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### RAPID COMMUNICATIONS

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#### Basis-set approach to calculating the radiative self-energy in highly ionized atoms

Steven A. Blundell and Neal J. Snyderman

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

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We present a complete numerical implementation of an alternative approach for evaluating the electron radiative self-energy in high- $Z$  hydrogenic ions. Using basis-set techniques, we demonstrate that the partial-wave expansion of the most numerically intensive term converges relatively rapidly as approximately  $1/L^3$ , making this an attractive calculational approach. Numerical results extrapolated to zero nuclear size are in agreement with Mohr [Ann. Phys. (N.Y.) **88**, 26 (1974); **88**, 52 (1974); Phys. Rev. Lett. **34**, 1050 (1975); Phys. Rev. A **26**, 2338 (1982)] for the  $K$  and  $L$  shells, and with the graphical results of Mohr and Kim (unpublished) for higher excited states. The algorithm is suitable for immediate generalization to non-Coulombic potentials.

The old problem of quantum electrodynamic (QED) corrections to atomic structure has recently acquired new significance on account of both experimental and theoretical advances. Experimentally, heavy atoms stripped of most of their electrons can now be studied with precision. For example, the  $2S_{1/2}$ - $2P_{1/2}$  transition in Li-like U has been measured to about 0.1 eV [1], and comparable accuracy has been obtained in a measurement of the  $3S_{1/2}$ - $3P_{1/2}$  transition in Na-like Pt [2] and  $4S$ - $4P$  transitions of Cu-like Th and U [3]. Theoretically, relativistic many-body calculations of the electronic correlation and Breit corrections to the Dirac Hartree-Fock approximation can now be performed with great accuracy for high- $Z$  ions with one electron outside a closed shell [4]. The remaining theoretical problem, then, is to compute the QED corrections, both to the single-particle levels in the many-electron atom and to the electronic correlations.

Of the QED corrections, the most important numerically, as well as the most difficult to calculate, is the radiative self-energy correction to single-particle levels. For high- $Z$  hydrogenic ions, Mohr and Kim [5] have recently presented results for the self-energy correction to excited states. These calculations generalized Mohr's algorithm for the  $K$  and  $L$  shells [6, 7], which involves highly accurate treatment of special functions particular to the point-nucleus Dirac-Coulomb problem. Con-

sequently, the extension of this work to many-electron ions is problematic, except for high- $Z$  He- and Li-like systems [8, 9]. There has also been progress by Cheng and Sapirstein [10] in extending earlier calculations by Desiderio and Johnson [11] and Cheng and Johnson [12], based in turn on the original approach of Brown, Langer, and Schaefer [13]. While this approach is more easily generalized to many-electron atoms [11], even for the  $K$ -shell hydrogenic problem there are troublesome convergence problems in both the partial-wave expansion and the photon frequency integration.

In this Rapid Communication we describe an alternative method for calculating the radiative self-energy, which we demonstrate to have rather rapid convergence properties, and which has a natural generalization to an arbitrary local potential. The approach is developed from the recent work of Snyderman [9].

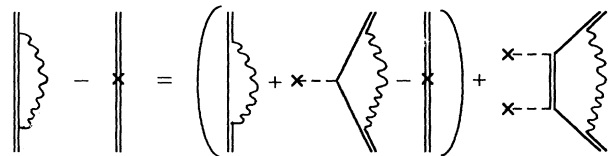


FIG. 1. Feynman diagrams for the bound-state radiative self-energy, and the decomposition used in this algorithm.

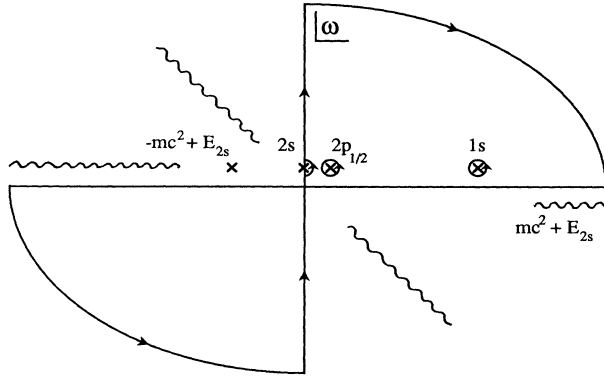


FIG. 2. Photon frequency plane singularities for the 2s-state hydrogenic self-energy graph. For finite nuclear size, the  $2S - 2P_{1/2}$  degeneracy is lifted. For the many-potential term there are multiple branch cuts at  $\pm mc^2 + E_{2s}$ , including those of the free electron propagators as well as the bound-state Green's function.

Part of the difficulty of the self-energy calculation arises because it is a difference of formally infinite quantities. In Fig. 1, the rearrangement of the Feynman graphs necessary to isolate the divergent parts is shown. The propagator for the virtual electron is expanded in terms of the binding potential  $V(r)$ . The first two terms together with the mass counterterm have canceling divergences. The last term is the finite *many-potential* term. This is the same grouping used by Baranger, Bethe, and Feynman [14] to isolate terms through order  $\alpha(Z\alpha)^5 mc^2$ , but here we evaluate to *all* orders in  $Z\alpha$  and  $\ln(Z\alpha)$ .

From Fig. 1, the *zero-potential* term is the matrix element between atomic states of the finite part of the free-electron self-energy, while the *one-potential* term involves an atomic matrix element of the finite part of the off-mass-shell vertex function [9]. The zero-potential term reduces to a single integral in momentum space, and the one-potential term to a triple integral.

The integration of the zero-potential term is straightforward. For the one-potential term, which contains integrable singularities and spikes, we have devised a weighted Gaussian integration scheme that gives five- or six-figure accuracy.

We now describe the numerical algorithm for the computationally intensive many-potential term. The photon frequency ( $\omega$ ) integral has the singularity structure shown in Fig. 2 for the particular case of a 2s atomic

$$E_{PV} = -\frac{\alpha}{\pi} \int_0^\infty d\omega \operatorname{Re} \sum_{i=1}^{2N} \frac{1}{E_A - E_i - i\omega} \times \left\langle \phi_i(-\omega) \psi_A \left| \alpha_1^\mu \alpha_{2\mu} \frac{1}{r_{12}} e^{-\omega r_{12}} \right| \psi_A \phi_i(\omega) \right\rangle, \quad (2)$$

where the sum over  $i$  is over all positive- and negative-energy states in the basis set for the potential  $V(r)$ . The states  $\phi_i(\omega)$  satisfy

$$\phi_i(\omega) = \sum_\alpha \psi_\alpha \frac{\langle \alpha | V(r) | i \rangle}{E_A - E_\alpha - i\omega}, \quad (3)$$

FIG. 3. Representation of the numerical calculation for the principal value contribution of the many-potential term. The heavy solid lines represent the effective wave functions  $\phi_i(\omega)$ .

state. The bound-state electron propagator contributes poles and branch cuts; the photon propagator gives branch cuts which pinch the real axis at the origin. To permit numerical evaluation of the  $\omega$  integral we rotate the contour to the imaginary axis, picking up pole terms from states of lower energy than the 2s, and a half-pole term from 2s itself. The remaining contour integral is then a principal-value integral, which we evaluate by Gaussian integration.

We express both the free-electron propagator and the electron propagator in the potential  $V(r)$  in the eigenfunction representation. Dirac eigenfunctions are solved for inside a cavity a few atomic units in radius, so that the positive and negative energy continua are discrete. The large and small radial wave functions are expanded in terms of  $N$  piecewise polynomials or *basis spline* [15] functions  $B_i(r)$ ,

$$\begin{pmatrix} g(r) \\ f(r) \end{pmatrix} = \sum_{i=1}^N \begin{pmatrix} c_i \\ d_i \end{pmatrix} B_i(r), \quad (1)$$

with coefficients determined by a variational principle. We thereby obtain a set of  $N$  positive-energy pseudostates and  $N$  negative-energy pseudostates and energy eigenvalues which we use to approximate sums over the infinite set of cavity states. For the basis set in the potential  $V(r)$ , the low-lying positive-energy states accurately approximate the discrete bound-state energies and eigenfunctions.

A compact and efficient way of using a basis set to evaluate the many-potential term is depicted graphically in Fig. 3. The principal-value part of the term is reexpressed as an effective exchange interaction between the atomic state of interest  $\psi_A$  and a frequency-dependent *effective basis state*  $\phi_i(\omega)$ ,

where the sum over  $\alpha$  is over all positive- and negative-energy free-electron basis states. For the single value  $i\omega = E_A - E_i$ , one may show  $\phi_i$  equals  $\psi_i$ , the  $i$ th basis state.

To illustrate the entire calculation, we give in Table I results for the 2s state of hydrogenic mercury,  $Z = 80$ . The basis set size ( $N = 110$ ) and the number of Gaussian

TABLE I. Self-energy of the  $2s$  state for hydrogenlike Hg ( $Z = 80$ ). The first two columns show the many-potential term for varying nuclear radii  $r_n$ ; the third gives the extrapolation to  $r_n \rightarrow 0$ . Nuclear charge density:  $\rho(r) = \rho_0 / \{1 + \exp[(r - r_n)/a]\}$ ,  $a = r_n/12.6$ . Units are rydbergs.

	$r_n = 6.6$ fm	$r_n = 3.3$ fm	Extrapolation <sup>a</sup> $r_n = 0$
Zero potential			-15.001
One potential			10.947
Principal value			
$L = 0$	-11.552	-11.555	5.744
$L = 1$	-4.274	-4.275	0.555
$L = 2$	0.184	0.184	0.184
$L = 3$	0.078	0.078	0.078
$L = 4$	0.039	0.039	0.039
$L = 5$	0.022	0.022	0.022
$L = 6$	0.013	0.013	0.013
$L = 7$	0.009	0.009	0.009
$L = 8$	0.006	0.006	0.006
$L = 9$	0.004	0.004	0.004
$L = 10-\infty$	0.015(2)	0.015(2)	0.015(2)
Pole terms			
$2s$	13.772	13.776	
$2p_{1/2}$	4.827	4.829	
$1s$	3.520	3.522	
Tot. many pot.	6.662(2)	6.666(2)	6.668(2)
Total			2.614(2)
Mohr <sup>b</sup>			2.616(3)

<sup>a</sup> The pole terms have been added on to the appropriate  $L$ -wave contribution.

<sup>b</sup> Reference [7].

points ( $n_G = 20$ ) in the  $\omega$  integration were increased until the digits shown were stable. The partial wave expansion was truncated at  $L = 9$ , and the contribution from  $L = 10-\infty$  was estimated by fitting to a polynomial in  $1/L$ . The  $L$ th partial wave is seen to drop off asymptotically as roughly  $1/L^3$ . By varying the number of terms in the fit, as well as the form of the fitting polynomial, we estimate a numerical error of about 10% in the extrapolate. This is the leading numerical error in the entire calculation.

Since our numerical techniques have been designed and optimized for the finite nucleus problem (the Coulomb singularity in the point-nucleus wave function is not well represented by basis splines), we must extrapolate to zero nuclear size to compare with the point-nucleus results of Mohr. This we do by a three-point polynomial extrap-

olation, but we show only two nuclear sizes in Table I. The momentum-space wave functions for use in the zero- and one-potential terms are evaluated from the analytic point-nucleus expressions, so that no extrapolation is required here.

In Table II we summarize results for the  $1s$  state for several values of  $Z$ , and in Table III we give results for excited states for  $Z = 80$ , in each case after extrapolation to zero nuclear size. We find precise agreement with the published  $K$  and  $L$ -shell results of Mohr [6, 7]. We also agree with the graphical results of Mohr and Kim [5] for excited states.

In the Feynman gauge used here, there are substantial gauge-dependent cancellations between the zero-, one-, and many-potential terms. The cancellations be-

TABLE II. Self-energy of the  $1s$  state in hydrogenlike systems, after extrapolation to zero nuclear size. Units are rydbergs.

	$Z = 70$	$Z = 80$	$Z = 90$
Zero potential	-27.828	-32.176	-37.075
One potential	20.021	25.348	33.140
Many potential			
$L = 0-9$	17.106	22.042	28.063
$L = 10-\infty$	0.011(2)	0.017(3)	0.017(4)
Tot. many pot.	17.117(2)	22.059(3)	28.081(4)
Total	9.310(2)	15.231(3)	24.145(4)
Mohr <sup>a</sup>	9.311(2)	15.232(6)	24.152(11)

<sup>a</sup> Reference [6].

TABLE III. Self-energy of excited states of hydrogenlike Hg ( $Z = 80$ ), after extrapolation to zero nuclear size. Units are rydbergs.

	$2p_{1/2}$	$2p_{3/2}$	$3s$	$3p_{1/2}$	$3p_{3/2}$
Zero potential	-17.177	-15.122	-8.660	-9.381	-8.657
One potential	10.400	9.279	6.357	6.292	5.841
Many potential					
$L = 0 - 9$	7.000	6.166	3.074	3.163	2.911
$L = 10 - \infty$	0.015(2)	0.015(2)	0.019(2)	0.018(2)	0.019(2)
Tot. many pot.	7.015(2)	6.181(2)	3.093(2)	3.182(2)	2.930(2)
Total	0.238(2)	0.338(2)	0.789(2)	0.093(2)	0.114(2)
Mohr <sup>a</sup>	0.2386(4)	0.3383(5)			
	$3d_{3/2}$	$3d_{5/2}$	$4s$	$4p_{1/2}$	$4p_{3/2}$
Zero potential	-9.223	-8.985	-5.708	-6.029	-5.688
One potential	6.216	6.099	4.266	4.263	4.038
Many potential					
$L = 0 - 9$	2.977	2.889	1.753	1.789	1.682
$L = 10 - \infty$	0.019(2)	0.020(2)	0.018(2)	0.020(2)	0.019(2)
Tot. many pot.	2.996(2)	2.909(2)	1.771(2)	1.808(2)	1.701(2)
Total	-0.012(2)	0.022(2)	0.330(2)	0.043(2)	0.051(2)

<sup>a</sup> Reference [7].

come more severe for higher- $l$  states, because the physical self-energy is reduced by about one order of magnitude for each unit increase in  $l$ , while the zero-, one-, and many-potential terms have nearly the same size for all states of a given  $n$ . Thus our error remains roughly constant in absolute terms at about 0.002 Ry or 0.03 eV, but our fractional error increases sharply as  $l$  increases.

We believe that the accuracy of the method can be improved by eliminating the spurious gauge-dependent terms that dominate the zero-, one-, and many-potential terms. The Fried-Yennie gauge is known to have the desired property [16, 9]. Based on preliminary calculations of the many-potential term, we believe that the Coulomb gauge also has the desired property. Thus, at the expense of the additional formal complexity entailed by using either of these gauges, one may be able to achieve substantially improved accuracy without further refinement of numerical techniques.

In summary, we have shown that an alternative approach to calculating the self-energy is numerically feasible and, with relatively few partial waves, reproduces the known results for a Coulomb potential. Furthermore, the

approach can readily be generalized to any local binding potential  $V(r)$  with no significant change in numerical technique. The algorithm for the many-potential term generalizes immediately for any potential in configuration space. To generalize the zero- and one-potential terms requires only numerically determined momentum-space atomic wave functions. By using a relativistic Hartree-Fock-Slater potential, as done by Desiderio and Johnson [11] for the  $K$  shell, we can approximately account for screening corrections in many-electron atoms. A discussion of these considerations, together with more details of the numerical algorithms used above, is planned to be presented in a lengthier future publication.

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