AN EVALUATION OF THE ACCURACY OF THE RELATIVISTIC DISTORTED-WAVE APPROXIMATION FOR THE CALCULATION OF CROSS SECTIONS FOR THE EXCITATION OF ATOMS BY ELECTRON IMPACT

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1. The Relativistic Distorted-Wave (RDW) method uses the standard formula for the T matrix for electron-atom scattering except that the target wave functions and distorted-waves are obtained as solutions of the Dirac equations. Thus the target states have wave functions for each fine-structure level which depend on the total angular momentum J of the atom including distinct energies for each level. The high energy behavior of the integrated cross sections depends on the J values of the initial and final levels for the excitation in question. The target wave functions are Dirac-Fock configuration-interaction wave functions obtained from the GRASP2K code and as such can reach arbitrary accuracy if enough configurations are included. Both the T-matrix and the Dirac equations for the distorted waves contain non-local exchange terms. The method is valid for incident electron energies exceeding two to three times the threshold value. Thus for excitation from the ground state of the noble gases, the method is applicable for incident energies of about 25 eV and above, less so for excitation from excited states where the threshold is smaller. Unitarization of the resulting cross sections would lower the energy at which this method is valid but would require an extensive set of cross sections, including elastic scattering from all of the levels included in the calculation of the target states.

2. The numerical methods used to obtain the target states, the distorted waves and the T-matrix elements are accurate to at least one part in $10^6$, well beyond the expected accuracy of the resulting cross sections. The method is valid for higher energies and does not give reliable cross sections near threshold and does not include any resonance behavior. Focusing on integrated cross sections, we note that for excitations where the direct term of the T matrix is non-zero, the majority of the contribution to the cross section comes from the forward scattering peak in the differential cross sections. For excitations which are solely due to the exchange of the incident electron with one of the bound target electrons, i.e. where the direct term of the T matrix is zero, significant contributions to the integrated cross section come from the whole angular range of scattering. The major source of uncertainty beyond the limitations of the method is the quality of the target wave functions themselves. In principle, these wave functions can be obtained from the GRASP2K code to arbitrary accuracy by including more states in the configuration-interaction description of the target. In practice, we are limited to a finite set of the most important configurations describing the target states.

3. The magnitude of the differential cross section for scattering at zero degrees is proportional to the optical oscillator strength calculated in the length formulation for the transition in question. (Note that in the discussion of my presentation, it was erroneously stated that the magnitude of the cross section was proportional to the square of the optical oscillator strength). Thus in order to ensure a correct magnitude of the integrated cross sections, the oscillator strength for the transition must be accurate. Extensive tables of experimental optical oscillator strengths for allowed transitions between fine-structure levels are available through the error estimates can be rather large. This detailed information provides another justification for the relativistic treatment of these electron excitation processes.

There are much less data available for direct excitations corresponding to transitions which are not optically allowed. One way to deal with this situation is to include intermediate levels in the description of the target wave functions which yield allowed optical oscillator strengths involving either the initial or final states of the excitation. (Note that the GRASP2K code produces these oscillator strengths as part of the calculations). Obtaining accurate values for both types of transitions indicates the accuracy of the target wave functions themselves.
There are other indicators of the accuracy of the target wave functions, such as the agreement between the length and velocity forms of the oscillator strengths, the energies of the various fine-structure levels and the correct energy ordering of these levels. Note that the geometric average of the length and velocity forms of the oscillator strength provides a result independent of the energy difference between the initial and final states of the transition, thus removing the influence of the errors in the calculated energy difference. However, it is the value of the oscillator strength in the length form that is proportional to the cross section and thus determines the accuracy of the final result.

This test of accuracy does not directly apply to excitations proceeding via exchange. However, obtaining accurate oscillator strengths involving the initial and final states of such excitation gives some confidence that the resulting cross section will be reliable. Nevertheless, the errors in such cross sections are likely to be larger in general that for cross sections for direct excitations.

BENCHMARK CALCULATIONS FOR ELECTRON COLLISIONS WITH COMPLEX ATOMS

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The B-spline R-matrix (BSR) approach [1,2] is based on the non-perturbative close-coupling method. As such it is, in principle, based on an exact expansion of the solution of the time-independent Schrödinger equation, as an infinite sum/integral of N-electron target states coupled to the wave function of the scattering projectile. The N-electron target states, again, can in principle be calculated with almost arbitrary accuracy using sufficiently large configuration-interaction expansions and the correct interaction hamiltonian. In practice, of course, the infinite expansions have to be cut off in some way and the exact hamiltonian may not be available. In the collision part of the BSR method, the integral over the ionization continuum and the infinite sum over high-lying Rydberg states are replaced by a finite sum over square-integrable pseudo-states. Also, a number of inner shells are treated as (partially) inert, i.e., a minimum number of electrons are required in those subshells.

There are several sources of errors that need to be considered. These include but are not limited to:

1) Errors in the structure description of the target states (energy levels, oscillator strengths, polarizabilities).
2) Errors associated with the cut-off in the close-coupling expansion, including inert subshells.
3) Approximations made in the treatment of relativistic effects.
4) Numerical approximations (integration/discretization schemes, use of an R-matrix box to account for exchange and full correlation only inside the box, etc.)

Similar to experiment, it is very difficult (if not impossible) to estimate systematic errors. Regarding the above sources of error, we will make a few statements below. These statements are most important for neutral targets, which are also the most difficult ones to deal with when it comes to correlation effects. We also emphasize that the uncertainty generally depends on several factors, such as the quantity of interest (rate coefficient, integrated cross section, differential cross section, specific transition, energy, etc). While it is impossible to make a general statement about the uncertainties that would cover (nearly) all cases, we will summarize a few important points. It is also critical to note that these statements are based on the assumption that no currently unknown effects, which one could classify as "new physics", are sufficiently important to change the outcome to the extent that the results really matter for plasma applications. Whether or not something really "matters", of course, depends on a sensitivity check, which would have to be carried out by the data user community.

1) The BSR approach with term-dependent (and hence non-orthogonal) orbitals allows for a highly accurate target description, which can be improved systematically, essentially limited only by the available computational resources. Hence we generally consider the associated error in the structure