Computer Physics Communications 196 (2015) 276–279

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Solving close-coupling equations in momentum space without singularities

A.W. Bray *, I.B. Abdurakhmanov, A.S. Kadyrov, D.V. Fursa, I. Bray

Curtin Institute for Computation and Department of Physics and Astronomy, Curtin University, GPO Box U1987, Perth, WA 6845, Australia

ARTICLE INFO

Article history:
Received 20 March 2015
Received in revised form
3 June 2015
Accepted 20 June 2015
Available online 29 June 2015

Keywords:
Electron–atom scattering

ABSTRACT

Solving the close-coupling equations for electron–atom scattering in momentum space involves the solution of coupled integral equations, which contain principal value singularities. These can be accurately treated numerically using an on-shell subtraction technique. Here we show how the singularities may be taken into account analytically, leading to an alternative approach to the solution of the integral equations. The robustness of the method is demonstrated by considering the S-wave model of e-H scattering across eight orders of magnitude of incident energies.

1. Introduction

Over the last two decades there has been considerable progress in the field of atomic scattering theory. Electron, positron and photon scattering processes, including ionisation, on simple atoms are readily calculated using several non-perturbative numerical approaches such as exterior complex scaling [1,2], R-matrix with pseudostates [3,4], time-dependent close-coupling [5], integro-differential close-coupling [6] and convergent close-coupling (CCC) [7].

The CCC method relies on the numerical formalism suggested by McCarthy and Stelbovics [8] for solving the coupled equations in momentum space, with a slight modification by Bray and Stelbovics [9] to allow the usage of only real arithmetic. Some of the numerical issues that require solving are the principal value singularities, which occur at a different energy in each open channel. The method of solution used up to now was based on the on-shell subtraction technique, of which there are several variants in the literature, see for example Walters [10] and Heller and Reinhardt [11], which generally works very well. By using a near-symmetric treatment on either side of the singularity with a Gaussian quadrature the magnitude of the subtractions can be minimised. Nevertheless, the on-shell point cannot be a part of the integration.

The subtraction procedure can be somewhat problematic near thresholds for excitation of open states, due to the vicinity of the singularity to zero. Also, in cases where the system is particularly ill-conditioned, as happens when large expansions are used in multi-centre problems, the addition and subtraction of large parts of the integrand on either side of the singularity is prone to precision loss. The near $n \leq 3$ positronium formation threshold study of positron–hydrogen scattering is one such example [12]. To push this to higher n requires a more robust numerical method.

Here we give an alternative approach to solving the CCC equations that eliminates the singularities. It is shown that the integrals can be done analytically and that the subsequent equations take the same form as the previous ones, but without singularities. To demonstrate the utility and robustness of the method we consider the Temkin–Poet S-wave model of e-H scattering [13,14]. In this model only states of zero orbital angular momenta are retained. In doing so the problem is stripped from the multidimensional complexity of the full problem, while retaining the essential issues associated with solving the coupled-equations. This model has been extensively used to develop and study a range of issues associated with the development of general numerical approaches to electron–atom scattering [15–19].

2. Theory

The convergent close coupling method (CCC) was developed by Bray and Stelbovics [9] in order to solve for scattering amplitudes in e-H collisions. It solves directly for the transition amplitude via

$$\langle \boldsymbol{k}_f \phi_f | T_S | \phi_i \boldsymbol{k}_i \rangle = \langle \boldsymbol{k}_f \phi_f | V_S | \phi_i \boldsymbol{k}_i \rangle + \sum_{n=1}^{N} \int d^3k \frac{\langle \boldsymbol{k}_f \phi_f | V_S | \phi_n \boldsymbol{k} \rangle \langle \boldsymbol{k} \phi_n | T_S | \phi_i \boldsymbol{k}_i \rangle}{E + i0 - \epsilon_n - \frac{1}{2}k^2}, \quad (1)$$

where $\boldsymbol{k}$ and ϕ are the projectile momentum and target state, respectively. The total energy (Hartree) of the system is $E = \epsilon_i +$

* Corresponding author. Tel.: +61 892667747.
E-mail address: alexander.w.bray@student.curtin.edu.au (A.W. Bray).

http://dx.doi.org/10.1016/j.cpc.2015.06.015
0010-4655/

$k_i^2/2 = \epsilon_f + k_f^2/2$, and the total spin is $S = 0, 1$. The $n = 1, \ldots, N$ target states ϕ_n are all square-integrable, and may be obtained by diagonalising the target Hamiltonian in a Laguerre basis [9], or by solving the target Schrödinger equation in a box-basis with $\phi_n(r) = 0$ for $r \geq R_0$, where R_0 is a free parameter [20]. The interaction potentials V_S are given in Ref. [9].

Eq. (1) is solved using real arithmetic by transformation to the K_S matrix, and upon partial wave expansion is solved separately for each partial wave of total orbital angular momentum

$$\langle k_f\phi_f|K_S|\phi_i k_i\rangle = \langle k_f\phi_f|V_S|\phi_i k_i\rangle + \sum_{n=1}^{N} \mathcal{P}\int_0^\infty dk \frac{\langle k_f\phi_f|V_S|\phi_n k\rangle\langle k\phi_n|K_S|\phi_i k_i\rangle}{E - \epsilon_n - \frac{1}{2}k^2}. \quad (2)$$

Here, for simplicity, we neglected any orbital angular momenta notation since in the S-wave model all are set to zero.

Following McCarthy and Stelbovics [8] the principal value singularity in Eq. (2) may be treated by a subtraction technique or equivalently symmetric positioning of quadrature points on either side of the singularity. To date the CCC method has utilised such an approach.

We now suggest an analytical approach to the integral for open, $k_n = \sqrt{2(E-\epsilon_n)}$, and closed, $k_n = \sqrt{2(\epsilon_n - E)}$, channels utilising the relation [21]

$$G_n(r', r'') = \mathcal{P}\int_0^\infty dk \frac{\langle r'|k\rangle\langle k|r''\rangle}{E - \epsilon_n - \frac{1}{2}k^2} = \begin{cases} \frac{\pi}{k_n}\sin(k_n r_<)\cos(k_n r_>), & \text{if open,} \\ \frac{\pi}{2k_n}\left[\exp(-k_n r_<) - \exp(k_n r_<)\right]\exp(-k_n r_>), & \text{if closed,} \end{cases} \quad (3)$$

where $r_< \equiv \min(r', r'')$ and $r_> \equiv \max(r', r'')$.

To implement this, we incorporate (3) in (2) as follows,

$$\begin{aligned} &\mathcal{P}\int_0^\infty dk \frac{|\phi_n k\rangle\langle k\phi_n|}{E - \epsilon_n - \frac{1}{2}k^2} \\ &= \mathcal{P}\int_0^\infty dk \int_0^\infty dk' \int_0^\infty dk'' \frac{|\phi_n k'\rangle\langle k'|k\rangle\langle k|k''\rangle\langle k''\phi_n|}{E - \epsilon_n - \frac{1}{2}k^2} \\ &= \mathcal{P}\int_0^\infty dk \int_0^\infty dk' \int_0^\infty dk'' \int_0^\infty dr' \int_0^\infty dr'' \\ &\quad \times \frac{|\phi_n k'\rangle\langle k'|r'\rangle\langle r'|k\rangle\langle k|r''\rangle\langle r''|k''\rangle\langle k''\phi_n|}{E - \epsilon_n - \frac{1}{2}k^2} \\ &= \int_0^\infty dk' \int_0^\infty dk'' \int_0^\infty dr' \int_0^\infty dr'' \\ &\quad \times |\phi_n k'\rangle\langle k'|r'\rangle G_n(r', r'')\langle r''|k''\rangle\langle k''\phi_n|. \end{aligned} \quad (4)$$

If we let $k'' \to k$ and define

$$\langle k_f\phi_f|V'_S|\phi_n k\rangle = \int_0^\infty dk' \int_0^\infty dr' \int_0^\infty dr'' \times \langle k_f\phi_f|V_S|\phi_n k'\rangle\langle k'|r'\rangle G_n(r', r'')\langle r''|k\rangle \quad (5)$$

then the original K-matrix is recovered simply from

$$\langle k_f\phi_f|K_S|\phi_i k_i\rangle = \langle k_f\phi_f|V_S|\phi_i k_i\rangle + \sum_{n=1}^{N}\int_0^\infty dk \langle k_f\phi_f|V'_S|\phi_n k\rangle\langle k\phi_n|K_S|\phi_i k_i\rangle, \quad (6)$$

where now there is no singularity as there was in Eq. (2).

Note that the above derivation used the relation $\langle k'|k\rangle = \delta(k' - k)$. However, this is difficult to implement numerically, and so instead we form a box-basis for the projectile which satisfies $\langle k_{n'}|k_n\rangle = \delta_{n'n}$. This ensures all integrals exist, and the integral in Eq. (6) becomes a simple sum over as many k_n as required for convergence. Note that now k_n may be included in the integrand of Eq. (6).

The integrals in Eq. (5) are essentially separable, due to the analytic nature of G_n, and so little extra computation is required. In the present case of the S-wave model studied, the evaluation of Eq. (5) is of a commensurate time as the original V-matrix elements. However, the computational time for Eq. (5) is independent of the complexity of the full problem. For general problems the extra overhead will be insignificant, particularly for two-centre problems such as positron–hydrogen scattering [22]. Convergence considerations with increasing N are the same as for Eq. (2). The primary difference now is that we have to choose a box size R_k for the projectile wavefunctions, and choose how many k quadrature points (N_k) we want to take. These can be taken to be exactly the same in every channel, open or closed, which was not possible previously. Taking R_k to be the same as for the Laguerre basis leaves N_k as the only free parameter.

3. Results

For the purpose of illustration we first take $N = 1$ and compare the old and new approaches pictorially for the case of an incident energy of 2 Hartrees. In Fig. 1 we present the integrands of Eq. (2) and Eq. (6), without the solution vector $K_S(k)$, labelled as "kernel", as well as the solution $K_S(k)$. To illustrate the behaviour of Eq. (6) under variation of R_k and N_k, two combinations are given. We see that the singularity is clearly visible at $k = \sqrt{3}$ a.u. ($E = 1.5$ Hartree) in the original form of the CCC equations labelled as "old". No such singularity exists in the new form, and yet both yield identical solution vectors $K_S(k)$ for the two total spins, as required. The new kernel V'_S has oscillations of a small amplitude which varies with the spacing between the individual momenta. This spacing depends on R_k taken for the projectile waves, but the solution must be, and is, independent of R_k. The doubling of R_k from 30 to 60 a.u. halves the momenta spacing, but then doubling N_k ensures the same maximum k.

Having shown that the method works for the simplest case, we now show its utility by providing a comprehensive approach to the S-wave model of e-H scattering that spans up to eight orders of magnitude above thresholds. To show convergence we compare $N = 30$ calculations using Eq. (6) with $N = 20$ using Eq. (2). The results for elastic, 2S and 3S excitation are given in Fig. 2. We see excellent agreement between the two sets indicating both convergence and utility of the new approach (as well as the old). Whereas in solving Eq. (2) great care needs to be exercised when calculating cross sections so close to threshold, no such concerns are required when solving Eq. (6), where only the total number of points needs to be determined.

There are some interesting features that are worth mentioning. Concentrating on 2S and 3S excitation, we see a strong suppression of the triplet cross section near the threshold compared to the singlet case. The singlet cross sections show a very similar shape, with the onset of the $n = 3$ and $n = 4$ thresholds leading to a sharp drop in cross sections for 2S and 3S states, respectively. Again, an accurate treatment of near threshold behaviour is required to get this behaviour accurately.

To complete our presentation the total ionisation cross sections are given in Fig. 3. These are the summed cross sections for all positive-energy states. Here we are unable to get arbitrarily close to threshold for finite N. We require at least one, and ideally several, positive-energy ($\epsilon_n > 0$) states which become open above the ionisation threshold of 0.5 Hartree. For $N = 20$ and $N = 30$ we may start around 0.005 Hartree above threshold. Once more we see that the two methods give good agreement indicating that convergence is to within a few percent. As in the case of 2S and 3S excitation the triplet cross section is considerably suppressed near threshold, due to the Pauli Exclusion principle, as has been found previously [19].