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FAST TRACK COMMUNICATION

A boundary adapted spectral approach for breakup problems

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Abstract
We present a spectral method to study three-body fragmentation processes. The basis set explicitly includes continuum asymptotic boundary conditions, and it is built upon generalized Sturmian functions. These functions are eigenvectors of a two-body problem where the magnitude of a potential is assumed as the eigenvalue. Comparison with a simple solvable analytical model demonstrates that our approach rapidly converges to the exact results, with basis sizes much smaller than other previous calculations. Preliminary calculations of H ionization by electron impact in the $L = 0$ approximation suggest that these convergence properties also apply to long-range Coulomb problems.

(Some figures in this article are in colour only in the electronic version)

In the last few years it has been stated that the three-body continuum problem has been solved [1]. This assertion is motivated by the fact that a theoretical quantum mechanical recipe has been found, and that its results are numerically convergent and agree with the available experimental data and other calculations. Of course, there are approximations which depend on the specific physical hypotheses and practical details of the method [2]. In this communication we introduce an alternative recipe, based on spectral expansions, presenting some important advantages when compared with other well-established techniques.

The theoretical methods developed to deal with ionizing collisions and, in general, with three-body systems, differ not only in the way the solution of the problem is reached, but also fundamentally in how these methods deal with the *asymptotic* conditions. Breakup and fragmentation problems require an adequate description of continuum states and their asymptotes. The converged close-coupling (CCC) [3] and the R-matrix [4] approaches use pseudo-states to describe the continuum. They set the asymptotic conditions in regions where two particles are close to each other, while the third one is far away. This type of channel expansion produces unphysical oscillations in the differential cross sections which are inherent to the method and cannot be removed unless an infinite number of basis elements is used [5, 6]. The exterior complex scaling (ECS) proposes an alternative way of working. It solves the problem on a numerical grid of coordinates, and fixes the boundary conditions in the fragmentation region where all the particles are far from each other (which is known as Ω_0). The procedure involves an external rotation of the coordinates in the complex plane. Since the scattered wavefunction must have pure outgoing behaviour in the asymptotic region, the rotated wavefunction must have a decreasing exponential one. For sufficiently large rotations, the exponential decay reaches zero and then the wavefunction can be numerically enforced to be zero on the border of each coordinate grid. Although this is only valid in the Ω_0 region, imposing this condition on the complete border of the grid produces cross sections which are in remarkably good agreement with experimental data for a variety of processes. The ECS has been implemented using a discretization of the two-dimensional Schrödinger equation, by finite differences on a grid, using numerical basis sets such as B-splines, or a combination of numerical and spectral methods within the discrete variable representation approach [7]. Even though there are basis sets involved in the ECS, they are of purely numerical nature and do not have any information

about the physics of the problem being studied, i.e. they do not diagonalize any of the interactions between the particles.

Beyond these physical considerations, some practical difficulties arise when solving the three-body continuum. A significant amount of computational resources are necessary to solve this problem. Progress in this field has been closely associated with the spectacular developments in parallel supercomputers. The advances of time-independent computational approaches such as the ECS [7], or CCC [3, 8] among others, rely on the capability to compute enormous amounts of integrals or to manage giant matrix systems. However, their extension to systems involving more than three particles faces huge challenges. No complete calculation within these time-independent methods has been reported for processes involving four particles such as the double ionization of helium by electron impact (e,3e). This is not due to the fact that the method itself cannot be extended to more particles, but because it is nowadays impossible to implement these approaches with the available computers [9]. Therefore, the theories have to be combined with time-dependent techniques [4, 10]. In any case, these methods are only available to those who have access to extremely large computer clusters.

In this work we address both these physical aspects as well as computational issues of previous theories. We propose a spectral method within a time-independent scheme with the potential of the ECS but requiring a considerably smaller amount of computational resources. Our assumption is that convergence rates can be substantially improved if the basis functions incorporate the physics of the problem, allowing the reduction of the computational resources needed and possibly opening the possibility of dealing with more complex systems. In the present communication we introduce an alternative method to solve the three-body problem in fragmentation processes. The asymptotic conditions are treated in a similar way to the ECS, but a Sturmian representation incorporating some of the physics of the problem is used.

Let us consider a system of two lights and a heavy particle. The three-body Schrödinger equation is $[H - E]\Psi^+ = [T + V - E]\Psi^+ = 0$, where T is the kinetic energy operator and $V = V_1 + V_2 + V_{12}$ is the usual addition of two-body interacting potentials. The wavefunction Ψ^+ for a fragmentation process is written as a sum of the initial state Ψ_0 (such that $[T + V_1 + V_2 - E]\Psi_0 = 0$), and the scattered wave $\Psi^+_{\rm sc}$, solution of

$$[E - T - V_1 - V_2]\Psi^+_{\rm sc} = V_{12}\Psi_0. \qquad (1)$$

The scattered wave $\Psi^+_{\rm sc}$ is then a solution of a non-homogeneous second-order multivariable differential equation, with a source term given by $V_{12}\Psi_0$, and with outgoing asymptotic conditions. For brevity, we restrict our analysis to an S-wave ($L = 0$) case, to avoid the long, well-known angular momenta algebra, although the use of the method for non-zero angular momenta is straightforward. At this point, we choose to expand $\Psi^+_{\rm sc}$ in a configuration interaction basis, i.e. $\Psi^+_{\rm sc}(r_1, r_2) = \sum_\nu c_\nu \phi_\nu(r_1, r_2)$ with

$$\phi_\nu(r_1, r_2) = A_S \frac{S^+_{n_a}(r_1)}{r_1}\frac{S^+_{n_b}(r_2)}{r_2} \qquad \nu = \{n_a, n_b\} \qquad (2)$$

where the operator A_S takes care of the proper symmetrization of the wavefunctions. The main contribution of this communication is to choose these $S^+_n(r)$ functions as *generalized Sturmians*. They are solutions of a two-body Schrödinger equation

$$[T_i + V_i - E_i]S^+_n(r_i) = -\beta_n \bar{V}_i S^+_n(r_i) \qquad i = 1, 2 \qquad (3)$$

where β_n (and *not* the energy) is considered the eigenvalue. This eigenvalue is the magnitude of a generating potential $\bar{V}_i$ such that for long distances $[T_i + V_i - E_i]S^+_n(r_i) = 0$. It is easy to see that they constitute a basis set with orthogonality and closure relations given by ($i = 1, 2$)

$$\int S^+_{n'}\bar{V}_i S^+_n \,\mathrm{d}r_i = \delta_{n'n},$$

$$\sum_n S^+_{n'}(r_i)\bar{V}_i(r_i)S^+_n(r'_i) = \delta(r_i - r'_i),$$

respectively. One should choose positive energies E_i for the fragmentation problem in (3). This Sturmian equation is then solved in such a way that $S^+_n(r)$ has outgoing behaviour for all n, and diagonalizes the interaction potential V_i. Thus, the Sturmians $S^+_n(r)$ have a 'built-in' non-zero flux for large distances, which is a condition of the fragmentation processes. Of course, the result is a set of complex eigenvalues β_n that, together with the interaction $\bar{V}_i$, introduce a complex short-range potential that generates this outgoing flux. The introduction of the asymptotic behaviour at the basis level avoids the exterior rotation of the coordinates into the complex plane, such as in the ECS approach. Although in principle arbitrary, the selection of $\bar{V}_i$ is dictated by the physical features of the full interaction V under study. Calculation of the basis set is performed by an expansion on Laguerre polynomials [11] or fully numerical on a radial grid [12]. The spatial extension of the basis is controlled by a coordinate scaling parameter λ in the Laguerre method [11], whereas the basis is computed in a box of a predefined radial size r_c in the grid one [13]. Other asymptotic conditions like incoming or standing-wave boundary conditions can be equally developed.

Replacing the CI expansion in the scattering equation (1), and projecting into the basis elements, the following linear system has to be solved:

$$[\mathbf{H} - (E - E_1 - E_2)\mathbf{S}]\mathbf{\Psi}^+_{\rm sc} = \mathcal{F},$$

where $\mathbf{H}$ is the matrix representation of the Hamiltonian in the basis $\phi_\nu(r_1, r_2)$, $[\mathbf{H}]_{\nu\nu'} = \langle\phi_\nu|H|\phi_{\nu'}\rangle$, while $[\mathbf{S}]_{\nu\nu'} = \langle\phi_\nu|\phi_{\nu'}\rangle$ is the overlap matrix, $\mathcal{F}$ represents the source $V_{12}\Psi_0$ projected into the basis set and $\mathbf{\Psi}^+_{\rm sc}$ is the vector of coefficients c_ν that completely determines the solution of the problem. It should be noted that the selection of the basis energies E_1 and E_2 is also arbitrary and can be different from the *physical* energies E_a and E_b. In addition, the Sturmian functions diagonalize the kinetic energy and the interaction potentials V_i. Therefore, only the interaction potential V_{12} and the generating potential $\bar{V}_i$ remain in the computation of $[\mathbf{H}]_{\nu\nu'}$, which substantially simplifies the evaluation of the matrix elements.

We can now proceed further and set up an analytically solvable three-body fragmentation problem which can be used to test our proposal. To this end we recall that the formal solution of equation (1) can be expressed in terms of the full

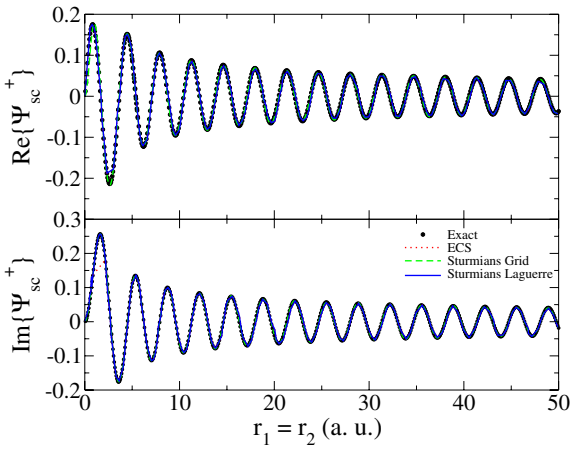

Figure 1. Comparison of the first-order exact wavefunction with calculations using the generalized Sturmian basis.

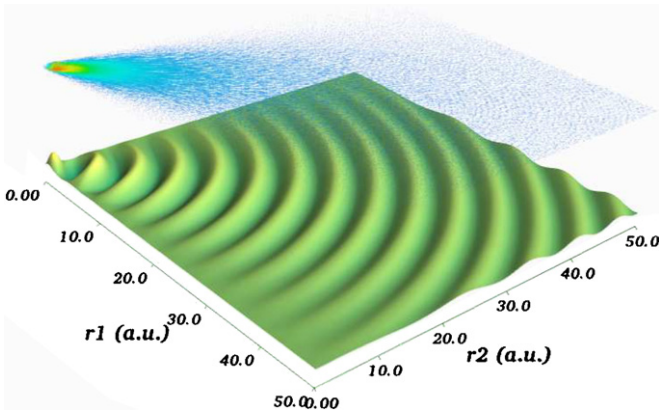

Figure 2. Real part of the first-order scattering wavefunction computed with the generalized Sturmian basis (below), for an incident energy of 24 eV. The vector field (above) represents the flux of the wavefunction as a function of r_1 and r_2. The breakup channel is seen clearly as a maximum of the flux around the line $r_1 \approx r_2$.

Green function $G^+ = [H - E]^{-1}$, as $\Psi^+_{sc} = G^+ V_{12} \Psi_0$. We can make use of the free Green function to write the solution up to first order as $\Psi^+_{sc} = \Psi_0 + \Psi^{(1)+}_{sc} = \Psi_0 + G^+_0 V_{12} \Psi_0$, with

$$[E - T]\Psi^{(1)+}_{sc} = V_{12}\Psi_0. \tag{4}$$

Since the analytic form of the free Green function is known [14], it is possible to obtain exact, closed form expressions for the solution $\Psi^{(1)+}_{sc}$ of equation (4), for certain classes of inter-particle potentials V_{12} and initial channel wavefunctions Ψ_0. One of such interactions is a product of exponential potentials $V_{12} \propto \exp(-ar_1 - br_2)$. This particular choice enables us to compute first the scattered function Ψ^+_{sc} as a series in terms of Hankel functions of the hyper-radius $\rho = \sqrt{r_1^2 + r_2^2}$ and Jacobi polynomials of the hyper-angle $\tan\alpha = r_2/r_1$. Finally, the scattering amplitude $f(\alpha)$ and the single differential cross section $(\mathrm{d}\sigma/\mathrm{d}\varepsilon = |f(\alpha)|^2/(k_a k_b))$ in terms of the energy sharing parameter $\left(\varepsilon = E_b/E_a = k_b^2/k_a^2\right)$ can be extracted from the asymptotic behaviour of the wavefunction [22]. This analytic model is a generalization of the one proposed in [15].

The first problem to analyse corresponds to the case where a constant value of 0.1 a.u. for Ψ_0 is considered in equation (4), to be able to compare with the results of the ECS approach [15]. In figure 1 we plot the scattered wavefunction against the exact results, for $r_1 = r_2$ and a total energy $E = 24$ eV. We make use of a basis of 30 Sturmians for each light particle, with an extension up to $r_c = 50$ a.u. with the grid method, while using 90 Sturmian functions with $\lambda = 1.5$ with the Laguerre expansion. In both calculations the generating potential is $\bar{V}_i = \mathrm{e}^{-0.3r_i}$. We find it convenient to choose $E_1 = E_2 = E$. Our results show an excellent agreement for both real and imaginary parts of the wavefunction compared to the analytic values, and also with previous calculations of Rescigno and co-workers [15].

We can compare the average efficiency of our method by computing the density of wavefunction basis per atomic unit, $d_b = N/V$, where N is the total basis size and V is the volume of the configuration space where the solution of the three-body problem is accurately described by the basis set. For the numerical Sturmian method, we have $V = r_c^2$, and for example, the density d_b for the calculations of figure 1 is 0.38 a.u.$^{-1}$. With the Laguerre expansion the corresponding d_b is 0.48 a.u.$^{-1}$ for $\lambda = 1.5$. This can be compared to $d_b = 25$ a.u.$^{-1}$ for time-dependent methods [16], and to $d_b \sim 2$ a.u.$^{-1}$ for ECS [17] or $d_b \sim 1.29$ a.u.$^{-1}$ [18] for similar problems. It is clear that our method requires less basis elements than all previous models.

Let us now turn to a more realistic fragmentation problem. We consider a light particle colliding with a two-body bound system, interacting with exponential potentials $V_i = 3\exp(-r_i)$, which supports only a bound state with energy $E_i = 11.2$ eV. We also assume the product of exponential potentials for the V_{12} interaction. The initial state Ψ_0 is the symmetrized product of the bound state and the $l = 0$ continuum partial wave that represents the incoming particle. In figure 2 we show the absolute value of our solution as a function of radial coordinates, as well as the numerical computation of the flux of the wavefunction, $\mathbf{j} = \Im\left(\Psi^+_{sc} \nabla \Psi^+_{sc}\right)$. We can clearly see that the general aspect of the function corresponds to a hyper-spherical wave depending on the hyper-radius ρ. The flux shows that the wavefunction has outgoing behaviour and that its maximum intensity is observed mostly in the region where $r_1 \approx r_2$, which corresponds to the breakup channel.

We also compute the differential cross section $\mathrm{d}\sigma/\mathrm{d}\varepsilon$ with both Sturmian bases. The comparison of our calculations against the exact results is shown in figure 3. We evaluate the cross section at different values of the hyper-radius ρ. In both methods, convergence to the exact values is achieved for increasing ρ. Small oscillations around the exact value are observed with both methods. They originate in the fact that outgoing waves are enforced on r_1 and r_2 when actually the outgoing behaviour should be expected on the hyper-radius. However, their magnitude decreases when ρ is increased. In addition, these oscillations concentrate on the borders of the configuration space where $r_1 \approx 0$, and r_2 is large, or vice versa. In these regions, the asymptotic conditions where one particle is far from the other two (Ω_1 and Ω_2 regions) would be more adequate. However, the outgoing conditions imposed to

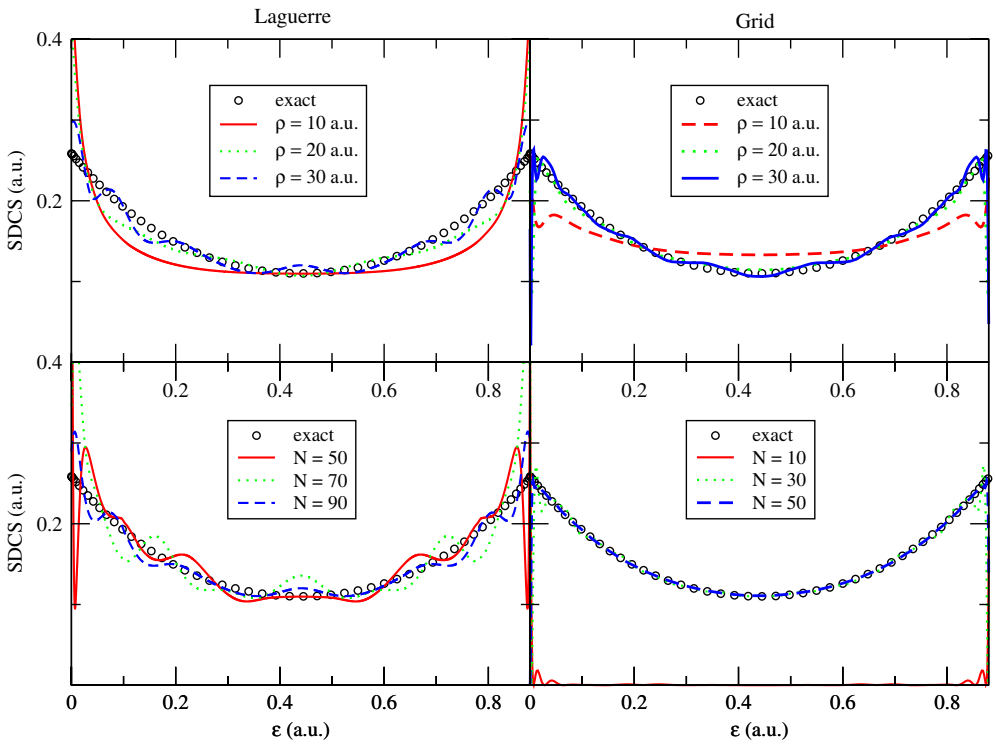

Figure 3. Single differential breakup cross section in terms of the energy sharing $\varepsilon = E_b/E_a = k_b^2/k_a^2$. The problem solved includes short-range exponential interactions $V_i = 3\exp(-r_i)$, $i = 1, 2$, while $V_{12} = \exp(-r_1 - r_2)$. Top row: SDCS as a function of ρ for both methods, the Laguerre basis uses $\lambda = 2.5$ and $N = 90$ basis functions per particle, while the numerical grid calculation extends up to $r_c = 50$ a.u. with a one-particle basis size of $N = 30$. Bottom row: SDCS for different basis sizes for both methods. Cross sections are computed at $\rho = 30$ a.u.

both coordinates work equally but at the expense of requiring more basis functions. The symmetry observed on the cross section arises naturally from the method, due to the proper boundary conditions included in the basis for both scattered particles.

Finally, we extended our calculation to the much more realistic Temkin–Poet problem, which models the ionization of one-electron atom by electronic impact, keeping only total angular momentum $L = 0$. This is a prototypical test for collision calculations, where the methods are faced with the long-range features of the Coulomb problems, but set aside the cumbersome angular momenta algebra. In figure 4 we present calculations of the single differential cross section of the singlet state for 54.4 eV impact energy. Computations were performed with the grid method for the Sturmian basis, with 150 Sturmians and $r_{\max} = 100$ a.u. Our basis diagonalizes the kinetic energy and some of the interaction potentials, reducing the size of the calculation and enabling us to solve this problem accurately with a single desktop PC.

Our result shows a good agreement with the benchmark calculations of ECS [19] and FDM [20], and with time-dependent calculations of Pindzola *et al* [21]. Cross sections are symmetric (which is not the case with CCC calculations, and therefore are not included in the comparison). Tiny oscillations can be attributed to the 'small' asymptotic hyper-radius $\rho = 80$ a.u. where the cross sections are obtained, and to the fact that asymptotic conditions are imposed on the $\{r_1, r_2\}$ space and not on the hype-radial coordinate, which should be the case. We recall that the results of ECS shown

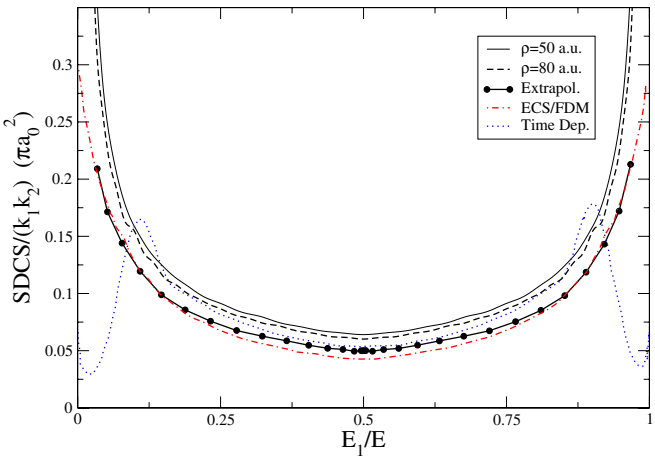

Figure 4. Single differential cross section (SDCS) for singlet ionization in the Temkin–Poet model, in terms of the energy of one of the particles. The impact energy is 54.5 eV. Solid thin black line: SDCS with the present method computed at $\rho = 50$ a.u., dashed black line: the present method at $\rho = 80$ a.u., black circles: extrapolation of the present results for $\rho \to \infty$, dot–dashed red line: SDCS obtained with ECS [19] or FDM [20], dotted blue line: time-dependent calculations [21].

in figure 4 were obtained with $\rho = 200$ a.u., whereas FDM needs $\rho = 240$ a.u. The figure shows that already for $\rho = 80$ a.u. our cross section has the proper shape and magnitude, putting in evidence the efficiency of our method. We have also computed the extrapolation for $\rho \to \infty$, which well agrees with ECS and FDM results. Differences with these theories

arise for (a) small energies of one of the ejected electrons, where the ECS and FDM also interpolate the cross sections and (b) $E_1 = E_2 = E/2$, where our results should be extended for larger distances.

In summary, we devised a method to deal with three-body fragmentation problems based on the use of Sturmian functions equipped with the appropriated asymptotic conditions. The problem is solved including the boundary condition of the Ω_0 region. We would like to stress the fact that these Sturmian functions diagonalize completely the kinetic energy as well as the interaction potentials. This means that the continuum breakup eigenstate of a given total energy E is represented by a spectral expansion in the magnitude of the potential $\bar{V}_i$, and therefore, the continuum itself is *not* discretized as in previous methods. Then, only the inter-particle interaction potential remains to be solved by the basis. Both grid and Laguerre Sturmian methods provide an accurate description of the process and are similarly efficient; their practical implementation presents differences in the way the potentials and boundary conditions are considered. We demonstrated in this communication that physically converged cross sections are obtained within this Sturmian theory, using a small number of basis functions and with fewer resources than those reported by the ECS or FDM. Moreover, our technique is also efficient in solving the Temkin–Poet model where long-ranged interactions are included. These encouraging results lead us to explore further the method for complete collisional ionizing problems.

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