

# Ionization channel in non-perturbative ion-atom collisions dominated by charge exchange.

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**Abstract.** The development of the described method has been motivated by studies of the proton-atomic oxygen collision system, where the accidental closeness of energy levels makes the charge exchange quasi-resonant. In slow collisions the ionization channel must compete with the resonant exchange channel. The present theoretical approach is to add target continuum states, found by solving numerically the self-consistent field Schrödinger equation, to the set of basis states on target and projectile, as used in close coupling treatment of excitation and exchange. We have shown that the chosen theoretical approach is feasible and report here first model studies using the new computer code. It is found that the large population of the ionization channel at the lowest collision velocities found in a previous study is not seen in the present approach.

## INTRODUCTION

One of the main motives for this work is the proton-atomic oxygen collision system, where the accidental closeness of energy levels makes the charge exchange quasi-resonant. The motivation to study this system, as well as our previous treatment of this system are described in ref. [1]. The results of the latter reference for ionization showed some unexpected features and the calculations have later been performed with a somewhat larger set of basis states, without a conclusive result [2]. In slow collisions the ionization channel must compete with the strongest resonant exchange channel. The situation is thus in many respects similar to the proton-hydrogen case, but it has different aspects, the most important is that a many electron system is studied and thus further approximations must be done to make the description of the many-electron problem feasible.

The present theoretical approach is to add to the set of basis states on target and projectile, as used in close coupling treatment of excitation and exchange [1], a set of target continuum states, found by solving numerically Schrödinger equation with a potential obtained from the self-consistent field calculation.

Ionization in nonperturbative collisions has been studied in many works, some of them quite early. In some studies of Greiner's Group [3], [4] the continuum was taken into account by expansion over a set of real continuum states, while in the papers of Reading's Group (first in ref.[5]), as well as e.g. in L-shell ionization studies of Shingal *et al* [6], various forms of pseudostates are used. More recent use of pseudostates in typical two-

centre collisions is very broad, a review can be found e.g. in [7]. The present theoretical treatment is thus an alternative or extension of previous methods, represented e.g. by the references [3], [5].

The studies of nonperturbative atomic collisions have become a large field where many innovative approaches have been developed. A very interesting set of ideas, named basis generator method (BGM) has been explored recently by Lüdde and collaborators [8]. Other approaches are based on purely numerical methods, e.g. direct numerical solution of Schrödinger equation on a mesh of spatially distributed points, e.g. in [9] and [10]. A special place has the approach of Sidky and Lin [11], [12], where the mesh is in the momentum space.

Here we explore a combination of two more traditional approaches, based on expansions in sets of certain eigenstates. We use a well established and tested coupled channels code, which uses atomic eigenstates (and pseudostates).

## THE COUPLED CHANNEL CODES

The code which is the starting point of the present work is PSgatcc of J.P. Hansen and A. Dubois. This code is a recent version of a long series of codes starting from atcc (atomic coupled channels) originally written in 1988-89, later generalized to gatcc and more recently in the middle of 1990's fully included general pseudostates (PSgatcc). The one-electron wavefunction is expanded in a set of atomic or model eigenstates. These eigenstates are ex-

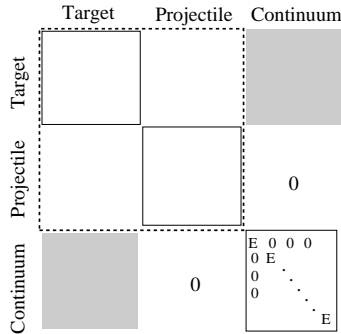
pressed as a linear combination of Slater orbitals on both target and projectile. Both direct and exchange matrix elements, are evaluated using Shakeshaft's method [13]. The basic routines of the original code have been published in [14]. The system of codes contains also a utility to plot the effective model molecular orbitals, which is useful for the discussion of collision dynamics.

Since the set of Slater type orbitals is larger than the set of atomic states, the positive energy solutions of the static problem can be used as pseudostates representing continuum, i.e. the ionization channel. A large number of studies has been performed using these codes, most recently e.g. [15]. and the paper [1] mentioned as one of the motives for this work.

## CONTINUUM EXTENDED COUPLED CHANNEL CODE

The effective potential used to construct the bound states on the target for the program PSgatcc is used to obtain radial functions of the continuum states, by solving the radial Schrödinger equation. The evaluation of matrix elements is performed using the method described e.g. in [16]. For bound-bound coupling of states on one centre such matrix elements are already included, and they could in principle be evaluated in the same way. In fact, some of the earlier versions of gatcc used a set of routines similar to those included now. In the present PSgatcc the one centre bound-bound matrix elements are calculated in a different way, suitable for the fact that the expansion Slater orbitals are not eigenstates of the hamiltonian.

In the present version we do not include continuum-continuum coupling and we do not allow the bound states to change their 'instantaneous energies', i.e. we effectively work with the hamiltonian shown in Fig. 1. These



**FIGURE 1.** Schematic representation of the total hamiltonian. The part in dashed frame is evaluated by the original code, shaded area and the diagonals are new parts.

limitations might seem rather severe in light of other

studies, e.g. [12] or [10], but for our purposes they in fact simulate important physical features (see the discussion). The coupling included is a sort of extension of perturbative ionization calculations. Perturbative ionization calculations have proven to be efficient even in many situations where the ionization channel dominates.

The inclusion of the continuum expansion in the coupled channel codes needs a method to discretize the continuum. This is implemented by normalizing the selected continuum states as explained in the next section.

## NORMALIZATION OF THE CONTINUUM STATES

This procedure is discussed in a monograph of Bransden and McDowell [17], and applied e.g. in the paper of Schwietz [18]. When we have a set of both continuum and discrete states, the expansion has a form

$$\Psi(\xi, t) = \sum_i c_i(t) \phi_i(\xi) + \int_0^\infty b_\epsilon(t) R_\epsilon(\xi) d\epsilon \quad (1)$$

where  $R_\epsilon$  is a continuum state with energy  $\epsilon$  and where  $\xi$  denotes the relevant electron coordinates. We need to consider only the second part of eq. (1), where our procedure should replace the integral by a summation. In [17] the discretization is introduced via so called eigendifferentials (there is a misprint obscuring the presentation in [17], therefore we discuss this in detail). For regular meshes of values  $\epsilon_i$  the expression

$$\sum_i \left\{ \sqrt{\Delta\epsilon} b_{\epsilon_i}(t) \right\} \left\{ \frac{1}{\sqrt{\Delta\epsilon}} \int_{\epsilon_i - \frac{1}{2}\Delta\epsilon}^{\epsilon_i + \frac{1}{2}\Delta\epsilon} R_\epsilon(\xi) d\epsilon \right\} \quad (2)$$

approaches the discussed integral as  $\Delta\epsilon$  approaches zero. Note that it is the expansion coefficient which is taken outside of the integrals. This expression is already in a form of summation

$$\sum_i \beta_i(t) \Phi_i(\xi) \quad (3)$$

where the functions  $\Phi_i(\xi)$  are defined by the second bracket of eq. (2) and they are called eigendifferentials. The expansion coefficients  $\beta_i$  are related to the original  $b_{\epsilon_i}$  in the first bracket of eq. (2).

It is easy to show that the eigendifferentials  $\Phi_i(\xi)$  form an orthonormal set for any mesh of  $\epsilon_i$ , when the continuum states are taken normalized on the energy scale

$$\int R_{\epsilon'}(\xi) R_\epsilon(\xi) d\xi = \delta(\epsilon' - \epsilon) \quad (4)$$

The eq. (2) is basis for the discretization, instead of a mesh with infinitesimal spacing a real mesh is chosen.

The fact that the set of  $\Phi_i(\xi)$  is orthonormal for any energy mesh does not at all guarantee that it also is complete. We know, however, that as the mesh gets finer and finer, the expansion would converge to the original eq. (1). The coupled equations can thus be solved in a normal way when we use the fully discrete expansion implied by eq. (3). One needs to evaluate the matrix elements between all the states  $\Phi_i(\xi)$  and  $\varphi_i(\xi)$  of the coupling terms of the hamiltonian.

The total probability of the electron being in continuum is given by

$$\sum_i |\beta_i(t)|^2 = \sum_i |b_{\varepsilon_i}(t)|^2 \Delta\varepsilon \rightarrow \int_0^\infty |b_\varepsilon(t)|^2 d\varepsilon \quad (5)$$

and if differential quantities are needed, they can be based on the above relation.

We consider a very simple approximation, i.e. that the variation of wavefunction with energy in the second bracket of eq. (2) can be neglected. In this approximation, the eigendifferentials  $\Phi_i(\xi)$  become

$$\Phi_i(\xi) \rightarrow \sqrt{\Delta\varepsilon} R_{\varepsilon_i}(\xi)$$

i.e. the energy-normalized continuum states with modified normalization states are used for the evaluation of the matrix elements. This method is adopted in the presented work.

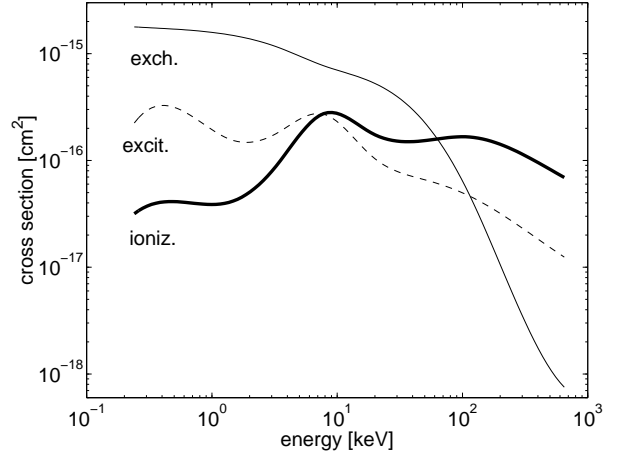
The same method has also been used in the paper of Soff *et al* [3], who introduced it simply by the relation

$$\int_0^\infty d\varepsilon \rightarrow \sum_i (E_{i+1} - E_i)$$

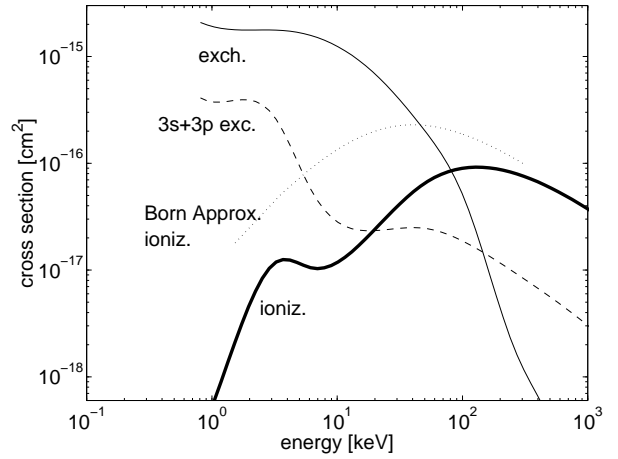
The continuum states  $R_\varepsilon$  must be normalized on the energy scale, eq. (4). This is done according to Bethe's prescription, section 1.4 of [19].

## COMPUTATIONAL ASPECTS

We use the possibility of the parallel execution by a small C-language code which performs in parallel multiple runs of the plain FORTRAN code without parallel modifications. This makes it possible to perform the same calculations also on any system with sufficient power but without parallelism. A large quantity of input and output data files are administered using standard Unix tools. The calculations are performed at the NOTUR site Parallax's Cray Origin 2000 for fast evaluation. However, it is possible to run the same code for example on any personal computer with Linux operating system, or any type of Unix workstation with standard FORTRAN compiler. The set of calculations for Fig. 3 would then take about one to two weeks of full time.



**FIGURE 2.** Comparison of cross sections for the three main channels in atomic O - H<sup>+</sup> collisions. Data from ref. [1].



**FIGURE 3.** Comparison of present model cross sections for the three main channels in atomic O - H<sup>+</sup> collisions and Born Approximation for ionization.

The code is written so that it can be viewed by a html-browser with pointers to subroutines and places of interest. We hope to make it available at the address <http://www.fi.uib.no/AMOS/gatcc> which now contains additional material on this work.

## DISCUSSION OF THE APPLICATION

It is well known (e.g. fig. 2.1 of [7]) that in proton-hydrogen collisions the exchange channel dominates and the ionization channel is much weaker than the excitation channel at low velocities. In the previous calculations on proton - atomic oxygen collisions [1] the situation was different, the ionization channel at low collision energies

follows the cross sections for the excitation channel. In these calculations the ionization channel has been represented by the positive energy eigenstates (pseudostates), as in many other current works.

Fig. 2 prepared from results in [1] shows the competition of the three channels in atomic O - H<sup>+</sup> collisions. Fig. 3 shows the results of the present model calculations, which only add the probabilities of electron removal from the 2p-states without proper statistical treatment.

The two figures cannot be directly compared, since the present calculations are not modified by the statistical factors discussed in detail in [1], and also the size of the atomic basis has been reduced. Nevertheless, it is found that large population of the ionization channel at the lowest collision velocities found in the previous study is not seen in the present approach.

The reason for a spurious population of the ionization channel might be a sort of diving of the positive energy states, i.e. due to the necessarily limited basis some of the positive energy states get negative energies for small internuclear distances. This could be seen using the MO-tool mentioned in the description of the codes. If the basis were larger, other weakly bound states would keep the continuum states higher up. In our approach this is simulated by neglecting altogether the off-diagonal terms for the positive energy states.

## CONCLUSION

We have modified a pseudostate-based coupled channel code to include a set of real continuum states obtained by solving electron Schrödinger equation with a realistic potential of the target atom. With this new code, which seems to be the first using such a combined approach, we have performed a set of model calculations for recently studied system proton on atomic oxygen. These calculations indicate that the previously obtained large cross sections for ionization are most probably spurious. The code has been shown functional and the results show a good agreement with perturbative calculations at high collision velocities. One of the above references [12] opens by a quote "to understand hydrogen is to understand all of physics" from ref. [20]. In accordance with this statement, we plan to study in the future the limitations of this model by applying it the proton-hydrogen case. Naturally, more extensive calculations on other suitable systems will also be performed in the near future.

## ACKNOWLEDGMENTS

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## REFERENCES

1. Hamre, B., Hansen, J.P., and Kocbach, L., *J.Phys.B: At.Mol.Opt.Phys.* **32**, L127-L131 (1999).
2. Hansen, J.P., Kocbach, L., and Ladadwa, I., *XXI. ICPEAC, Abstracts of contributed papers*, ed. Y. Itikawa et al, Sendai, Japan, 1999, Volume II., p. 478
3. Soff, G., Reinhardt, J., Müller, B., and Greiner, W., *Z. Physik A* **294**, 137-147 (1980).
4. Mehler, G., Greiner, W., and Soff, G. *J.Phys.B: At.Mol.Opt.Phys.* **32**, 2787-2801 (1987).
5. Ford, A. L., Fitchard, E., and Reading, J.F., *Phys. Rev. A* **16**, 133-143 (1977).
6. Shingal, R., Malhi, N. B., and Gray, T. J., *J. Phys. B: At. Mol. Opt. Phys.* **25**, 2055-2063 (1992).
7. Fritsch, W., and Lin, C. D., *Phys. Reports* **202**, 1-97 (1991).
8. Kroneisen, O.J., Lüdde, H.J., Kirchner, T., and Dreizler, R.M., *J. Phys. A: Math.Gen.* **32**, 21411-2156 (1999).
9. Grün, N., Mühlhans, A., and Scheid, W., *J. Phys.B: At.Mol.Opt.Phys.* **15**, 4043-4061 (1982).
10. Wells, J. C., Schultz, D. R., Gavras, P., and Pindzola, M. S., *Phys. Rev. A* **54**, 593-604 (1996).
11. Sidky, E. Y., and Lin, C. D., *J. Phys. B: At. Mol. Opt. Phys.* **31**, 2949-2960 (1998).
12. Sidky, E. Y., Illescas, C., and Lin, C. D., *Phys. Rev. Lett.* **85**, 1634-1637 (2000).
13. Shakeshaft, R., *J. Phys. B: Atom. Molec. Phys.* **8**, 134-136 (1975).
14. Hansen, J.P., *Computer Phys. Comm.* **58**, 217-221 (1990); Hansen, J.P. and Dubois, A., *ibid.* **67**, 456-464 (1992).
15. Lundsgaard, M. F. V., Nielsen, S. E., Rudolph, H., and Hansen, J.P., *J.Phys. B: At. Mol. Opt. Phys.* **31**, 3215-3232 (1998).
16. Kocbach, L., *Z. Physik A* **279**, 233-236 (1976).
17. Bransden B. H., and McDowell, M. R. C., *Charge Exchange and the Theory of Ion-Atom Collisions* Oxford: Clarendon Press, 1992.
18. Schiwietz, G., *Phys.Rev. A* **42**, 296-306 (1990).
19. Bethe, H. A., and Salpeter, E. E., *Quantum Mechanics of One- and Two-Electron Atoms* Berlin: Springer, 1957.
20. Kleppner, D., *Physics Today* **52**, 11 (1999).