TRANSITION PROBABILITIES FOR ATOMS

by

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TRANSITION PROBABILITIES FOR ATOMS

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Current status of advanced theoretical methods for transition probabilities for atoms and ions is discussed. An experiment on the $f$ values of the resonance transitions of the Kr and Xe isoelectronic sequences is suggested as a test for the theoretical methods.
Accurate transition probabilities for allowed and forbidden transitions of neutral atoms and ions are needed in a wide range of problems in atomic physics, astrophysics, and recently in the diagnostics of high temperature plasmas for magnetic fusion.

Theoretically, the interaction of a photon with an atom or ion is easier to describe than that of charged particles such as electrons and ions. Basically it reduces to calculating a transition matrix element of the form

\[ M_{AB} = \langle A | Op | B \rangle, \]

where \( A \) and \( B \) are the levels involved in the transition, and \( Op \) is an operator representing the multipole transition of interest. The actual form of the operator depends on the degree of sophistication (e.g., relativistic formulation, frequency dependence, etc.); nevertheless it is well defined.\(^1\) The traditional approach is to calculate wave functions for levels \( A \) and \( B \) separately, and then to evaluate \( M_{AB} \) from the wave functions. An alternative approach is to compute \( M_{AB} \) directly without producing the wave functions, as is done in the random phase approximation (RPA) and the many-body perturbation theory (MBPT).

In both approaches, the accuracy depends strongly how well the relativistic and electron correlation effects are accounted for. The relativistic effects are important only for medium to heavy atoms, mainly in transitions involving inner-shell electrons, although there are examples of the relativistic effects in the outer shells of heavy atoms.\(^2,3\) In the case of forbidden transi-
tions, relativity can be important even for low Z atoms as in the case of the M1 transitions $1s2s2^3S_1 \rightarrow 1s^21^1S_0$ near the neutral end of the He sequence.$^4$-$^7$ For the outer shells of neutral atoms and ions of low ionicity, the correlation effects are dominant. Thus, studies of transition probabilities along isoelectronic sequences provide fertile ground for testing various theories of the relativistic and correlation effects.$^8$-$^9$ Also, such a study readily identifies shifts in coupling schemes that often manifest themselves as level crossings and configuration mixing. Many articles have been published on the behavior of transition probabilities along isoelectronic sequences,$^{10}$-$^{14}$ but I shall focus on the resonance transitions of the Be I sequence to illustrate the relativistic and correlation effects.

In Figure 1, electric dipole oscillator strengths, $f$, for the $2s^21^1S_0 \rightarrow 2s2p^3,1^1P_1^o$ transitions of the Be-like ions are presented. The difference between the dotted curve and the lower solid curve as nuclear charge Z increases is due to the relativistic effects such as change in transition energies and contraction of wave functions. Shift from the LS to the jj coupling for high values of Z is responsible for the rise of the f values for the "forbidden" $^3P_1^o$ transitions. Disagreement at $Z = 4$ among various theoretical values of the oscillator strength results from different degrees of correlation effects accounted for in the theories cited.

For instance, the relativistic RPA results$^{15}$ for the $^1P_1^o$ transitions are superior to those from the relativistic multiconfiguration Hartree-Fock (MCHF) method,$^{10}$ particularly near the neutral end of the sequence. However, the
two methods produce practically identical results for higher Z values. The results for the singlet transitions from the Bethe-Goldstone method, though not shown in Figure 1, agree closely with the relativistic RPA results. On the other hand, for the triplet transitions, the RPA and the MCHF methods give different values for high Z ions such as Mo$^{38+}$. With the RPA method, the results for forbidden transitions are less reliable than those for allowed transitions.

The standard RPA method uses a single-determinant HF wave function as a starting point. As a result, the transition energies (or ionization potentials for photoionization) are not as reliable as the transition probabilities. The relativistic MCHF method can give better transition energies but it is less reliable than the RPA method in transition probabilities. Development of an RPA method that starts with MCHF wave functions will eventually eliminate most of the problems mentioned above. Current status of the relativistic MCHF, relativistic RPA, and MBPT methods are compared in Table I. At present, the MCHF method has less restrictions and is easier to use, but the results are less accurate than those obtained from the other methods.

Finally, I would like to mention an experiment that can be done with a synchrotron light source. In neutral Kr and Xe, the np$^6$ 1$S_0$ $\rightarrow$ np$^5$(n+1)s 3$P^o_1$ transitions are no more "forbidden" than the "allowed" 1$P^o_1$ transitions, as can be seen from Table II. The f values for the transitions are affected by the correlation effects both in the valence (5p) and inner (e.g., 4d) shells, and also by relativistic effects such as the spin-orbit interaction. The absolute f
values are not known accurately, experimentally, or theoretically. The lifetimes of the P levels are of the order of nanoseconds. Reliable experimental data on the f values or lifetimes for the resonance lines of Kr I and Xe I sequence—particularly near the neutral end—will help to test existing and new theories.

The author wishes to thank Professor W. R. Johnson and Dr. K. T. Cheng for valuable discussions.

Table I. Current Status of Advanced Theories for Transition Probabilities

<table>
<thead>
<tr>
<th></th>
<th>MCHF</th>
<th>RPA</th>
<th>MBPT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Open shell</td>
<td>yes</td>
<td>not yet</td>
<td>yes, in principle</td>
</tr>
<tr>
<td>Relativity</td>
<td>yes</td>
<td>yes</td>
<td>not yet</td>
</tr>
<tr>
<td>Continuum correlation</td>
<td>indirect, difficult</td>
<td>direct, RPA equation</td>
<td>direct, brute force</td>
</tr>
<tr>
<td>Gauge invariance</td>
<td>no</td>
<td>yes</td>
<td>depends</td>
</tr>
<tr>
<td>Accuracy</td>
<td>good</td>
<td>better</td>
<td>best, in principle</td>
</tr>
<tr>
<td>Isoelectronic sequences</td>
<td>yes</td>
<td>yes, but limited</td>
<td>not yet</td>
</tr>
</tbody>
</table>
Table II. Dipole Oscillator Strengths for the np $^6\,^1S_0 \rightarrow np\,^5\,(n+1)s\,^3,^1P_1^0$ Transitions of Kr and Xe.

<table>
<thead>
<tr>
<th>Level</th>
<th>$3P_{1}^0$</th>
<th>$1P_{1}^0$</th>
<th>$3P_{1}^0$</th>
<th>$1P_{1}^0$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Excitation energy, eV</strong></td>
<td>10.03</td>
<td>10.64</td>
<td>8.44</td>
<td>9.57</td>
</tr>
<tr>
<td><strong>f values</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Theory</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Relativistic Hartree-Fock$^{17}$</td>
<td>0.222</td>
<td>0.175</td>
<td>0.312</td>
<td>0.168</td>
</tr>
<tr>
<td>Effective operators$^{18}$</td>
<td>0.176</td>
<td>0.177</td>
<td>0.246</td>
<td>0.268</td>
</tr>
<tr>
<td><strong>Experiments</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lewis$^{19}$</td>
<td>0.204</td>
<td>0.184</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wilkinson$^{20}$</td>
<td>0.159</td>
<td>0.135</td>
<td>0.260</td>
<td>0.270</td>
</tr>
<tr>
<td>Chashchina and Schreider$^{21}$</td>
<td>0.21</td>
<td>0.21</td>
<td>0.28</td>
<td>0.23</td>
</tr>
<tr>
<td>Wieme and Mortier$^{22}$</td>
<td></td>
<td></td>
<td>0.214</td>
<td>0.180</td>
</tr>
<tr>
<td>Electron impact$^{23}$</td>
<td>0.173</td>
<td>0.173</td>
<td>0.26</td>
<td>0.19</td>
</tr>
<tr>
<td>Electron impact$^{24}$</td>
<td></td>
<td></td>
<td>0.183</td>
<td>0.169</td>
</tr>
</tbody>
</table>
References

*Work performed under the auspices of the U.S. Department of Energy.

9. C. F. Fischer, in Proc. 6th Intern. Conf. Atomic Physics, R. Damburg and
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    (1976); W. Fielder, Jr., D. L. Lin, and D. Ton-That, Phys. Rev. A 19,
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FIG. 1.—Dipole oscillator strengths for the np$^6 1S_0 + np^5(n+1)s \ 3P^0_1$ transitions of the Be sequence. The solid curves are the relativistic MCHF results (Ref. 10), the dotted curve is the non-relativistic MCHF results (Ref. 10), the triangles are the relativistic RPA values (Ref. 15), the circles are those from non-relativistic configuration-mixing calculations by Sims and Whitten (Ref. 25), and the squares are the values recommended by Smith and Wiese (Ref. 26). Note the different scales for the triplet and singlet transitions.