Rydberg states of He I using the polarization model

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The polarization-model calculation of the hydrogenic He I excited states ($l \geq 2$) is reexamined. Compact expressions for the $\langle nl | R^{-m} | nl \rangle$ matrix elements allow the elimination of spurious irregularities. The agreement with recent sophisticated calculations is greatly improved.

Recently, a great deal of attention has been devoted both experimentally[1] and theoretically[2-5] to an accurate determination of the hydrogenic ($l \geq 2$) excited states of neutral helium. Indeed, the basic stimulus to this study was mainly provided by the very accurate determination of the bound-state energies using microwave and microwave-optical-resonance spectroscopy.[1]

Sometime ago, I proposed[2] a polarization-model approach for the calculation of the He I Rydberg levels. Unfortunately, the numerical results were plagued with some errors arising mainly from the very tedious expressions we used for the hydrogenic matrix elements $\langle nl|R^{-7}|nl\rangle$. The corresponding discrepancies have led some authors[5] to distrust this polarization approach, which has the merits of simplicity and transparency. As a consequence, one may be inclined to consider that only sophisticated techniques based either upon the extrapolation of scattering data[4] or the use of Brueckner-Goldstone diagrams could produce quantitative agreements with experiment. The purpose of this work is to show clearly that this is not the case, and that the previous polarization approach[2] does not only provide a very transparent formula [Eq. (1) below] but also results in quantitative agreements with other techniques,[3-5] provided the ortho-para difference is ignored.

The basic assumption of the static polarization model[2] consists in the recognition of the preeminence of the configurations ($1s\, nl$) where the first electron remains in the ground state of He II, while the second travels between the excited states (n, l) labeled with the hydrogenic quantum numbers n and l. Moreover, the two electrons are supposed to remain distinguishable, so that any exchange effect (singlet-triplet) is neglected.

The main result of this analysis is the explicit formula

$$T_{nl} = T_\infty - R_{\mathrm{He}^4}\left(\frac{1}{n^2} + \langle nl\,|\frac{9}{32}R^{-4} - \frac{17.25R^{-6}}{64} - \frac{213}{256}R^{-7} + \cdots |nl\rangle\right), \tag{1}$$

with $T_\infty = 198\,310.750$ cm^{-1} and $R_{\mathrm{He}^4} = 109\,722.357$ cm^{-1}. R denotes the optical electron position. Equation (1) is made explicit with the hydrogenic matrix elements

$$\langle nl|R^{-4}|nl\rangle = \frac{3n^2 - l(l+1)}{2n^5(l-\frac{1}{2})l(l+\frac{1}{2})(l+1)(l+\frac{3}{2})}, \tag{2}$$

$$\langle nl|R^{-6}|nl\rangle = \frac{35n^4 - n^2[30l(l+1) - 25] + 3(l-1)l(l+1)(l+2)}{8n^7(l-\frac{3}{2})(l-1)(l-\frac{1}{2})l(l+\frac{1}{2})(l+\frac{3}{2})(l+2)(l+\frac{5}{2})}, \tag{3}$$

and[6]

$$\langle nl|R^{-7}|nl\rangle = \frac{63n^4 - n^2[70l(l+1) - 105] + 15(l-1)l(l+1)(l+2) - 20l(l+1) + 12}{8n^7(l-2)(l-\frac{3}{2})(l-1)(l-\frac{1}{2})(l+\frac{1}{2})(l+1)(l+\frac{3}{2})(l+2)(l+\frac{5}{2})(l+3)}. \tag{4}$$

Equation (4), explicated recently by Bockasten[7] through the relation

$$\langle nl|r^{-(m+2)}|nl\rangle = \left(\frac{2Z}{a_0}\right)^{2m+1}\frac{(2l-m)!}{(2l+m+1)!} \times \langle nl|r^{m-1}|nl\rangle, \quad l \geq \tfrac{1}{2}m,$$

obtained previously by many authors,[6] allows us to evaluate Eq. (1) in a much more secure way than previously.[2] In order to make contact with the dynamical-polarization-techniques[4] results, we also consider the term values in the form

$$T'_{nl} = \frac{10^6}{n^2} + \frac{T_{nl} - 198\,310.760}{0.109\,722\,357} \tag{5}$$

in units of 10^{-6} Ry, with T_{nl} in cm^{-1} given by Eq.

TABLE I. Polarization excitation energies T_{nl} (in cm^{-1}) and T'_{nl} (10^{-6} Ry) with the R^{-7} corrections included (columns 3 and 4) and neglected (columns 5 and 6).

n	l	T_{nl}	T'_{nl}	T_{nl}	T'_{nl}
3	2			186 106.060	−121.456
4	2			191 447.162	−54.232
4	3	191 452.005	−10.093	191 451.987	−10.254
5	2			193 918.746	−28.432
5	3	193 921.238	−5.718	193 921.224	−5.84
5	4	193 921.710	−1.419	193 921.710	−1.421
6	2			195 261.089	−16.656
6	3	195 262.535	−3.480	195 262.525	−3.570
6	4	195 262.817	−0.910	195 262.816	−0.912
6	5	195 262.885	−0.2916	195 262.884	−0.291
7	2			196 070.369	−10.564
7	3	196 071.280	−2.256	196 071.274	−2.319
7	4	196 071.467	−0.607	196 071.461	−0.608
7	5	196 071.506	−0.202	196 071.506	−0.202
7	6	196 071.519	−0.0779	196 071.519	−0.0779
8	2			196 595.568	−7.109
8	3	196 596.179	−1.539	196 596.174	−1.584
8	4	196 596.302	−0.421	196 596.302	−0.422
8	5	196 596.332	−0.143	196 596.332	−0.143
8	6	196 596.342	−0.0571	196 596.342	−0.0571
8	7	196 596.345	−0.0251	196 596.345	−0.0251
9	2			196 955.613	−5.10
9	3	196 956.043	−1.094	196 956.039	−1.21
9	4	196 956.130	−0.303	196 956.129	−0.304
9	5	196 956.151	−0.104	196 956.151	−0.104
9	6	196 956.158	−0.0424	196 956.158	−0.0424
9	7	196 956.161	−0.0192	196 956.161	−0.0192
9	8	196 956.162	−0.00935	196 956.162	−0.00935

(1).

In Table I, we display the numerical results for Eqs. (1) and (5) in columns 3 and 4. In order to get the $(n, 2)$ terms, and also to evaluate quantitatively the importance of the $\langle nl|R^{-7}|nl\rangle$ corrections in Eq. (1), we give in columns 5 and 6 additional data for T_{nl} and T'_{nl}, respectively, with this last correction put equal to zero. It turns out that the $\langle nl|R^{-7}|nl\rangle$ corrections are non-negligible mainly for $l \leq 3$. The T'_{nl} data are in excellent agreement with the singlet Temkin-Silver results.[4] Moreover, for $l \leq 3$ and the $\langle nl|R^{-7}|nl\rangle$ corrections present, they get closer to the polarized-orbital values, which are more accurate than the extended polarization results. Notice also the improved $T_{72} = 196\,070.359$ cm^{-1} value. Moreover, we display in Table II some T_{nG}-T_{nF} differences in order to demonstrate clearly that the irregularities referred to in Ref. 5 were only spurious ones and did not result from any shortcomings of the polarization-model approach.

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TABLE II. T_{nG}-T_{nF} level differences (in cm^{-1}).

n	T_{nG}-T_{nF}
7	0.181
8	0.123
9	0.087
10	0.064

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