A study of cross sections for excitation of pseudostates

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(September 18, 1998)

Using the electron-hydrogen scattering Temkin-Poet model we investigate the behavior of the cross sections for excitation of all of the states used in the convergent close-coupling (CCC) formalism. In the triplet channel, it is found that the cross section for exciting the positive-energy states is approximately zero near-threshold and remains so until a further energy, equal to the energy of the state, is added to the system. This is consistent with the step-function hypothesis [Bray, Phys. Rev. Lett. 78 4721 (1997)] and inconsistent with the expectations of Bencze and Chandler [Phys. Rev. A 59 3129 (1999)]. Furthermore, we compare the results of the CCC-calculated triplet and singlet single differential cross sections with the recent benchmark results of Baertschy et al. [Phys. Rev. A (in press)], and find consistent agreement.

34.80.Bm, 34.80.Dp

In recent times the electron-impact ionization of atoms has attracted considerable attention and controversy. Whereas we would argue that the convergent close-coupling (CCC) approach to the problem has been one of the most successful to date, Bencze and Chandler argue that there are fundamental flaws in the CCC formalism due to its simplicity (only states of zero orbital angular momentum involved), and yet it is sufficient to address all of the issues involved. Accordingly, we shall write momenta as scalars.

In performing CCC calculations we first obtain a set of $N$ states $\phi_i^{(N)}$ with energies $\epsilon_i^{(N)} (n = 1, \ldots, N)$ by diagonalising the target Hamiltonian in an orthogonal Laguerre basis. These are then used to approximate the target space identity operator $I_2$ by

$$I_2 \approx I_2^{(N)} = \sum_{n=1}^{N} |\phi_i^{(N)}\rangle \langle \phi_i^{(N)}| .$$

Subsequently, the total e-H wave function is expanded using

$$|\psi_{S}^{(+)}\rangle \approx (1 + (-1)^S P_r) |\psi_{S}^{(+)}\rangle \approx (1 + (-1)^S P_r) I_2^{(N)} |\psi_{S}^{(+)}\rangle ,$$

where $P_r$ is the space exchange operator and $|\psi_{S}^{(+)}\rangle$ is an unsymmetrized form of the total wave function. In the CCC approach we calculate the $T$-matrix elements

$$\langle k_f | \phi_i^{(N)} | T_S | \phi_i^{(N)} k_i \rangle = \langle k_f | \phi_i^{(N)} | V_S | \phi_i^{(N)} k_i \rangle + \sum_{n=1}^{N} \int_0^{\infty} dk \frac{\langle k_f | \phi_i^{(N)} | V_S | \phi_i^{(N)} k \rangle \langle k_0 | \phi_i^{(N)} | T_S | \phi_i^{(N)} k_i \rangle}{E + i\epsilon_i^{(N)} - k^2/2} ,$$

where $V_S$ is the effective interaction potential. The ionization scattering amplitudes are defined as

$$f_S^{(N)}(k_f, q_f) = \langle q_f^{(-)} | \phi_i^{(N)} \rangle \langle k_f | \phi_i^{(N)} | T_S | \phi_i^{(N)} k_i \rangle ,$$

where $\langle q_f^{(-)} |$ is a Coulomb wave with normalization of $\sqrt{2/\pi}$ (no $1/q_f$ factor) of energy $q_f^2/2 = \epsilon_f^{(N)}$, and such amplitudes may be defined for all $0 < \epsilon_f^{(N)} < E$. Bencze and Chandler are quite happy with this definition of the ionization amplitude and claim that in the limit of infinite $N$ it leads to the true scattering amplitudes that...
must, therefore, satisfy the symmetrization relation \[\sigma_{\text{ion}}^{(N,S)} = \sum_{n: 0 < \epsilon_n^{(N)} < E} |\langle k_n \phi_n^{(N)} | T_S | \phi_i^{(N)} k_i \rangle|^2 \]

\[= \int_0^{\sqrt{2E}} dk |f_S^{(N)}(k,q)|^2 \]

\[= \int_0^E de |f_S^{(N)}(k,q)|^2 / \sqrt{2e} \]

\[= \int_0^E de \frac{de}{d\epsilon}^{(NS)}(e). \tag{9} \]

The CCC(\(N\)) calculations have been performed for \(N = 21, \ldots, 25\). For the triplet channel all of the CCC calculations lie on the smooth curve of the ECS-calculated SDCS, but only for secondary energies less than \(E/2\). At higher energies the latter increases symmetrically about \(E/2\), whereas the CCC calculations all yield near-zero cross sections. To our mind this is a very satisfactory result. All of the physics is contained in the secondary energy range \([0, E/2]\). Clearly, CCC has converged to the correct result on this energy range, and no double counting of the ionization cross section occurs even though the integration endpoint in \(\sigma_{\text{ion}}^{(N,S)}\) is \(E\).

Unfortunately, the singlet case is more complicated. The unphysical oscillatory CCC-calculated SDCS has not converged with increasing \(N\), but oscillates about the ECS-calculated SDCS on the \([0, E/2]\) secondary energy range. The ECS calculations show that the SDCS at \(E/2\) is substantial, unlike the triplet cases where it is zero due to the Pauli Principle. We believe that as \(N \to \infty\) the CCC(\(N\))-calculated SDCS would converge to the step-function formed by the ECS SDCS on the secondary energy range \([0, E/2]\) and zero elsewhere. These results are consistent with our earlier expectations \(\[\sigma_{\text{ion}}^{(N,S)} = |\langle k_n \phi_n^{(N)} | T_S | \phi_i^{(N)} k_i \rangle|^2 \]

\[\text{for the excitation of the pseudostates.} \tag{10} \]

![Graph](attachment:image.png)

**FIG. 1.** The singlet and triplet (spin-weights included) SDCS for the Temkin-Poet model e-H problem at a total energy \(E = 7\) Ry. The SDCS calculated by the external complex scaling (ECS) method are due to Baertschy et al. \[\[\text{Fig. 3 we give the triplet } \sigma_{\text{ion}}^{(N,S)} = |\langle k_n \phi_n^{(N)} | T_S | \phi_i^{(N)} k_i \rangle|^2 \text{ for the excitation of the pseudostates.} \tag{10} \]

**FIG. 2.** The 25 long tics are the energy levels in the CCC(25) calculations. The short tics and arrow indicate the true discrete energies and the continuum, respectively.

To demonstrate this explicitly we take a single \(N = 25\) basis, whose energies are given in Fig. \[\[\text{and perform CCC(25) calculations at very many total energies } E. \text{ The exponential fall-off parameter } \lambda = 1.0 \text{ in all cases. This yields eight negative-energy states (lowest six good eigenstates) and 17 positive-energy states. The cross section for the excitation of states with } n \leq 3 \text{ has been given before } \[\[\text{and so we start with } n = 4. \text{ In Fig. 3 we give the triplet } \sigma_{\text{ion}}^{(N,S)} \text{ for } 4 \leq n \leq 8 \text{ plotted against total energy above threshold } E - \epsilon_n^{(25)}. \text{ Nothing particularly remarkable is observed. The cross sections start very small and rise visibly at around 0.1 Ry after} \]

...
threshold. The $n = 8$ cross section is of greater magnitude than the $n = 7$ owing to it attempting to take into account $n > 8$ true discrete eigenstates.

What is more interesting is the behavior of the cross sections for the excitation of positive-energy states, given in Fig. 4. Other than for a rise in magnitude the $n = 9$ and $n = 13$ (and those inbetween) cross sections are much the same as the $n = 8$ cross sections. This is contrary to the expectations of Bencze and Chandler, at least in the limit of infinite $N$. A symmetric SDCS could only be obtained if the cross section for exciting the positive-energy pseudostates was non-zero at threshold, diminished to (in the present case) zero at $E/2$, and then began to increase. Instead, as we increase $n$ further we see that the cross section remains very small until approximately an energy equal to $\epsilon_n^{(25)}$ above threshold. By the Pauli Principle the true result is exactly zero at this point. The CCC calculations give a very good approximation to this.

Thus, we found that the bigger the energy of the pseudostate the more energy above threshold is required before the cross section for its excitation begins to rise. This remarkable feature demonstrates the consistency of our interpretation of the CCC-calculated ionization amplitudes. Whereas previously we have taken a particular $E$ and showed, by variation of $N$, the plausibility of the step-function hypothesis [3] at that $E$. Here, we have taken a single $N$ and showed, by variation of $E$, the plausibility of the step-function hypothesis at all $E$, at least for the triplet channel.

For the singlet channel the situation is less clear due to lack of convergence problems, see Fig. 5. Here the cross sections rise rapidly after the arrow (indicating $\epsilon_n^{(25)}$) and are relatively small at the lower total energies above threshold.

FIG. 3. Triplet cross sections for excitation of the specified negative-energy states of the CCC(25) calculation in the Temkin-Poet model.

FIG. 4. Triplet cross sections for excitation of the specified positive-energy states of the CCC(25) calculation in the Temkin-Poet model. The arrows indicate the energy $\epsilon_n^{(25)}$ of the state.
threshold. We suspect that for infinite $N$ these cross sections would be zero at energies smaller than the energy of the state, and jump to be substantially nonzero at higher energies.

A consequence of the present study is that we are still confident in the correctness of our interpretation of the application of the CCC method to ionization processes [3]. We are particularly pleased to see the ECS theory being able to calculate accurately the true SDCS, as these are necessary to rescale the CCC-calculated angle-differential cross sections [3,15]. In the present context the step-function in the SDCS hypothesis [3] may be restated as: cross sections for the excitation of positive-energy $\epsilon_n^{(N)}$ pseudostates remain zero past threshold ($E = \epsilon_n^{(N)}$) until the total energy $E$ is in excess of $2\epsilon_n^{(N)}$. We suspect that this claim is applicable to all implementations of the close-coupling method.

We thank Tom Rescigno for permission to use unpublished data. We are grateful to Emily McPherson, Ryan Coad and David Pike of the Australian CSIRO Student Research Scheme for the many useful discussions. Support of the Australian Research Council and the Flinders University of South Australia is acknowledged. We are also indebted to the South Australian Centre for High Performance Computing and Communications.

FIG. 5. Singlet cross sections for excitation of the specified positive-energy states of the CCC(25) calculation in the Temkin-Poet model. The arrows indicate the energy $\epsilon_n^{(25)}$ of the state.

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