An Integrated Approach to Bound and Continuum States: Application to Beryllium-like Ions

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Modern research in the theory of atomic physics is characterised by a desire to understand the collective behavior of charged particles and their response to added energy or radiation, from quantum-mechanical first principles (*ab initio*); the concomitant aim being the quantitative prediction of atomic properties and the establishment of standards for areas of science and technology where atoms play a role – whether in laboratory plasmas or in environments such as astrophysics.

Because of the implied *ab initio* approach, the theme of much recent research is the incorporation of more effects into the wavefunction: the unification of processes formerly treated as independent. So atomic properties associated with bound and continuum states, electron impact excitation and ionization cross sections, photon excitation and ionization, and fine-structure levels, can be calculated in an integrated way. [1]

Resonances are perhaps the most obvious manifestation of interference effects in quantum mechanics. One of the most widely used, and perhaps most fully developed, of the sophisticated models available to atomic physics is the R-matrix approach [2]. This model was first introduced in nuclear physics specifically to study resonance reactions[3], the idea being that a resonance could be described in terms of the colliding particles forming a compound state, the total wavefunction being expanded as a complete set of these states. The complicated interaction zone, the internal region of configuration space, is delineated by a sphere of radius $r = a$ around the centre of mass, with the external region reducing to a simpler two-body problem. These ideas were developed for atomic physics by Burke and others and encapsulated in a computer program package for electron scattering and photoionization from atoms and ions [4].

It may seem suprising for a method originating in the study of resonances and continuum processes, but R-matrix techniques – and indeed any multiconfigurational close-coupling approach – can be applied to the bound state problem with great success.

This was exploited in the drive for quality data for stellar opacity applications by Seaton and others [5], who extended the R-matrix method and programs to photoabsorption processes relevant to stellar envelope opacities, in particular for bound-bound and photoionization transitions. The Opacity Project (OP) provided an important data base for atomic physics, the TOPBASE facility at the Centre de Donnèes Astronomiques de Strasbourg [6].

Within this paradigm, we are now concerned to explore the potential of close-coupling *ab initio* methods for high precision atomic structure calculations. Particularly for excited and continuum states, such methods should eventually be superior to atomic structure methods which use the same functional basis from $r = 0$ to $r = \infty$. Recent developments are again based on the R-matrix model, within the high optimization offered by close-coupling. These include exploitation of the 'QB' method[7] for systematic resonance analysis, use of target 'core base states' and pseudo-states for accurate representation of inner-shell and continuum processes, and incorporation of radiative and relativistic effects via the Opacity Project codes together with terms of the Breit-Pauli Hamiltonian.

Table 1: Comparison of $2s^2 - 2s2p$ gf-values for C^{++} $J = 0^e - 1^o$, taken from the recent R-matrix calculation of all bound and autoionizing fine-structure energy levels to $n = 10$ [10], with other theories (OP [5], CIV3 [12] and MCHF [13]) and experiments.

Transition	Present[10]	NIST[8]	Other
$2s^2 - 2s2p^3P_1^o$	1.93E-7	1.87E-7	1.89±0.07E-7[12], 1.87±0.002E-7[9]
$2s^2 - 2s2p^1P_1^o$	0.761	0.759	0.780[5], 0.757[13], 0.754±0.014[11]

Oscillator strengths for all ions of C, N and O were subject to a review and assessment by Wiese et al in 1996 [8]. This review, together with a more recent lifetime measurement on C^{++} using the heavy ion storage ring at Heidelberg [9], provide a sensitive test of theory. Using the theoretical techniques described above, a complete set of data has just been calculated [10] for fine-structure energy levels for bound and autoionizing states of the form $1s^2 2snl$ and $1s^2 2pnl$ ($J = 0^e$ and $J = 1^o$) up to $n = 10$ for the Be-like ion C^{++}, together with electric dipole oscillator strengths whose accuracy is estimate to be within ∼3% by comparison with experiment (table 1). Work is progressing on other ions, for example Ne, Ar, P and Cl, to upgrade the OP database and to extend it to fine-structure transitions.

In a higher energy regime, similar theoretical techniques can be used to quantify so-called 'hollow atom' effects. Although the methods are developed for complex atoms, consider the four-body problem in atomic physics, which is the simplest system to show hollow atom interference between direct and indirect ionization involving excitation-autoionization and triply excited intermediate states. In the particular case of hollow lithium, this occurs when both K electrons from the ground state configuration become excited into the L shell during a collision, and there has been much interest in the properties of this system. In a recent application of the R-matrix and QB method (described above), hollow atom interference effects and resonances in Li have been examined and quantified. Outer-shell and inner-shell effects, excitation and ionization channels, direct and indirect ionization processes, resonant and non-resonant behavior are combined for photon and electron impact processes. This includes resonance analysis (table 2), electron impact ionization of ground state Li^+ and photoionization of Li (table 3), electron excitation and ionization of metastable states and double photoionization. Good agreement with experiment where available is obtained, with a tabulation of all 480 $2l2l'nl''$ states for $n \leq 9, l'' \leq 3$, and a demonstration of the chaotic behavior of overlapping series [14].

These bound and continuum state techniques are in progress to being extended to more complex atoms, particularly for atoms (eg. C, O, Ne, Mg etc.) where there is current interest in the dynamics of atoms and ions at X-ray energies in astrophysical and technology applications.

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Table 2: Li resonances coupled to $2s^2\ ^1S$: effective n and width (Γ meV). Identifications (ID) assume a $2s^2$ core, except those labelled ^3P ($2s2p$) and $Q \equiv 2s2p^2$.

ID	$n_{^1S^e}$	Γ	ID	$n_{^1S^e}$	Γ	ID	$n_{^1S^e}$	Γ	ID	$n_{^1S^e}$	Γ
	$^2\mathbf{S}^e$			$^2\mathbf{P}^o$			$^2\mathbf{D}^e$			$^2\mathbf{F}^o$	
Q	1.664	82	$2p$	1.215	123	Q	1.425	98	$4f$	3.985	0.9
$3s$	2.243	141	$2p^3$	2.239	55	$3d$	2.968	97	^3P3d	4.490	4.8
$4s$	3.181	22	$3p$	2.430	65	^3P3p	3.244	17	$5f$	4.981	0.5
^3P3p	3.677	8.5	^3P3s	2.860	19	$4d$	3.944	23	$6f$	5.980	0.4
$5s$	4.228	8.2	$4p$	3.471	18	$5d$	4.924	8.1	$7f$	6.979	0.2
$6s$	5.212	5.0	$5p$	4.440	6.9	$6d$	5.911	3.8	$8f$	7.978	0.2
$7s$	6.205	3.1	^3P3d	4.798	5.7	$7d$	6.888	2.1	$9f$	8.977	0.1
$8s$	7.198	2.1	$6p$	5.387	3.2	^3P4p	7.561	4.9			
$9s$	8.187	1.5	^3P4s	5.958	3.9	$8d$	7.976	2.3			
^3P4p	9.971	1.9	$7p$	6.560	2.8	$9d$	8.933	1.1			
			$8p$	7.506	1.5						
			$9p$	8.490	1.0						

Table 3: Total ionization cross sections (10^{-18}cm^2) for e^-+Li^+ $1s^2$ and γ+Li $1s^2 2s$, as a function of e^- energy (eV) relative to Li $1s^2$.

e^-(eV):	146.13	147.00	147.02	147.14	147.20	147.33	147.43	150.33	153.93
e^-+Li^+	2.918	2.962	2.962	2.973	2.977	2.975	2.980	3.097	3.244
γ+Li	0.603	0.928	0.962	0.508	0.523	0.606	0.533	0.540	0.512

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