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Theoretical Treatment of Charge Transfer Processes of Relevance to Astrophysics

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Abstract. Charge transfer is an important process in many astrophysical and atmospheric environments. While numerous experimental and theoretical studies exist for H and He targets, data on other targets, particularly metals and molecules, are sparse. Using a variety of theoretical methods and computational techniques we are developing methods to estimate the cross sections for electron capture (charge transfer) in slow collisions of low charge state ions with heavy (Mg, Ca, Fe, Co, Ni and Zn) neutrals. In this ongoing work particular attention is paid to ascertaining the importance of double electron capture.

1. Introduction

Multiply charged ions X^{q+} exist in significant abundances in many astrophysical environments. In collisionally-ionized gas their recombination, and hence the ionization balance, is dominated by radiative and dielectronic recombination with electrons. However, in photoionized gas the electron density may be small and neutrals Y may coexist spatially with the multiply charged ions. In photoionized and nonthermally ionized gas, recombination may therefore largely be driven by charge transfer:

$$X^{q+} + Y \rightarrow X^{(q-1)+} + Y^{+}.$$

The majority of theoretical and experimental studies have been performed on H and He targets. However, a variety of astrophysical situations exists in which H and He are deficient or absent entirely, as is the case with the inner-core of a supernova (SN) ejecta. In these instances the dominant neutral species are often metals. The iron-core of a Type Ia (SN) contains only ions and neutrals of Fe, Co and Ni. Charge transfer plays a role in the ionization balance which must be modeled accurately to reproduce observed nebular spectra [1] . However, state-of-the-art quantum molecular-orbital close-coupling (MOCC) calculations become a formidable task due to the large number of electrons, high angular momenta and large spin.

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Lacking these nearly intractable results, model calculations can in some cases provide cross sections with satisfactory accuracy. In particular, we have utilized the Quantum Decay Model (QDM) [2], the Classical Trajectory Monte Carlo (CTMC) method [3], the Landau-Zener (LZ) [4] model (based on either asymptotic diabatic molecular terms or, when possible, *ab initio* molecular potentials), MOCC [5] and the Hidden Crossings (HC) method [6]. To begin with, these techniques have been applied to collisions systems for which experimental results exist to access their suitability for investigations of astrophysically interesting systems.

2. Test Systems

Considering the simplest cases, QDM has been tested against the existing experimental data for single electron capture (SEC) in collision of H^+ with H (Fig. 1) and against the recommended cross section [7] for double electron capture (DEC) in the He^{2+} + He system (Fig. 2). Provided the reaction is resonant, QDM is accurate in the low energy regime for both processes. Variants of the CTMC method (CTMC, rCTMC) underestimate the cross sections at low energies due to the absence of a tunneling mechanism in their description of the process, but are more reliable in the intermediate to high energy range.

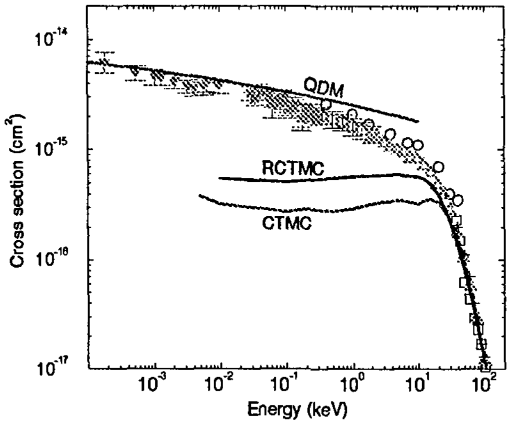

Figure 1. $H^+ + H \rightarrow H + H^+$.

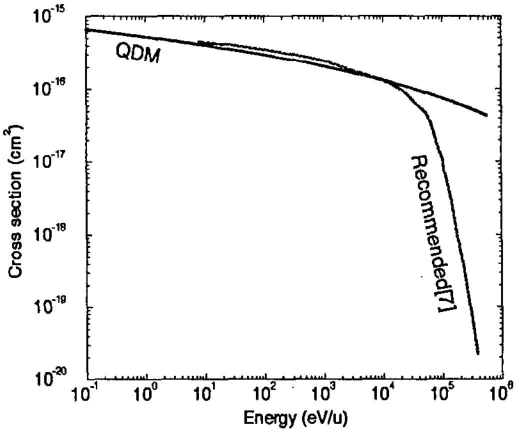

Figure 2. $He^{2+} + He \rightarrow He + He^{2+}$.

In resonant SEC and DEC for many-electron atoms (Ca^+ + Ca in Fig. 3 and Mg^{2+} + Mg in Fig. 4), both QDM and CTMC (when the potential barrier is shallow enough) accurately predict cross sections to within a factor of 2. However, SEC to the doubly ionized projectile could be a nonresonant process even with multielectron atoms/ions. In such a case both QDM and CTMC greatly overestimate the cross sections at low energy as shown in Figs. 5 and 6 for $Mg^{2+} + Mg \rightarrow Mg^+ + Mg^+$ and $Mg^{2+} + Zn \rightarrow Mg^+ + Zn^+$, respectively. The present multichannel LZ calculations, based on *ab initio* MO potentials (Fig. 5), estimate the cross section with acceptable accuracy. Even the LZ model with model Olson-Salop [8] coupling gives a qualitatively correct trend (Fig. 6).

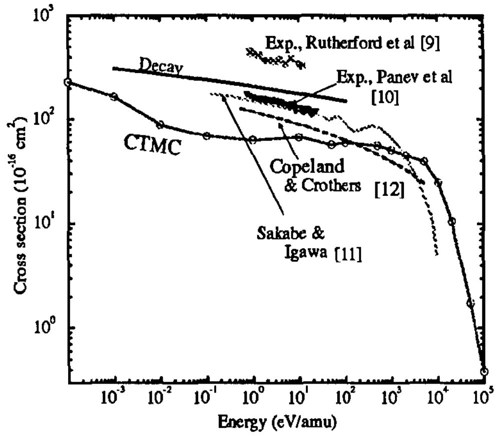

Figure 3. $Ca^+ + Ca \rightarrow Ca + Ca^+$.

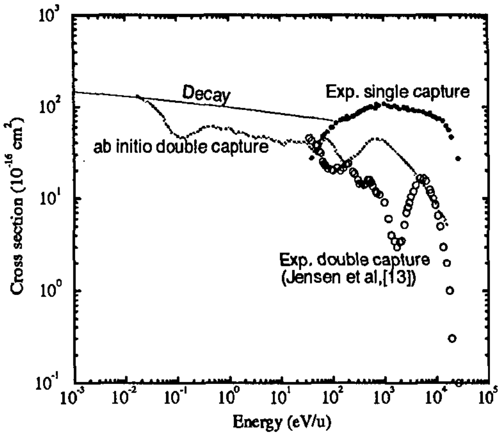

Figure 4. $Mg^{2+} + Mg \rightarrow Mg + Mg^{2+}$.

Thus, the most inexpensive method for production of resonant SEC and DEC cross sections at low collision energies even with metal projectiles and targets is QDM. Any extension to a asymmetric process must be augmented by careful examination of the possible fulfillment of the quasiresonant conditions.

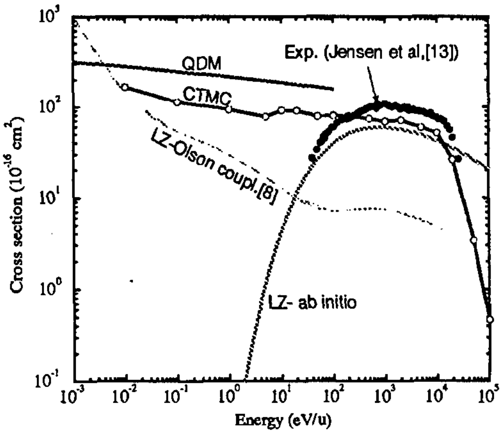

Figure 5. $Mg^{2+} + Mg \rightarrow Mg^+ + Mg^+$.

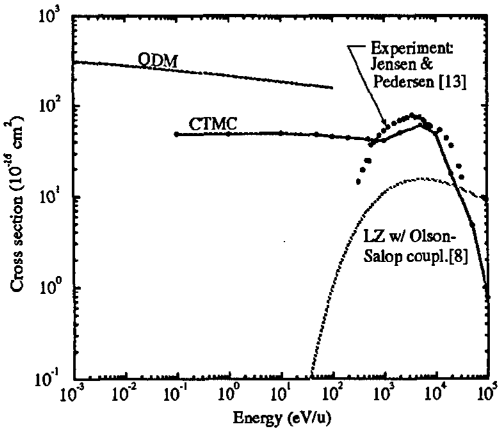

Figure 6. $Mg^{2+} + Zn \rightarrow Mg^+ + Zn^+$.

3. Collision Systems of Astrophysical Interest

In Fig. 7 we present the rate coefficients for SEC between multiply charged transition metals which are important for modeling the ionization balance of the iron-core of Type Ia SNe [1]. According to the considerations above, one could expect the $q = 1$ results to be accurate, while $q = 2$ and 3 cases rely on (quasi)resonance between the initial and final states. If the charge q is high enough, the final state is in the Rydberg region of the ion providing the needed quasi-resonance. The intermediate cases need further justification for the considered systems through *ab initio* calculation of the MO potential curves. This is the subject of an going study.

Some sub-Chandrasekhar mass models of Type Ia SNe produce helium in the iron-core as a result of alpha freeze-out [15]. If there is sufficient neutral iron, He^+ can be produced via SEC from He^{2+} + Fe collisions. Helium recombination lines could then possibly be observable in the nebular phase. We used the multi-channel LZ approach (with Butler-Dalgarno model coupling [4]) and QDM to estimate the cross section for this reaction (Fig. 8).

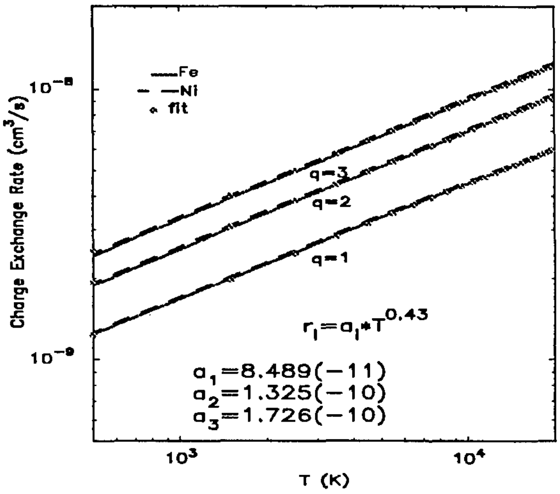

Figure 7. Fe, Co and Ni SEC.

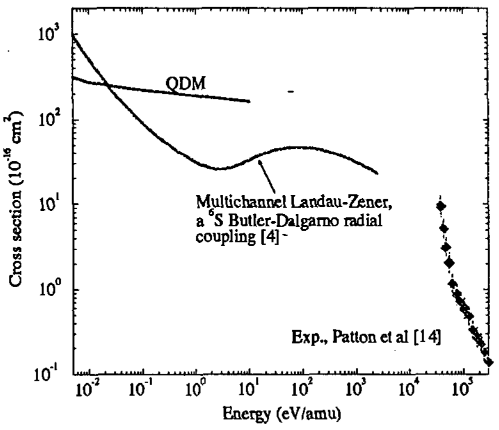

Figure 8. $He^{2+} + Fe \rightarrow He^+ + Fe^+$.

C I lines are observed in the interstellar medium, but as C has a lower ionization potential (11.26 eV) than H, the carbon exists mostly as C^+. Since formation of neutral carbon by radiative recombination is slow, Péguingnot *et al* [16] suggested that SEC from neutral H could neutralize the carbon. Using a variety of theoretical approaches, in conjuction with new merged-beams measurements, we obtained the cross sections shown in Fig. 9 [?] . The resulting rate coefficient is significantly bigger than obtained by Butler and Dalgarno [18], but still too small to have an effect on the carbon ionization balance.

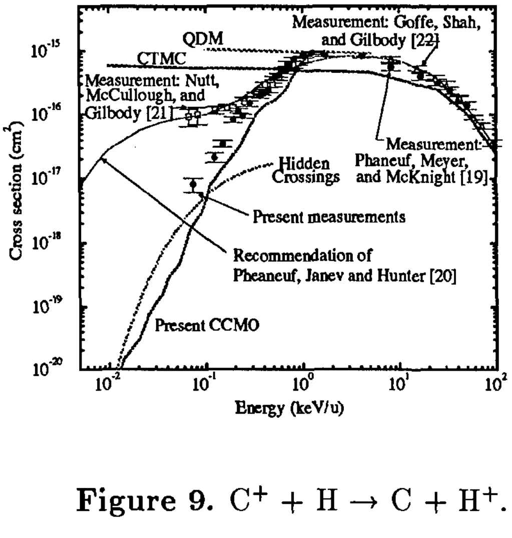

Figure 9. $C^+ + H \rightarrow C + H^+$.

4. Conclusions

We have begun evaluation of methods to treat single and double charge transfer among astrophysically relevant metallic ions and atoms. Due to the lack of existing data and the near intractability of full quantum mechanical treatments we have compared results of these simple methods to existing data to access their limits and degree of applicability. Ongoing work to provide at least a few fully quantal benchmarks for the most complex systems continues.

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