BENCHMARK CALCULATIONS OF ATOMIC DATA FOR PLASMA AND LIGHTING APPLICATIONS

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Accurate and complete sets of atomic structure and collision data are important for many applications in plasma physics, in particular the modeling and diagnostic of discharges. In recent years, we have developed a general *B*-spline *R*-matrix (BSR) approach [1, 2] that has been applied with great success to the calculations of such data both for the target structure (energy levels and oscillator strengths) and electron collisions with atoms and ions. A general computer code of the nonrelativistic and semirelativistic versions, with the latter accounting for relativistic effects through the most important terms of the Breit-Pauli Hamiltonian, was published [3], and we now have a fully relativistic (Dirac) DBSR program working as well. The latter was already applied to a variety of heavy targets, including Cs [4], Au [5, 6], Hg [7, 8], and most recently the heavy noble gases Kr and Xe [9].

The principal idea behind these calculations is the solution of the close-coupling equations for electron scattering, using an *R*-matrix approach. The distinguishing features of our implementation compared to the well-known Belfast suite of computer programs [10] are i) the use of a highly flexible *B*-spline basis and ii) the possibility to employ non-orthogonal sets of one-electron orbitals. The latter generally allow for a highly accurate target description with relatively small (compared to standard approaches with orthogonal orbitals) configuration-interaction expansions.

Table 1: Selected target states of Hg used in the DBSR calculation [8]. Most of the experimental energies are taken from the NIST database [11], except for energies marked with an asterisk. The latter were given by Lear and Morris [12].

Configuration	Term	Expt. (eV)	Theory (eV)	Diff. (eV)
$6s^2$	$^1S_0$	0.000	0.000	0.000
$6s6p$	$^3P^o_0$	4.667	4.590	-0.078
$6s6p$	$^3P^o_1$	4.887	4.821	-0.065
$6s6p$	$^3P^o_2$	5.461	5.401	-0.060
$6s6p$	$^1P^o_1$	6.704	6.848	0.144
$6s7s$	$^3S_1$	7.730	7.794	0.064
$6s7s$	$^1S_0$	7.926	7.953	0.027
$5d^96s^26p$	$^3P^o_2$	8.541	8.533	-0.007
...				
ionization limit		10.438		
$5d^96s^26p$	$^3F^o_2$		10.602	
$5d^96s^26p$	$^3P^o_1$	11.005	11.104	0.099
$5d^96s^26p$	$^3P^o_0$		11.111	
$6p^2$	$^3P_0$	11.170	11.224	0.054
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Table I shows a small selection of the target states included in the recent calculation for e−Hg collisions [8]. We see that the DBSR method allowed us to reproduce all excitation energies with an accuracy of better that 0.15 eV, including the core-excited states.

The oscillator strengths for transitions from the ground state and the corresponding contributions to the polarizability are given in Table II. The result for the $(6s^2)^1S_0 \rightarrow (6s6p)^1P^o_1$

Table 2: Contributions to the static dipole polarizability of the Hg ground state in the DBSR model. Here kp,kf and np,nf stand for contributions from the ionization continuum and the remaining states in the Rydberg series. The oscillator strengths are given as the unweighted average of several sets of experimental values. See Migdalek [13] for references and more details.

Upper level	oscillator strength	polarizability (a_0^3)	experiment
$(5d^{10}6s6p)^1P_1^o$	1.147	18.474	1.16
$(5d^{10}6s6p)^3P_1^o$	0.018	0.435	0.024
$(5d^{10}6s7p)^1P_1^o$	0.022	0.208	
$(5d^{10}6s8p)^1P_1^o$	0.019	0.154	
$(5d^96s^26p)^1P_1^o$	0.203	1.583	
$(5d^96s^26p)^3P_1^o$	0.495	2.976	
$(5d^96s^26p)^3D_1^o$	0.182	0.994	
$(5d^96s^27p)^1P_1^o$	0.086	0.386	
$(5d^96s^28p)^1P_1^o$	0.027	0.110	
$(5d^96s^27p)^3P_1^o$	0.044	0.154	
$6skp$		3.426	
$5d^96s^2(np+kp)$		2.143	
$5d^96s^2(nf+kf)$		2.993	
Total		34.036	33.9 [14]

resonance transition obtained using the above method is close to the average value of the available experimental results. This transition provides the principal contribution to the polarizability of the ground state. Nevertheless, core excitations to the $5d^96s^2np$ and $5d^96s^2nf$ states are also very important, along with excitation to the $5d^{10}6snp$ Rydberg and $5d^{10}6skp$ continuum states.

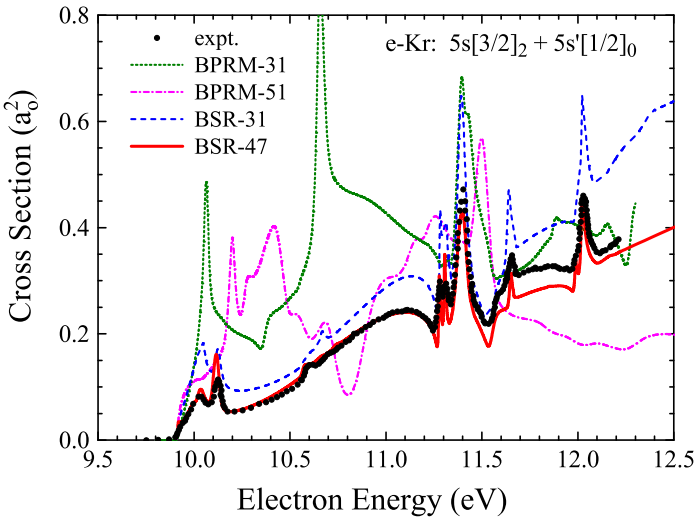

Fig. 1: Metastable electron-impact excitation function of the $4p^55s$ ($J=0,2$) states in Kr [9]. The experimental data of Buckman *et al.* [15] are compared with 31-state (BSR-31) and 47-state (BSR-47) results as well as predictions from previous 31-state (BPRM-31) [16] and 51-state (BPRM-51) [17] standard Breit-Pauli *R*-matrix calculations. The published experimental data were multiplied by 0.67 for a good visual fit to the BSR-47 results. The BSR predictions include cascade contributions from all higher-lying states included in the respective models.

Figure 1 shows the electron-impact metastable excitation function in Kr, i.e., the angle-integrated cross section for excitation of the $4p^5 5s$ ($J = 0, 2$) states [9]. The 31-state (BSR-31) model already dramatically improves the agreement between theory and experiment [15] compared to the previous standard Breit-Pauli *R*-matrix calculations by Zeman *et al.* [16] (BPRM-31) and by Bartschat and Grum-Grzhimailo [17] (BPRM-51). Nevertheless, there are still small problems regarding the near-threshold resonance structure. These problems, however, are removed by the 47-state BSR-47 model, which produces excellent agreement with the measured energy dependence. Note, however, that the published data of Buckman *et al.* [15] were multiplied by 0.67 in order to obtain a good visual fit to the BSR-47 results. This factor is well within the experimental uncertainty of the absolute normalization [18].

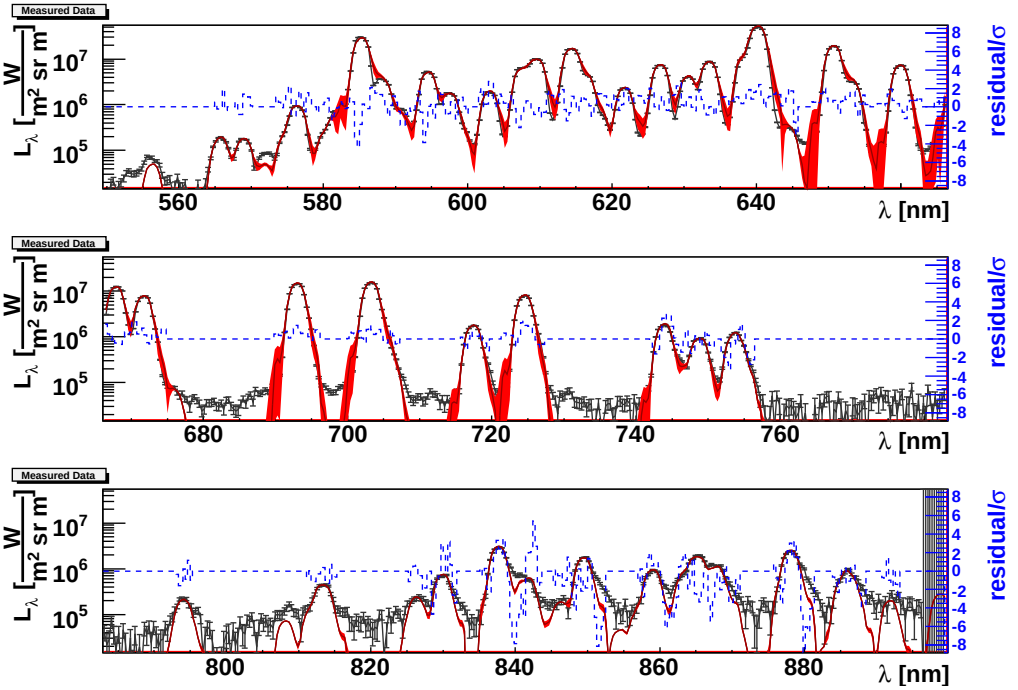

Fig. 2: Intensity of light emitted from a neon discharge as a function of wavelength. The light-colored (red) curve depicts the modeled spectrum, including the uncertainty of the apparatus function. The measured spectrum with the experimental error bars is partly hidden behind the modeled spectrum. The dashed (blue) line represents the difference between model and measurement in units of standard deviations. For details, see [19].

Figure 2 exhibits an example where BSR results for oscillator strengths and electron collision cross sections were used to model the intensity of light from a neon discharge over a wide range of wavelengths [19]. The dashed (blue) curve shows the difference between model and measurement in units of standard deviations. It can be seen that almost every feature of the neon spectrum in the considered range of wavelengths is incorporated in the model (note the logarithmic scale). This is possible due to the extensive set of atomic structure and collision data available from the BSR calculations.

More examples will be presented at the conferenece, in order to provide an overview of what theory can do today and where its current limitations are. Anticipated directions of future developments will also be discussed.

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