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SPECTROSCOPY OF HIGHLY-IONIZED HELIUM-LIKE AND LITHIUM-LIKE ATOMS

A.E. LIVINGSTON

Department of Physics, Notre Dame University, Notre Dame, IN 46556, U.S.A.

Abstract -- Recent precision spectroscopic measurements of 2s - 2p transition energies in high-Z helium-like and lithium-like ions are sensitive to relativistic and QED contributions. Comparisons are presented between the latest experimental results and theoretical calculations for these transitions along the helium-like and lithium-like isoelectronic sequences.

INTRODUCTION

The spectroscopy of highly-ionized atoms provides crucial tests of the capabilities of atomic structure calculations for high-Z few electron systems. Measurements of 2s - 2p transition energies in helium-like and lithium-like ions are capable of sensitivity to higher order relativistic and QED (Lamb shift) contributions at high Z. Recent precision measurements of such transition energies using vacuum ultraviolet spectroscopy have motivated interest in accurate theoretical calculations of excited state energies in these ions. An early discussion of the importance of such measurements in two and three electron systems was presented by Berry et al. (1). Several recent reports on experiment and on theory for both the helium-like and the lithium-like systems appear in the proceedings of the 1987 Symposium on Atomic Spectroscopy and Highly-Ionized Atoms (2). The reader is referred to these proceedings for experimental and theoretical background as well as for references to earlier work. The present paper is restricted to a discussion of the current status of measurements and calculations of 2s - 2p transition energies in highly-ionized two and three electron atoms.

HELIUM-LIKE IONS

The most precise values for the 1s2s 3S1 - 1s2p 3P0,2 transition energies in high-Z two electron ions are provided by fast ion (beam-foil) and recoil ion measurements that are sensitive to total Lamb shift contributions at the 1% level, which is comparable to the precision of n=2 Lamb shift measurements in high-Z one electron ions. This spectroscopic precision requires the measurement of transition wavelengths to ~10⁻²Å of the typical linewidths, and thus the understanding of the Doppler shifted wavelength scale to ~10⁻²Å. A recent review of the spectroscopy of two electron systems is given in reference 3. A survey spectrum of highly ionized sulfur produced by carbon foil excitation of 80 MeV sulfur ions (4) is shown in figure 1. The helium-like 1s2s 3S1 - 1s2p 3P0,2 transitions are observed, as are lithium-like and beryllium-like 2s-2p transitions and several hydrogenic transitions, the latter involving low-lying Rydberg states. Such 2s-2p and hydrogenic transitions are often suitable as reference lines for the helium-like measurements (5). However, hydrogenic structures in ions with four or more electrons are usually sufficiently perturbed to be inadequate for use as reference transitions (6).

Fig. 1. Fast-ion spectrum of foil-excited 80 MeV sulfur ions between 380-760 Å produced at the Notre Dame Tandem Accelerator Laboratory.

Fig. 2. Plot of Lamb shift contributions for the 1s2s \(^3S_1\) - 1s2p \(^3P_2\) transition in helium-like ions.
The electron screening corrections to the Lamb shift for helium-like 2s-2p transitions are expected to be a few percent of the total Lamb shift for Z=20-40 (7-10), so that current measurements are able to test these contributions to 10-50%. Figure 2 shows a plot of the contributions of the total Lamb shift and the estimated Lamb shift screening, expressed as a percentage of the 1s2s 3S_1 - 1s2p 3P_2 transition energy for helium-like ions. The screening effect is seen to grow with Z more slowly than the total Lamb shift by about one power of Z. A summary of the contributions to this transition energy as calculated by Drake (7) for helium-like nickel (Z=28) is given below.

<table>
<thead>
<tr>
<th>Contribution</th>
<th>Value (cm^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nonrelativistic</td>
<td>226,574</td>
</tr>
<tr>
<td>Relativistic</td>
<td>220,815</td>
</tr>
<tr>
<td>Mass polarization</td>
<td>-119</td>
</tr>
<tr>
<td>Nuclear size</td>
<td>-77</td>
</tr>
<tr>
<td>OED</td>
<td>-5267</td>
</tr>
<tr>
<td>Total</td>
<td>441,926 ± 74</td>
</tr>
</tbody>
</table>

The Lamb shift for the analogous hydrogen-like transition 2s_{1/2} - 2p_{3/2} for Z=28 is -5387 cm^{-1} (11), which when compared with the above tabulation enables the screening effects to be estimated. The theoretical uncertainty of 0.2 Z^4 a_0^4 represents an estimate of the size of uncalculated higher order terms.

Previous high-Z measurements for the 1s2s 3S_1 - 1s2p 3P_2 transition energy showed excellent agreement with theory for Z=14-17 (8), but suggested the possibility of a slight systematic discrepancy from calculations for Z=20-29 (3,12). However, the measurements for Z>17 all possessed sufficiently large uncertainties to preclude confirmation of this discrepancy. During the past year two new higher precision measurements have been reported, in nickel, Z=28 (5) and in krypton, Z=36 (13), both of which display excellent agreement with theory. The spectrum of nickel showing the 3S_1 - 3P_2 transition as well as nearby lithium-like and beryllium-like lines is shown in figure 3. Several of the transitions appear in the second order of dispersion.

Fig. 3. Portion of the fast-ion spectrum of highly-ionized nickel produced at the ATLAS facility at Argonne National Laboratory.
A list of wavelength values for the transitions used as reference lines in the nickel experiment appears below, including minor modifications of the list in reference 5, to which the reader is referred for the original sources.

<table>
<thead>
<tr>
<th>Spectrum</th>
<th>Transition</th>
<th>Wavelength (Å)</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>XXVI</td>
<td>2s $^2S_{1/2}$ - 2p $^2P_{3/2}$</td>
<td>165.40 ± 0.02</td>
<td>a</td>
</tr>
<tr>
<td>XXVI</td>
<td>6 - 7</td>
<td>182.75 ± 0.02</td>
<td>b</td>
</tr>
<tr>
<td>XXVII</td>
<td>5 - 6</td>
<td>102.15 ± 0.02</td>
<td>b</td>
</tr>
<tr>
<td>XXVI</td>
<td>5 - 6</td>
<td>110.15 ± 0.02</td>
<td>b</td>
</tr>
<tr>
<td>XXV</td>
<td>2s$^2$1S0 - 2s2p $^1P_1$</td>
<td>118.00 ± 0.01</td>
<td>a</td>
</tr>
<tr>
<td>XXV</td>
<td>2s2p $^3P_2$ - 2p $^2D_2$</td>
<td>120.52 ± 0.03</td>
<td>c</td>
</tr>
<tr>
<td>XXVI</td>
<td>2s $^2S_{1/2}$ - 2p $^2P_{1/2}$</td>
<td>234.14 ± 0.02</td>
<td>a</td>
</tr>
</tbody>
</table>

(a) Hinnov et al., tokamak plasma. (b) Calculated. (c) Edlén, semi-empirical.

The experimental result for nickel of 226.27 ± 0.04 Å tests the Lamb shift screening contribution to about 30%, which is approximately the same magnitude as the theoretical uncertainty for this transition energy.

A comparison between experiment and theory for the $^3S_1 - ^3P_2$ transition energy in the helium isoelectronic sequence is shown in figure 4. The data are plotted with respect to the theoretical values of Drake (7), and are scaled by $Z^4$ in order to provide a $Z$-independent display of the theoretical uncertainties. The confirmation of theory for this fine structure transition up to $Z=36$ provides motivation for precision measurements at higher $Z$, where the theoretical uncertainties are expected to be less reliable.

![Figure 4](image_url)

**Fig. 4.** Comparison of experiment and theory for the 1s2s $^3S_1 - 1s2p$ $^3P_2$ transition in helium-like ions, plotted with respect to the theoretical values of ref. 7. The experimental values are from references 3,5,12,13,14 and the theoretical values from (a) ref. 8, (b)&(c) ref. 9, (d)&(e) ref. 11.
For the $1s2s\,^3S_1 - 1s2p\,^3P_0$ fine structure transition there are no precision wavelength measurements available for helium-like ions with $Z>18$ (3), and thus the accuracy of theoretical calculations at high $Z$ has not been checked. It is noteworthy that for sulfur ($Z=16$) the measurement of reference 8 is in disagreement with the value calculated by Drake (7). This discrepancy has been confirmed for $Z=16$, although with a smaller deviation, by the newer measurement of reference 4. On the other hand, the recoil ion result for argon ($Z=18$) displays reasonable agreement with theory (14). A comparison of experiment with theory for this transition is shown in figure 5. It is apparent that additional precise high-Z measurements of the $1s2s\,^3S_1 - 1s2p\,^3P_0$ transition wavelength are needed in order to check the theoretical calculations. These measurements, in conjunction with those for the $^3S_1 - ^3P_2$ transition, will of course also provide values directly for the $1s2p\,^3P_2 - ^3P_0$ fine structure interval.

Fig. 5. Comparison of experiment and theory for the $1s2s\,^3S_1 - 1s2p\,^3P_0$ transition in helium-like ions, plotted as in figure 4.

LITHIUM-LIKE IONS

The $1s^22s\,^2S_{1/2} - 1s^22p\,^2P_{1/2,3/2}$ fine structure transitions in high-Z lithium-like ions possess similar total energies and Lamb shift contributions to their 2s-2p counterparts in helium-like ions. Figure 6 shows a plot of the total Lamb shift and the estimated Lamb shift screening, expressed as a percentage of the $^2S_{1/2} - ^2P_{1/2}$ transition energy for lithium-like ions. More extensive measurements are available for these ground state transitions at high $Z$ from spectra of solar flares, tokamak plasmas, and fast-ion excitation. However, available theoretical calculations for these transition energies show only fair agreement with experiment, primarily due to the absence of accurate calculations for the Lamb shift screening contributions. Very recent many-body calculations (15) have included explicit non-perturbative computation of higher order Breit interaction contributions for these lithium-like 2s-2p transition energies. This leaves only the QED contributions uncalculated and, by combining these new results with existing unscreened Lamb shift values (11), comparison with experiment yields an estimate of the Lamb shift screening contributions. Figure 7 displays such a comparison, by plotting experimental values for the $^2S_{1/2} - ^2P_{1/2}$ transition energy for lithium-like ions with respect to the combined theoretical values of references 11 and 15. The scaling of $Z^{2.5}$ is chosen simply to emphasize that the Lamb shift screening contribution appears to possess a uniform $Z^{2.5}$ dependence for $Z=10-36$. Both the variational screening results (1), curve (a), and the
Fig. 6. Plot of Lamb shift contributions for the $2s^2 S_{1/2} - 2p^2 P_{1/2}$ transition in helium-like ions.

Fig. 7. Comparison of experiment with theory for the $2s^2 S_{1/2} - 2p^2 P_{1/2}$ transition in lithium-like ions (see text for details of plot).
semi-empirical values (16), curve (b), begin to show slight deviations from experiment at high Z, although the semi-empirical extrapolation is based only upon data for Z<26. Curve (c) is the relativistic Hartree-Fock results of reference 17. All the experimental results for Z>26 are from recent tokamak spectra (18), with the exception of a new fast-ion value (13) for krypton, Z=36. The new many-body calculations and the recent high-Z experimental results provide incentive for explicit calculations of Lamb shift screening contributions in these lithium-like transitions. Measurements at higher Z will provide valuable tests of the apparent Z dependence of these screening effects.

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