in momentum space for the test case is given by

$$\tilde{E}_{2P} = 365.613\,427. \quad (47)$$

Turning to the coordinate space part of the calculation, we note that the double derivative with respect to E_a can be carried out using the recursion relations for spherical Bessel functions. While this results in a somewhat complicated integrand, the numerical integral is of the same form as used for the other parts of the coordinate space calculation and the results are of the same accuracy. We list the partial waves for the test case up to $\ell = 30$ in the third column of Table II.

A check on the calculation can now be made by comparing the partial wave expansion of $\tilde{E}_{2P}$ with the momentum space form, which can be evaluated with high precision. From Table II, the partial wave sum of $\tilde{E}_{2P}$ up to $\ell = 30$ is 365.5675, which agrees with the momentum space result in Eq. (47) to 0.01%. While this check reflects the accuracy possible for the partial wave expansion, that accuracy is still limited for the same reason DJA is limited—the relatively slow convergence of the partial wave expansion. However, the partial wave expansion of DJB has two features that make the method much more accurate. The first is that the cancellation with E_{MP}, shown in the sixth column of Table I and re-shown in the second column of Table II, makes the higher partial waves smaller by over two orders of magnitude as shown in the fourth column of Table II. Indeed, the cumulative sum of $\tilde{E}_{MP} = E_{MP} - \tilde{E}_{2P}$, shown as Sum_$B$ in the fifth column, can be seen to converge readily to 6.2515 at $\ell = 30$ instead of Sum_A's 6.0256 in Table I. The second feature is that the convergence of $\tilde{E}_{MP}$ is more rapid at $1/\ell^4$. Using a range of extrapolation methods as done with the DJA method, we find that, at $\ell = 30$, they all give consistent high-ℓ corrections at ~0.0001, improving the present self-energy result to 6.2516, same as the high-precision results of Ref. [12] down to the fourth decimal point as seen in the last two rows in Table II. For higher-Z ions than the present test case of $Z = 5$, 10–20 partial waves would likely be sufficient for the DJB method and high-ℓ extrapolations may not even be necessary except for accuracy checks. DJB is a marked improvement over DJA.

TABLE II. DJB partial wave contributions to the self-energy of the $Z = 5$ point-Coulomb 1s state. $\tilde{E}_{MP} = E_{MP} - \tilde{E}_{2P}$. Sum_$B$ is the cumulative partial-wave sum of $\tilde{E}_{MP}$.

ℓ	E_{MP}	$\tilde{E}_{2P}$	$\tilde{E}_{MP}$	Sum_B
0	755.9480	349.1413	406.8067	4.6921[a]
1	11.5556	10.1811	1.3744	6.0665
2	2.9329	2.8131	0.1198	6.1863
3	1.2709	1.2374	0.0335	6.2198
4	0.6845	0.6708	0.0136	6.2334
5	0.4157	0.4090	0.0067	6.2401
6	0.2728	0.2690	0.0038	6.2439
7	0.1890	0.1868	0.0023	6.2462
8	0.1365	0.1350	0.0015	6.2476
9	0.1017	0.1007	0.0010	6.2486
10	0.0777	0.0771	0.0007	6.2493
11	0.0607	0.0602	0.0005	6.2498
12	0.0482	0.0479	0.0004	6.2502
13	0.0389	0.0387	0.0003	6.2505
14	0.0318	0.0316	0.0002	6.2507
15	0.0263	0.0262	0.0002	6.2508
16	0.0220	0.0219	0.0001	6.2510
17	0.0185	0.0184	0.0001	6.2511
18	0.0158	0.0157	0.0001	6.2512
19	0.0135	0.0134	0.0001	6.2512
20	0.0116	0.0116	0.0001	6.2513
21	0.0101	0.0100	0.00005	6.2513
22	0.0088	0.0088	0.00004	6.2514
23	0.0077	0.0077	0.00003	6.2514
24	0.0068	0.0068	0.00003	6.2514
25	0.0060	0.0060	0.00002	6.2515
26	0.0053	0.0053	0.00002	6.2515
27	0.0048	0.0047	0.00002	6.2515
28	0.0043	0.0042	0.00002	6.2515
29	0.0038	0.0038	0.00001	6.2515
30	0.0034	0.0034	0.00001	6.2515
High-ℓ correction $\Delta\ell_{2,5}^{-4}$			0.00010	6.2516
Ref. [12]				6.2516

[a]Include momentum-space contributions from E_{01P} in Eq. (32) and $\tilde{E}_{2P}$ in Eq. (47).

V. APPLICATIONS

Now that we have shown the details of the DJB method for the test case, it is clear that the present DJB result of $E_{1s}(5\alpha) = 6.2516(1)$, with an uncertainty of 1 in the last digit, cannot match the accuracy of 6.251 627 078(1) in Ref. [12]. Nevertheless, the present result is still accurate to five significant figures, which is more than enough for most applications. More importantly, the present approach is not limited to point-Coulomb cases, as bound-state wave functions and electron Green's functions are solved numerically instead of derived analytically. Thus the DJB method has a wide range of applications and can be used to calculate, for

TABLE III. DJA and DJB partial wave contributions to the self-energy of the $2s$ state of Li-like boron ($Z = 5$) in a finite-nucleus, Kohn-Sham potential. $\tilde{E}_{MP} = E_{MP} - \tilde{E}_{2P}$. Sum_$A$ and Sum_B are cumulative partial-wave sums of E_{MP} and $\tilde{E}_{MP}$, respectively. $\Delta\ell_{2,5}^{-4}$ are high-ℓ corrections of Sum_B by fitting $\tilde{E}_{MP}$ with Eq. (38). Total_B = Sum_$B + \Delta\ell_{2,5}^{-4}$.

ℓ	E_{MP}	Sum_A	$\tilde{E}_{2P}$	$\tilde{E}_{MP}$	Sum_B	$\Delta\ell_{2,5}^{-4}$	Total_B
0	577.4753[a]	−8.2795[b]	298.9027	278.5726	2.2123[c]		
1	6.9704	−1.3091	6.3045	0.6659	2.8782		
2	1.7532	0.4441	1.7022	0.0509	2.9291		
3	0.7848	1.2289	0.7707	0.0141	2.9432		
4	0.4390	1.6679	0.4333	0.0058	2.9490		
5	0.2773	1.9452	0.2744	0.0029	2.9518	0.0052	2.9570
6	0.1893	2.1345	0.1877	0.0016	2.9535	0.0035	2.9570
7	0.1365	2.2710	0.1355	0.0010	2.9544	0.0025	2.9569
8	0.1024	2.3734	0.1018	0.0006	2.9551	0.0018	2.9569
9	0.0793	2.4527	0.0789	0.0004	2.9555	0.0014	2.9569
10	0.0630	2.5157	0.0627	0.0003	2.9558	0.0011	2.9569
11	0.0511	2.5668	0.0508	0.0002	2.9560	0.0009	2.9569
12	0.0421	2.6089	0.0419	0.0002	2.9562	0.0007	2.9569
13	0.0352	2.6441	0.0351	0.0001	2.9563	0.0006	2.9569
14	0.0298	2.6739	0.0297	0.0001	2.9564	0.0005	2.9569
15	0.0255	2.6994	0.0254	0.0001	2.9565	0.0004	2.9569
16	0.0220	2.7214	0.0220	0.0001	2.9565	0.0003	2.9569
17	0.0192	2.7406	0.0191	0.00005	2.9566	0.0003	2.9569
18	0.0168	2.7575	0.0168	0.00004	2.9566	0.0003	2.9569
19	0.0149	2.7723	0.0148	0.00003	2.9567	0.0002	2.9569
20	0.0132	2.7855	0.0132	0.00003	2.9567	0.0002	2.9569

[a]Include the pole contribution of 34 654.400 87.
[b]Include the E_{01P} contribution of −585.754 79.
[c]Include the $E_{01P} + \tilde{E}_{2P}$ contribution of −276.360 31.

example, electron screening and finite-nuclear size corrections to electron self-energies.

Choosing the $2s$ state of Li-like boron as an example, we start by using a Kohn-Sham potential for the $1s^2 2s$ ground state to account for the screening effect. Finite-nuclear size potential is modeled by a Fermi charge distribution with parameters $c = 1.8104$ fm and $t = 2.3$ fm. Partial wave results up to $\ell = 20$ are shown in Table III. Specifically, E_{MP} in column 2 and Sum_A in column 3 correspond to DJA results with one-potential expansions, while $\tilde{E}_{2P}$ in column 4, $E_{MP} - \tilde{E}_{2P}$ in column 5, and Sum_B in column 6 are DJB results with the additional two-potential expansions. High-ℓ corrections $\Delta\ell_{2,5}^{-4}$ to Sum_B from least-square rational polynomial fits of the form given in Eq. (38) are shown for $\ell \geqslant 5$ in column 7 and Total_B = Sum_$B + \Delta\ell_{2,5}^{-4}$ are shown in column 8. As in Tables I and II, the E_{MP}, Sum_A, and Sum_B terms have the pole and momentum-space terms included in the $\ell = 0$ partial waves so that the cumulative sums of Sum_A, Sum_B, and Total_B will converge to the self-energy $E_{2s}(5\alpha)$.

At the DJA level, it can be seen that $E_{MP}(20)$ only goes down to 0.0132 and Sum_A(20), at 2.7855, is far from convergence. With DJB, however, $E_{MP} - \tilde{E}_{2P}$ is already down to 0.0000 3 at $\ell = 20$ and Sum_B(20), at 2.9567, is nearly converged to the last digit. When high-ℓ corrections $\Delta\ell_{2,5}^{-4}$ are added, Total_B actually converges to 2.9569 with only eight partial waves even though high-ℓ correction is still rather large at 0.0025. While $\Delta\ell_{2,5}^{-4}$ continues to drop by an order of magnitude to 0.0002 at $\ell = 20$, Total_B remains constant to the fourth decimal point. This is a good check on the accuracy of the final result and affirms the use of high-ℓ extrapolation methods to accelerate the partial wave convergence. Comparing to the test case, it is clear that the DJB method converges much faster with non-Coulomb potentials even for higher-n ($2s$ vs $1s$) states. There is also no doubt that DJB is an important improvement over DJA even though the latter can give accurate enough results in most cases with larger partial wave expansions.

VI. CONCLUSION

We have deliberately used only a modest number of partial waves in this paper. This is because we wish to emphasize that relatively simple calculations can allow quite accurate self-energies to be computed. However, one application that requires extremely high accuracy is the self-energy of hydrogen. As with our test case, it has been evaluated with extremely high accuracy in Ref. [12]. Because that accuracy is needed in the treatment of the finite size of the proton, a check using different methods would be useful.

One of the advantages already present in the DJA method is the fact that the numerical methods used allow one to go up to values of $\ell \approx 60$, though extreme care and very fine radial grids are needed. In fact, it is possible to control the high-ℓ extrapolation so well that the DJB method is usually not qualitatively more accurate, but it works just as well as DJA with fewer partial waves and can deal with low Z better than DJA. DJB thus supersedes DJA as a general approach to self-energy calculations. However, calculations at $Z = 1$ of radiative corrections are particularly challenging even for DJB. Sophisticated summation schemes were required in the framework of the Mohr method in Ref. [12] to reach the very high accuracy results presented there. To reach similar accuracy with potential-expansion methods, many numerical issues would have to be addressed. Techniques that are more than adequate for calculations demanding parts per million accuracy may fail at higher levels.

We are at present working on evaluating the self-energy of hydrogen and hydrogenic ions with low Z. Because of the numerical problems that may be present that we have not detected, we are also looking into the use of different gauges. There are advantages to the use of both the Coulomb gauge and Yennie gauge that are known to help with the infrared behavior of radiative corrections [15]. While very accurate calculations have in fact already been carried out in Feynman gauge, getting the same result using another gauge would clearly be a check on the calculation and getting different answers could uncover numerical problems that had been missed. However, we conclude by emphasizing the utility and relative ease of using the DJB method described in this paper for those interested in evaluating the self-energy part of the Lamb shift.

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