Electron collisions with beryllium and its ions

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Abstract. An overview is provided of the convergent close-coupling calculations for electron-impact on neutral beryllium, as well as its various ionic stages. The calculations were performed from near threshold to high energies with initial states having principal quantum number \( n \leq 4 \). Excitation to states with \( n \leq 5 \) and total ionisation cross sections have been calculated with an estimated accuracy of below 10% at all energies considered.

1. Introduction
Electron scattering on atoms and ions is of both fundamental and practical interest. From the fundamental perspective, few-body physics on the atomic scale has only the Coulomb potential governing the interactions, and so has the capacity for accurate solution. Complexities arise from the number of particles involved and the long-ranged nature of the Coulomb potential. From a practical perspective, such interactions are important in the laser, lighting, atmospheric, plasma processing, and fusion energy applications.

During the course of the last two decades there has been immense progress in the field of electron scattering on atoms and ions. Whereas in the early 1990s there were discrepancies between theory and experiment for the fundamental electron-hydrogen scattering problem [1], today much more complex problems are solved routinely, which are accurate for excitation and ionisation processes on the full energy range of interest [2, 3, 4]. The key factor governing the capacity of theory to provide accurate results is that the electron-atom interaction should be dominated by one- or two-electron processes. This is the case for electronic configurations that have one [5] or two [6] valence electrons.

Given that the first wall of ITER will have a substantial amount of beryllium, it is important to have a quantitative knowledge of electron interactions with its neutral and all ionic stages. We write such collision systems as e-Be\(^{q+}\), for \( q = 0, 1, 2, 3 \). Here we provide an overview of the calculations performed for such systems.

2. Theory
We use the convergent close-coupling (CCC) theory for the e-Be\(^{q+}\) collisions. The H-like Be\(^{3+}\) and the Li-like Be\(^{+}\) targets are able to be treated as one valence electron systems [5]. The He-like Be\(^{2+}\) and neutral Be require the more complicated two-valence electron target implementation [6]. The details of the CCC method are given in Refs. [5, 6]. Briefly, the underlying building block of the method is a complete Laguerre basis. Diagonalisation of the target Hamiltonian in this basis ensures that all of the target states are square-integrable, yet
completeness is approach as the size of the basis is increased. The negative-energy states converge
to the true discrete eigenstates, whereas the positive-energy states yield an increasingly dense
discretisation of the target continuum. The square-integrable nature of the basis ensures that
implementation within the close-coupling formalism is possible with all integrals existing.
The key aspect of the CCC method is that the convergence of the results of interest to a
specified accuracy should be able to be established by simply increasing the size of the Laguerre
bases $N_l$, for $l \leq l_{\text{max}}$. The Laguerre basis exponential fall-off parameter $\lambda_l$ may also be varied,
but for simplicity of convergence studies we generally fix it at some realistic value, and only vary
$N_l$ and $l_{\text{max}}$. Furthermore, we often simplify things further by setting $N_l = N_0 - l$.

2.1. e-Be$^{3+}$ scattering
The Be$^{3+}$ ion is H-like, and as such represents least computational difficulty. The CCC
calculations were performed with $\lambda_l = 8$, $l_{\text{max}} = 4$ and $N_l = 20 - l$. These resulted in 85-
state calculations, with the energy levels given in figure 1. In Laguerre-based diagonalisation
typically only the highest negative-energy state is a pseudostate, with the lower-energy states
being good eigenstates. From the figure we see that the calculations have good $n \leq 4$ eigenstates,
and a rather dense discretisation of the continuum. Accordingly the calculation yields scattering
amplitudes for excitation to $n \leq 4$ states, and also ionisation from the $n \leq 4$ states.

In figure 2 the cross sections for e-Be$^{3+}$ scattering are given for three selected transitions.
Comparison is given with the distorted wave approximation (DWBA) and first-order many body
theory (FOMBT) $^1$. We see generally good agreement between the calculations for both the 2P
excitation and total ionisation cross section (TICS). However, only close-coupling based methods
are able to resolve any resonance structure at energies below the ionisation threshold.

$^1$ http://aphysics2.lanl.gov/tempweb/
2.2. e-Be$^{2+}$ scattering
The Be$^{2+}$ ion is He-like, and requires a good deal more developmental and computational effort. The CCC calculations were performed with $\lambda_l = 4$, $l_{\text{max}} = 4$ and $N_l = 25 - l$. Here the target states were constructed utilising the orbitals obtained from first diagonalising Be$^{3+}$ in the Laguerre basis, and then diagonalising Be$^{2+}$ in explicitly symmetrised two-electron configurations. The configurations consisted of the frozen-core $\{1s,nl\}$ type, augmented by two $s$-, $p$-, and $d$-orbitals for both electrons to improve the quality of the ground state. The resulting 284 energy levels are given in figure 3. From the figure we see that the calculations have good $n \leq 5$ eigenstates, and again a dense discretisation of the continuum. The extra states with energies a little above 100 eV are due to the doubly excited states arising from the non-frozen-core configurations.

In figure 4 the cross sections for e-Be$^{2+}$ scattering are given for four selected transitions. Once more comparison is given with the DWBA and FOMBT approaches. We see substantial discrepancy between CCC and the first-order methods for the important $1^1S \rightarrow 2^1P$ transition. Surprisingly, agreement considerably improves for the two presented TICS cases. Given the unitarity of the CCC formalism, it is expected to be equally accurate for all transitions.

2.3. e-Be$^+$ scattering
The Be$^+$ ion is Li-like, and so is only marginally more complicated to work with than the H-like Be$^{3+}$. The primary difference is that the 1s$^2$ core electrons are treated via the self-consistent Hartree-Fock (SCHF) method, with the valence electron moving in the resulting frozen-core Hartree-Fock (FCHF) potential. The CCC calculations were performed with $\lambda_l = 2$, $l_{\text{max}} = 4$ and $N_l = 20 - l$. These resulted in 84-state calculations, with the energy levels given in figure 5, where we see that the calculations have good $n \leq 5$ eigenstates.

In figure 6 the cross sections for e-Be$^+$ scattering are given for two selected transitions. As
Figure 3. Energy levels in the CCC(284) calculations of e-Be$^{2+}$ scattering.

Figure 4. Selected cross sections for e-Be$^{2+}$ scattering calculated using the CCC method, and distorted-wave and first-order many-body theories.
Figure 5. Energy levels in the CCC(84) calculations of e-Be$^+$ scattering.

Figure 6. Selected cross sections for e-Be$^+$ scattering calculated using the CCC method, and distorted-wave and first-order many-body theories.
Figure 7. Energy levels in the CCC(284) calculations of e-Be$^{2+}$ scattering.

Previously, comparison is given with the DWBA and FOMBT theories. We see generally good agreement between the calculations.

2.4. e-Be scattering

Lastly, neutral Be is the most complex of the targets considered. The core 1s electrons are obtained via the SCHF treatment of Be$^+$. The orbitals for generating the two-electron configurations were generated by diagonalising the Be$^+$ Hamiltonian in a Laguerre basis with $\lambda_l = 2$, $l_{\text{max}} = 2$ and $N_l = 25 - l$. The frozen core configurations $\{2s, nl\}$ were supplemented by the symmetric ones using two lowest s-, p-, and d-orbitals. The Be Hamiltonian is then diagonalised in these configurations to yield the target states to be used in the close-coupling formalism. The resulting 292 energy levels are given in figure 7. From the figure we see that the calculations have good $n \leq 5$ eigenstates. The doubly excited states are interspersed with the $\{2s, nl\}$ continuum ones around 10 eV.

In figure 8 some fundamental cross sections for e-Be scattering are given for four selected transitions, and compared with the DWBA and FOMBT approaches. We see some substantial discrepancy between CCC and the first-order methods. Given that this is a neutral target perhaps this is not so surprising, with agreement being approached at the higher energies. Interestingly, the total ionisation cross section from the $2^3P$ state shows unexpectedly good agreement.

3. Conclusions

We have given a brief overview of the recently performed e-Be$^{q+}$, $q = 0, 1, 2, 3$, scattering calculations using the CCC method. These were a part of the IAEA Coordinated Research Project, motivated by the fact that the first wall of ITER will contain beryllium. The Laguerre basis sizes were sufficiently large to ensure that the accuracy of the results would be within 10%
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