Addendum to "Effects of transverse photon exchange in helium Rydberg states: Corrections beyond the Coulomb-Breit interactions"

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We present numerical results for the correction potential beyond the Coulomb-Breit and the Araki-Sucher interaction potentials due to transverse photon exchange between the Rydberg electron and the core in helium Rydberg atoms.

In an earlier paper, Au[1] has shown that the effective potential due to transverse photon exchange between the Rydberg electron and the core ion in helium Rydberg atoms is fairly well represented at short distances by the Breit and Araki-Sucher interactions. However, at larger distances, as might be the case in high-Rydberg states of helium, this approximation may be inadequate. Au pointed out that this approximation can be corrected by an effective potential V'' that accounts for the difference between the actual effective potential and the Breit and Araki-Sucher interaction potentials. In terms of the generalized oscillator strengths f_j and the excitation energies ω_j of the core He^+ ion, this potential V'' can be expressed as

$$V''(R)=\frac{\alpha^4 a^2}{\pi R^6}\sum_j{}' \frac{f_j}{\omega_j^3} Q''(\omega_j R) , \tag{1}$$

where the prime over the summation sign indicates inclusion of the continuum, a is the Bohr radius, α is the fine-structure constant,

$$Q''(z)\equiv Q'(z)-\frac{\pi z^2}{2}\frac{7z^3}{6} , \tag{2}$$

TABLE I. The effective potential $V'(R)$ due to transverse photon exchange between the outer electron and the core ion in helium Rydberg atoms and its excess over the Breit and Araki-Sucher potentials $V''(R)$. R is the distance in Bohr radii a, and the potentials are given in natural units of $1/a$ where $1/a$ is the Hartree (2 Ryds). d is the scale distance defined in the text. The numbers in square brackets indicate powers of 10 to be multiplied.

d	R	V'	V''
1[−4]	3.426[−3]	7.052[+02]	2.340[−06]
1[−3]	3.426[−2]	7.050[−02]	2.324[−08]
1[−2]	3.426[−1]	7.026[−06]	2.229[−10]
1[−1]	3.426[00]	6.809[−10]	1.830[−12]
1[+0]	3.426[01]	5.372[−14]	9.385[−16]
1[01]	3.426[02]	1.943[−18]	2.108[−17]
1[02]	3.426[03]	2.668[−23]	2.551[−20]
1[03]	3.426[04]	2.767[−28]	2.612[−23]
1[04]	3.426[05]	2.777[−33]	2.618[−26]
1[05]	3.426[06]	2.778[−38]	2.619[−29]

$$Q'(z)\equiv P(z)-\frac{3\pi}{2}+\frac{11z}{4} , \tag{3}$$

$$P(z)\equiv\frac{13z}{4}-\frac{z^3}{2}+(3-5z^2+z^4)f(2z) +(6z-2z^3)g(2z) , \tag{4}$$

and f and g are the auxiliary functions for the sine and cosine integrals.[2] In comparison, the effective potential corresponding to transverse photon exchange in the electric-dipole approximation V' is given by[3,4]

$$V'(R)=\frac{\alpha^4 a^2}{\pi R^6}\sum_j{}' \frac{f_j}{\omega_j^3} Q'(\omega_j R) . \tag{5}$$

The small and large argument expansions of P give

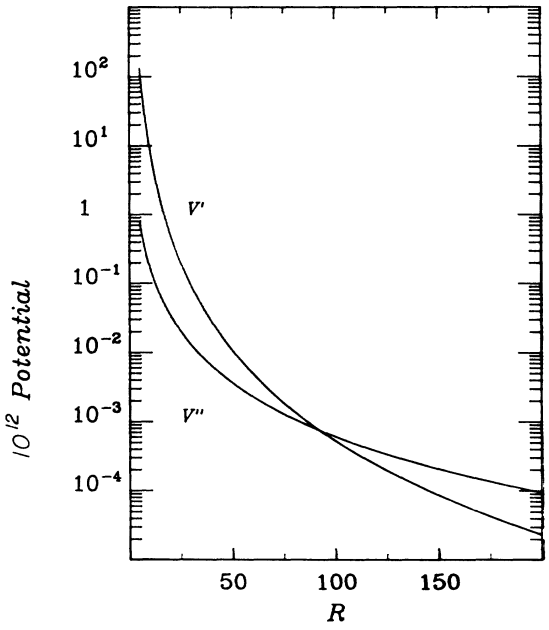

FIG. 1. The effective potential $V'(R)$ due to transverse photon exchange between the outer electron and the core ion in helium Rydberg atom and its excess $V''(R)$ over the Breit and Araki-Sucher interaction potentials. The distance R is in units of the Bohr radii a and the potentials are in natural units of $1/a$.

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$$\lim_{z\to 0} P(z)=\frac{z}{8}\left[\frac{12\pi}{z}-22+4\pi z-\frac{28z^2}{3}+\frac{8\pi z^3}{3}+\frac{[165\gamma+165\ln(2z)-193](2z)^4}{225}+\frac{\pi(2z)^5}{6}\right.$$
$$\left.-\frac{(4830\gamma+4830\ln(2z)-8831)(2z)^6}{44100}+O(z^7)\right], \tag{6}$$

and

$$\lim_{z\to\infty} P(z)=\frac{23}{4z}-\frac{129}{8z^3}+\frac{639}{4z^5}+O(z^{-7}) . \tag{7}$$

The small argument expansion of P given in Eq. (6) follows from the series expansions of the auxiliary functions f and g. We see that Q'' corresponds to having the first four terms in the small argument expansion removed from P. Thus the accurate numerical computation of Q''

TABLE II. The expectation values of V' and V'' for various states.

N	L	$\langle V'\rangle$ (kHz)	$\langle V''\rangle$ (kHz)	N	L	$\langle V'\rangle$ (kHz)	$\langle V''\rangle$ (kHz)
3	2	45 969.5	250.634	12	2	918.985	3.489 17
4	2	21 923.8	102.036		3	145.474	2.104 71
	3	2 969.20	63.7631		4	37.1501	1.399 31
5	2	11 824.4	51.0162		5	12.3191	0.988 72
	3	1719.37	31.5641		6	4.811 74	0.728 92
	4	382.044	21.5249		7	2.098 39	0.554 73
6	2	7031.16	29.0400		8	0.988 08	0.432 79
	3	1057.51	17.8386		9	0.490 72	0.344 55
	4	249.321	12.0792		10	0.252 35	0.278 94
	5	73.0762	8.690 57		11	0.132 12	0.229 07
7	2	4499.27	18.0721	13	2	724.360	2.737 20
	3	689.664	11.0426		3	114.933	1.649 05
	4	167.701	7.438 03		4	29.4504	1.094 96
	5	51.7193	5.323 91		5	9.811 67	0.772 69
	6	18.1319	3.974 84		6	3.856 56	0.568 93
8	2	3045.23	12.0014		7	1.695 99	0.432 44
	3	472.319	7.304 01		8	0.807 54	0.336 98
	4	116.987	4.900 13		9	0.407 08	0.267 96
	5	37.1181	3.493 56		10	0.213 63	0.216 70
	6	13.6085	2.598 34		11	0.115 08	0.177 77
	7	5.412 25	1.994 32		12	0.062 77	0.147 64
9	2	2153.71	8.373 31	14	2	580.949	2.186 89
	3	336.679	5.080 39		3	92.3483	1.316 16
	4	84.3945	3.397 80		4	23.7261	0.873 00
	5	27.2553	2.415 07		5	7.933 38	0.615 40
	6	10.2584	1.790 84		6	3.133 42	0.452 64
	7	4.24655	1.370 58		7	1.386 77	0.343 69
	8	1.85557	1.075 15		8	0.665 80	0.267 56
10	2	1577.85	6.073 02		9	0.339 29	0.212 56
	3	248.020	3.675 91		10	0.180 62	0.171 73
	4	62.6851	2.452 50		11	0.099 19	0.140 76
	5	20.4861	1.738 96		12	0.055 56	0.116 80
	6	7.842 45	1.286 45		13	0.031 39	0.097 98
	7	3.326 80	0.982 29	15	2	472.9805	1.774 88
	8	1.507 42	0.768 86		3	75.2965	1.067 28
	9	0.708 75	0.613 99		4	19.3862	0.707 29
11	2	1189.80	4.544 45		5	6.500 98	0.498 14
	3	187.775	2.745 46		6	2.577 48	0.366 08
	4	47.7411	1.828 17		7	1.146 38	0.277 73
	5	15.7337	1.293 78		8	0.553 90	0.216 03
	6	6.093 90	0.955 29		9	0.284 58	0.171 48
	7	2.627 37	0.728 09		10	0.153 10	0.138 44
	8	1.218 06	0.568 88		11	0.085 24	0.113 38
	9	0.592 06	0.453 51		12	0.048 62	0.094 02
	10	0.295 26	0.367 65		13	0.028 16	0.078 82
					14	0.016 41	0.066 71

requires extremely high precision in the numerical computation of f and g.

The potentials V'' and V' are calculated with the sum-over-state method as well as the finite-basis-set method, using the pseudostates given by Martin and Fraser[5] for a wide range of the distance R in the logarithmic scale. The results from either method are found to agree to within 0.1%. Table I shows the values of V' and V'' for various distances R calculated with the fine-basis-set method. Since for a He^+ ion core $2\omega R$ is of order $4\alpha R/a \equiv d$, we use a logarithmic scale for d. A much denser set of calculated data is used to generate the graphs shown in Fig. 1 (Ref 6). As the graph shows, V'' overtakes V' around $d \sim 1$ or more exactly around $R \sim 90a$. This indicates that for very high Rydberg states of helium, or for all the states of muonic helium, the use of the Breit and Araki-Sucher interaction potentials to approximate the effects of transverse photon exchange between the outer electron and the core is very inadequate. Table II gives the expectation values of V' and V'' in the various Rydberg states. The results for V' are in excellent agreement with those of Babb and Spruch.[7] For high-L Rydberg states, $\langle V'' \rangle$ accounts for a significant fraction of $\langle V' \rangle$. We remind the reader that $\langle V'' \rangle$ is to be added to calculations (such as those by Drake[8]) that use the Breit and Araki-Sucher potentials to account for the effects of transverse photon exchanges. Figure 2 is a graphical presentation of the values of $\langle V' \rangle$ and $\langle V'' \rangle$ for helium Rydberg states with principal quantum numbers 12 and 15.

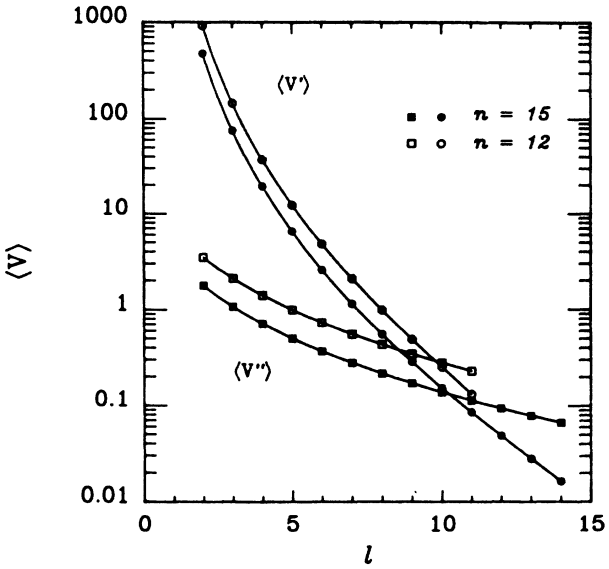

FIG. 2. The expectation values of V' and V'' for selected Rydberg states of helium with principal quantum numbers $n = 12$ and 15.

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