Energy calculation of $^1S_e$ autoionizing states of He and H$^-$

Abstract. A serious error has been found in a previous calculation of the energy of the lowest $^1S_e$ autoionizing state of He and H$^-$ made by Holstein in 1958 using the 20-order subset in the basis. The error lies in the incorrect root which is associated with the state. New results obtained by re-examination of the particular roots associated with the two lowest autoionizing states are compared in detail with those obtained by experiment and other approximate methods.

When experimental results (Simpson et al. 1963, Rudd 1964) for the positions of the two lowest autoionizing states with specific symmetry $^1S_e$ of He became known, we wondered about the large discrepancy between the theoretical value obtained by the truncated scaling variation orthogonalization procedure (Holstein 1958 a) and the experimental value for the lowest state, in view of the striking agreement for the next state (Holstein 1958 b). This discrepancy stimulated us to make a re-diagonalization of the 1958 matrix of order 20. Unfortunately, the lowest roots were not mapped at this time for the 20-order subset, as was done for the lower subsets of order 4 and 10 (Holstein 1961-2; the same error appears also in this paper).

In the re-examination all the 10 lowest roots of the same (20 × 20) matrix are completely mapped by a continuous variation of the scale parameter within the range 0.20–0.50. The results of this scaling procedure show that the 1958 results for the root associated with the lowest state, denoted by asterisks in the table, are erroneous both for He and H$^-$. The erroneous results for the (2s2s) roots have obviously led to some misleading conclusions in the literature about the ability of the truncated orthogonalization procedure to ensure bounds on the true energies of the autoionizing states. It has often been argued that the convergence of the procedure will break down when more states in the basis are added. We are now making a new investigation of this matter in which additional states in the basis are included up to a maximum of 54. The results of this investigation will be published elsewhere.

The new results for the (20 × 20) matrix, experimental results and results obtained by other approximate methods are compared in the following table.
# Energy of the (2s^2)1S^o and (2p^2)1S^o states in units of Z^2 ryd

<table>
<thead>
<tr>
<th>Atom</th>
<th>States</th>
<th>Energy</th>
<th>Optimal scale parameter</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>2s^2</td>
<td>-0.38689(57.93)</td>
<td>0.38</td>
<td>57.9</td>
<td>57.83</td>
<td>57.94</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2p^2</td>
<td>-0.30945(62.14)</td>
<td>0.40</td>
<td></td>
<td>62.1</td>
<td>62.16</td>
<td>62.30</td>
</tr>
<tr>
<td>H^-</td>
<td>2s^2</td>
<td>-0.29183(9.63)</td>
<td>0.32</td>
<td>9.56</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

A, results by Simpson et al. 1963; B, result by Rudd 1964; C, results obtained by the Feshbach projection method (O'Malley and Geltman 1965); D, results obtained by the truncated diagonalization procedure (Lipsky and Russek 1966); a, most reliable experimental result (McGowan, private communication).

The unit of length is \( \frac{1}{2} a_0 Z^{-1} \). Energies above the ground state are given in parentheses in ev.

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