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Final Technical Report

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Project: *The Screening of the Lamb Shift in Heavy Helium-like Ions*

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submitted by
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Introduction

The project was undertaken in collaboration with Dr. Neal Snyderman of Lawrence Livermore National Laboratory (LLNL) through a project under the directorship of Dr. Kennedy Reed of LLNL. It is a collaboration of the work started at LLNL during the summers of 1994 and 1995, and continued at Spelman College. Spelman students Adrienne Stiff and Joy Harris were supported under this project.

The main question under investigation was whether a Sturmian representation of the electron Green function[1] is suitable for numerical calculations of QED effects in high-Z helium-like atoms. The frequency-independent part of the two-photon exchange graphs was calculated with this representation and compared with the results of other recent calculations.[2,3,4] Only the Coulomb part of these graphs were calculated under this project.

The Two-Photon Graphs

The main focus of the calculation is the correlation graph ladder (Lγ) and crossed-ladder (Xγ) exchange of two photons. The Feynman diagrams are shown in Figure 1.

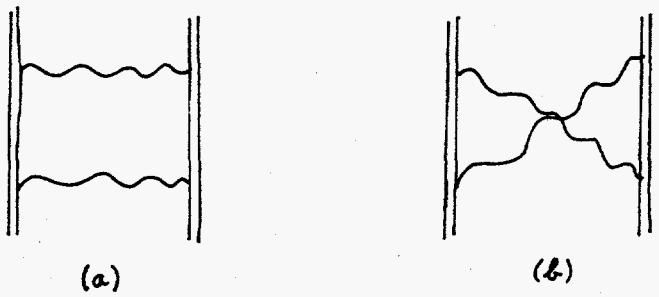

Figure 1. Feynman diagrams of two-photon exchange between bound electrons represented by the double lines.

The calculation for both graphs proceed approximately the same. Therefore, only one will be described. The calculation for the other graph is just a matter of changing the way that the external wavefunctions is linked to the photon. This will affect the spin-angular part of the calculation. For the ladder exchange graph in Figure 1a, the energy in natural units is given by[5]

$$\alpha^2 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \bar{\psi}_c(x)\, \gamma_\mu\, G(x,x'';E_A-\omega)\, \gamma_\nu\, \psi_A(x'')\, \bar{\psi}_D(x')\, \gamma^\mu\, G(x',x''';E_B+\omega)\, \psi_B(x''')$$

$$\frac{e^{i\omega|x-x'|}}{|x-x'|}\, \frac{e^{i\omega|x''-x'''|}}{|x''-x'''|}\, d^3x\, d^3x'\, d^3x''\, d^3x'''\, C^{j_A\, j_B\, J}_{m_A\, m_B\, M}\, C^{j_A\, j_B\, J}_{m_c\, m_D\, M'}, \qquad (1)$$

where *A,B,C.D* refer to the initial and final electron states; *G* refers to the Coulomb-Dirac Green function; and the magnetic quantum numbers of the Clebsch-Gordon coefficients are summed with the corresponding ones of the wavefunctions. In the photon propagators (the exponential), the ω in the exponents is more precisely $\sqrt{\omega^2+i\epsilon}$.

The integrals in equation (1) may be separated into a product of two double integrals if the Coulomb-Dirac Green function $G(x_1,x_2,E)$ may be written as a product of a function of x_1 and a function of x_2, which would greatly facilitate the calculation. This is usually not the case as it is written in terms of $x_< \equiv \min(x_1,x_2)$ and $x_> \equiv \max(x_1,x_2)$. However, there is a convenient representation described in the next section which accomplishes this, and it is used in the present calculation.

The Representation for *G*

The Coulomb-Dirac Green function is a 4X4 matrix. It is expanded in terms of the spin-angular eigenfunctions, $\mathcal{Z}_{\chi,m}(\theta,\phi)$, which are spinor matrices, to give[6]

$$G(x,x';E) = \sum_{\chi m} \begin{pmatrix} G^{11}_\chi(r,r';E)\, \mathcal{Z}_{\chi m}(\theta,\phi)\, \mathcal{Z}^{+}_{\chi,m}(\theta,\phi) & i\, G^{12}_\chi\, \mathcal{Z}_{\chi,m}\, \mathcal{Z}^{+}_{-\chi,m} \\ i\, G^{21}_\chi\, \mathcal{Z}_{-\chi,m}\, \mathcal{Z}^{+}_{\chi,m} & -G^{22}_\chi\, \mathcal{Z}_{-\chi,m}\, \mathcal{Z}^{+}_{-\chi,m} \end{pmatrix} \qquad (2)$$

The radial part, $G^{ij}{}_\kappa$, is expanded in terms of a Sturmian basis.[1] For example, for $G^{11}{}_\kappa$, it has the form[7]

$$G^{11}_\chi(r,r';E) \sim (r,r')^{\gamma-1}\, e^{-p(r+r')} \left\{ (\chi+\tfrac{\nu}{E}) \sum_{n=0}^{\infty} \frac{n!}{\Gamma(2\gamma+1+n)}\, \frac{L^{2\gamma}_n(x)\, L^{2\gamma}_n(x')}{n+\gamma+1-\nu} \right.$$

$$-\left[(\chi-\tfrac{\nu}{E})+2(\gamma+\nu)\right] \sum_{n=0}^{\infty} \frac{n!}{\Gamma(2\gamma+1+n)}\, \frac{L^{2\gamma}_n(x)\, L^{2\gamma}_n(x')}{n+\gamma-\nu}$$

$$\left. + \sum_{n=0}^{\infty} \frac{n!}{\Gamma(2\gamma+n)}\, \frac{L^{2\gamma-1}_n(x)\, L^{2\gamma}_n(x') + L^{2\gamma}_n(x)\, L^{2\gamma-1}_n(x')}{n+\gamma-\nu} \right\}, \qquad (4)$$

where

$$p = \sqrt{1-E^2}\ , \quad \chi = 2\rho n\ , \quad \omega = \frac{Z\alpha E}{\rho}\ , \quad \gamma = \sqrt{\chi^2 - (Z\alpha)^2}\ , \tag{4a}$$

and L^a_b are Laguerre functions. The main advantage that this representation has is that the argument of the Laguerre polynomials is x or x', and not $x_<$ or $x_>$. This allows the separation of the radial integrals which can now be performed and written as confluent hypergeometric functions, as is described in the next section.

The Frequency-Independent Calculation

The photon propagator in equation (1), the factor with the exponential, was used with $\omega = 0$, essentially the Coulomb potential. This is expanded in partial waves, i.e., spherical harmonics.[8] The integral in equation (1) is now evaluated. The calculation is separated into Coulomb-Coulomb (C-C, i.e., $\mu = \nu = 0$), Coulomb-Breit (C-B, i.e., $\mu = 0$, $\nu \neq 0$), and Breit-Breit (B-B, i.e., $\mu \neq 0$, $\nu \neq 0$). There is a pole at $\omega = 0$ in G for the $\kappa = -1$ or 2 term in the expansion in equation (2). The radial integrals for C-C in equation (1) are of the form

$$\int dn_1 dn_2 dn_3 dn_4\ (n_1 n_2 n_3 n_4)^2 \left[P(n_1)\, G^{11}_\chi(n_1, n_3; E_{1S} + i\omega)\, P(n_3) + P G^{12}_\chi Q + Q G^{21}_\chi P + Q G^{22}_\chi Q \right] \left(\frac{n_<^{\ell_1}}{n_>^{\ell_1+1}} \right)_{12} \left(\frac{n_<^{\ell_2}}{n_>^{\ell_2+1}} \right)_{34} \tag{4}$$

$$\left[P(n_2)\, G^{11}_\chi(n_2, n_4, E_{1S} - i\omega)\, P(n_4) + P G^{12}_\chi Q + Q G^{21}_\chi P + Q G^{22}_\chi Q \right],$$

where P and Q are the upper and lower radial eigenfunctions, respectively. The radial components of G, denoted G^{ij}_κ, are now written as in equation (4). Thus, they are products of Laguerre polynomials. With this representation for G, the integral in equation (4) can be written as a product of two double integrals with variables r_1, r_2 and r_4, r_4. A typical integral, then, is of the form

$$\int dn_1 dn_2\ e^{-an_1} e^{-bn_2}\ \frac{n_<^{\ell}}{n_>^{\ell+1}}\ n_1^k n_2^j\ L^{\beta_1}_{n_1}(c_1 n_1)\ L^{\beta_2}_{n_2}(c_2 n_2)\ , \tag{5}$$

where the exponential factors are from the radial eigenfunctions. By writing out the Laguerre polynomials, each term integrates to a confluent hypergeometric function. Thus, equation (5) is a double sum of these confluent hypergeometric functions. The result of performing the integral in equation (5) is

$$\sum_{s=0}^{n_1}\sum_{t=0}^{n_2}\frac{\Gamma(n_1+\beta_1+1)\,\Gamma(n_2+\beta_2+1)}{\Gamma(n_1-s+1)\,\Gamma(\beta_1+s+1)\,\Gamma(n_2-t+1)\,\Gamma(\beta_2+t+1)}\frac{(-c_1)^s(-c_2)^t}{s!\,t!}\rightarrow \tag{6}$$

$$\times\frac{\Gamma(k+j+s+t+1)}{(a+b)^{k+j+s+t+1}}\left[{}_2F_1\left(1,k+j+s+t+1,k+s+l+2,\frac{a}{a+b}\right)+{}_2F_1\left(1,k+j+s+t+1,j+t+l+2,\frac{b}{a+b}\right)\right.$$

These finite series were evaluated using the software Mathematica.

The radial integrals were performed for about 8 to 10 values of ω. In order to complete the ω-integration, the results were fitted to a curve separately for $\omega < 1$ and $\omega > 1$ and the ω-integral in equation (1) performed using these fitted functions. The results for the calculations we performed are summarized in Tables 1 and 2.

Table 1. Pole contributions to the ladder (Lγ) and crossed-ladder (Xγ) graphs, where $Z = 100$. The numbers are in atomic units.

	Lγ	Xγ	Total
C-C, κ = -1	-0.105491	-0.105491	-0.210982
C-B, κ = -1	-0.084417	-0.084417	-0.168844
B-B, κ = -1	-0.012411	+0.004104	-0.008207
B-B, κ = +2	0	+0.002542	+0.002542
			-0.485481

From reference [4] where ΔE = -0.48100 a.u. for the result in Table 1, one sees that our calculation compares favorably. The difference is probably due to the nuclear size effect which was accounted for in the calculation in reference [4], but it was not accounted for in our calculation.

Table 2. The results for various contributions of the various values of κ in the electron Green function for C-C. Energies are in atomic units.

κ	C-C
-1, pole	-0.210984
-1	-0.04129
+1	-0.00495
-2	-0.02444
+2	-0.00058
-4	-0.00465
+4	-0.00040
-4	-0.00255
	-0.27764

The non-pole terms were evaluated for various values of κ. The results are given in Table 2. The κ-values from +4 to ∞ were approximated and added to the total in Table 2 to get a value -0.282 a.u. The result from relativistic many body perturbation theory from reference [4] is -0.27690 a.u. Again, the difference is probably due to the nuclear size effect not accounted for in our calculation.

Summary and Conclusions

The favorable comparison of our results to the results of other calculations establishes this method as suitable for high-Z atomic structure calculations. This method utilizes a Sturmian representation for the electron Green function. This representation overcomes some of the numerical difficulties and could yield analytic results for various radial integrations in terms of confluent hypergeometric functions as it does in the present calculation.

Future calculations are: 1) complete the C-B and B-B contributions to the present calculation along with more values of κ; 2) include a frequency-dependent photon propagator; 4) apply the method to other calculations such as other Feynman graphs or to excited states or to Li-like atoms.

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