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Collision problems treated with the Generalized Hyperspherical Sturmian method

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Abstract.

An hyperspherical Sturmian approach recently developed for three–body break–up processes is presented. To test several of its features, the method is applied to two simplified models. Excellent agreement is found when compared with the results of an analytically solvable problem. For the Temkin–Poet model of the double ionization of He by high energy electron impact, the present method is compared with the Spherical Sturmian approach, and again excellent agreement is found. Finally, a study of the channels appearing in the break–up three–body wave function is presented.

1. Introduction

The incorporation of appropriate boundary conditions on break–up three–body problems is a very difficult task. Various approaches have been developed to provide *ab initio* solution of such problems. Some of them, like the convergent close–coupling [1] or the J–Matrix [2] methods, impose the boundary conditions explicitly. Other approaches, such as the exterior complex scaling [3] or the Generalized Sturmian Functions (GSF) [4] approach, circumvent an explicit imposition. In the latter methods, at large distances, the outgoing flux conditions are enforced separately on each one of the outgoing particles (e.g. two electrons) coordinates. It turns out that this generates for the scattering wave function an overall hyperspherical outgoing asymptotic shape. Even though this is the expected behavior for a three–body collision problem, it is not completely clear how this front is generated. Hyperspherical coordinates should provide, in principle, the most effective framework to generate a basis set to build up, naturally, this expected asymptotic behavior. However, as different ionization channels are simultaneously present and coupled (single ionization with or without excitation, and double ionization) it is very useful to investigate which scheme (spherical or hyperspherical or a combination) is best suited. In order to do so, and to identify the advantages of each, we have used the Generalized Sturmian approach in both systems of coordinates (for a review see [4] and [5]). It consists of a spectral method with the essential feature that the asymptotic behavior can be explicitly imposed on the basis functions. In this way, Generalized Sturmian functions need to expand only the reaction zone, rendering the method very efficient.

2. Theory

2.1. General scattering problem

In any scattering process there is always a prepared initial state defining the initial channel, and a final state which is the result of the collision itself. When performing a quantum study of the process within a time–independent representation, one can split the wave function Ψ as the sum of two terms $\Psi = \Psi_0 + \Psi_{\rm sc}$. The initial channel wave function Ψ_0 satisfies an initial channel hamiltonian. The scattering solution $\Psi_{\rm sc}$, on the other hand, possesses all the information about the collision problem and satisfies a driven Schrödinger equation

$$[H - E]\,\Psi_{\rm sc}\,(\mathbf{r}_1, \mathbf{r}_2) = -\,[H - E]\,\Psi_0\,(\mathbf{r}_1, \mathbf{r}_2) \equiv \varphi\,(\mathbf{r}_1, \mathbf{r}_2)\ , \tag{1}$$

where H is the three–body hamiltonian, and $\varphi\,(\mathbf{r}_1, \mathbf{r}_2)$ is named the driven term. The Peterkop–type asymptotic behavior [6]

$$\Psi^{+}_{\rm sc}\,(\mathbf{r}_1, \mathbf{r}_2) \longrightarrow A\,(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2, \alpha)\ \frac{e^{iK\rho + i\gamma \ln(2K\rho)}}{\rho^{5/2}}, \tag{2}$$

should be imposed on the solution in the Ω_0 region where all three particles are far from each other. In Eq. (2), $K = \sqrt{2E}$ defines the hyper–momentum, $\rho = \sqrt{r_1^2 + r_2^2}$ the hyper-radius and $\alpha = \tan^{-1}(r_2/r_1)$ the hyperangle, and the hyperspherical Sommerfeld parameter is defined as

$$\gamma = \frac{1}{K}\left[\frac{1}{\cos\alpha} + \frac{1}{\sin\alpha} - \frac{1}{\sqrt{1 - \hat{\mathbf{r}}_1 \cdot \hat{\mathbf{r}}_2 \sin 2\alpha}}\right] \equiv \frac{\mathcal{C}(\omega_5)}{K} \tag{3}$$

which clearly depends on the angular coordinates $\omega_5 = \{\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2, \alpha\}$.

2.2. The Hyperspherical Generalized Sturmian method

The GHSF have been thoroughly described, e.g. in [7, 8]. Here we just recall that the kinetic–energy operator reads

$$T = -\frac{1}{2\mu}\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) - \frac{\Lambda^2}{\rho^2}\right] \tag{4}$$

where Λ^2 is the grand orbital angular momentum. The interaction between all the particles

$$V(\rho, \omega_5) = \frac{\mathcal{C}(\omega_5)}{\rho}. \tag{5}$$

can be viewed as a Coulomb potential having a $1/\rho$ behavior and a charge depending on all the angular variables.

To solve Eq. (1) we use the following expansion in terms of GHSF basis set [8, 9]

$$\Psi^{NUM}(\rho, \alpha) = \frac{1}{\rho^{\frac{5}{2}}}\sum_m \sum_n a_{n,m}\ S^{+}_{n,m}(\rho)\ \Omega_n(\alpha) \tag{6}$$

where $\Omega_n(\omega_5)$ and $S_{n,m}(\rho)$ are the angular and radial GSF, respectively. In this contribution we deal only with S–wave models so that the $\Omega_n(\omega_5)$ functions depend only on the α coordinate. In particular we will use $\Omega_n(\alpha)$ functions being the eigenfunctions of the grand angular momentum, $\Lambda^2\Omega_n(\alpha) = (q_n^2 - 4)\Omega_n(\alpha)$; the eigenvalues are $(q_n^2 - 4) = \lambda_n(\lambda_n + 4)$ with $\lambda_n = 2n$ $(n = 0, 1, \ldots)$. The hyperradial Sturmian functions satisfy the following equation

$$\left[-\frac{1}{2\mu}\frac{\partial^2}{\partial\rho^2} + \frac{q_n^2 - 1/4}{2\mu\rho^2} + \mathcal{U}(\rho) - E\right] S_{n,m}(\rho) = \beta_{n,m}\,\mathcal{V}_g(\rho)\,S_{n,m}(\rho), \tag{7}$$

where $\mathcal{U}(\rho)$ is called the auxiliary potential, $\mathcal{V}_g(\rho)$ the generating potential, $\beta_{n,m}$ are the eignevalues while the energy E is externally fixed. By choosing a short range generating potential, all hyperradial Sturmian functions will possess the same asymptotic behavior dictated by the long range behavior of the auxiliary potential (outgoing behavior is taken in Eq. (6)).

3. Application Example: a scattering model problem

Before tackling the full double ionization problem, we wanted to make sure that all developed numerical tools were working properly and proceeded in the following way. Knowing that the full Coulomb interaction involves $\mathcal{C}(\omega_5)$, we started first by analyzing a problem where the charge is taken as a constant $\mathcal{C}(\omega_5) = \mathcal{C}$, and named this the model problem. Then, we increased the difficulty by considering $\mathcal{C}(\omega_5) = \mathcal{C}(\alpha)$, i.e., a Temkin–Poet model. In this contribution, we first present results of these two models and then some preliminary results corresponding to the full problem.

3.1. Model Problem

In this case we considered the Coulomb potential $\mathcal{C}/\rho$ and a driven model source [9, 10]

$$\varphi(r_1, r_2) = e^{-a\rho}\frac{1}{2}\left[\frac{\sin(r_1)}{r_1}\frac{\sinh(r_2)}{r_2} + \frac{\sin(r_2)}{r_2}\frac{\sinh(r_1)}{r_1}\right], \tag{8}$$

which simulates a symmetrized bound-free initial state multiplied by a Coulombic potential (a is a parameter such that $\Re(a) > 1$). The proposed model three–body problem is non separable in either spherical or hyperspherical coordinates. It has an analytical solution [9] which provides a solid benchmark to test the proposed numerical expansion (6). The latter is built to have the desired outgoing asymptotic behavior

$$\lim_{\rho\to\infty} \Psi^{+}(\rho, \alpha) = f(\alpha)\frac{e^{iK\rho - i\eta\ln(2K\rho)}}{\rho^{\frac{5}{2}}}, \tag{9}$$

expected for a Coulomb scattering problem [6] ($\eta = \mathcal{C}\mu/K$ is the Sommerfeld parameter). This limit provides an analytical expression also for the transition amplitude $f(\alpha)$. Numerically, for the radial GSF, the auxiliary potential $\mathcal{U}(\rho)$ is taken to be equal to the interaction potential $\mathcal{C}/\rho$, while the generating potential $\mathcal{V}_g(\rho)$ is set as a Yukawa potential in ρ. With this choice, asymptotically, Eq. (7) reduces to a Coulomb homogeneous equation providing all basis functions (and thus the hypersherical GSF) a unique – and appropriate – asymptotic behavior

$$\lim_{\rho\to\infty} S^{+}_{n,m}(\rho) \propto e^{iK\rho - i\eta\ln(2K\rho)}. \tag{10}$$

Then the transition amplitude can be easily extracted

$$f(\alpha) = \sum_n \left(\sum_m a_{n,m}\right)\Omega_n(\alpha) \tag{11}$$

and compared to the analytical result.

In Ref. [9, 10], several kinematic situations were studied and overall excellent agreement was found between the numerical hyperspherical expansion $\Psi^{NUM}(\rho, \alpha)$ and the analytical solution. An example is provided by Fig. 1.

The model problem allowed one to explore how the scattering wave function behavior is modified for different hyperradial domains, and how far one should go to extract the transition amplitude from the wave function itself. It was found that, although the driven term vanishes for $\rho > 5$ a.u. for $a = 2$, the required hyperradial distances are very large, especially for low energies, as illustrated in Fig. 2. As a rule of thumb, to obtain converged transition amplitudes one should get the scattering solution up to $\rho_\sigma > 3000/K$, implying enormous distances. It should

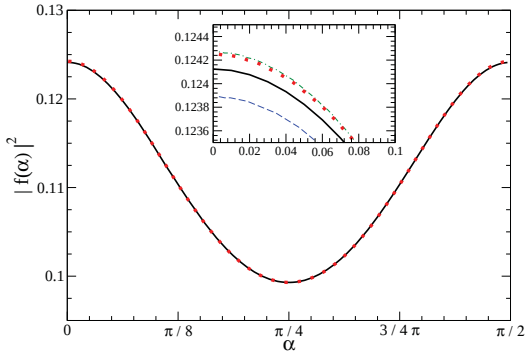

Figure 1. The analytical (full line) and numerical (dotted line) transition amplitude for $K = 1$ a.u., are shown as a function of α. Inset: partial summations (different hyperangular quantum numbers n in Eq. (11) for the numerical transition amplitudes, with 2 terms (dashed line), 3 terms (dot–dashed line), and 8 terms (dotted line).

be emphasized that with the GHSF method, we are able to reach the truly outgoing asymptotic region, where no other numerical method (besides the propagations performed by Malegat *et al* [11]) can handle the calculations. In this sense our hyperspherical approach is highly efficient in comparison with spherical methods. It is worth noting that, in general, other methods cannot reach the required asymptotic distances and therefore need to extrapolate the numerical wave functions; our method will allow to explore the validity of such extrapolation technique. While integral formulae succeed in providing transition amplitudes from a much smaller domain, it is interesting to know how far it is necessary to go to really reach the asymptotic region.

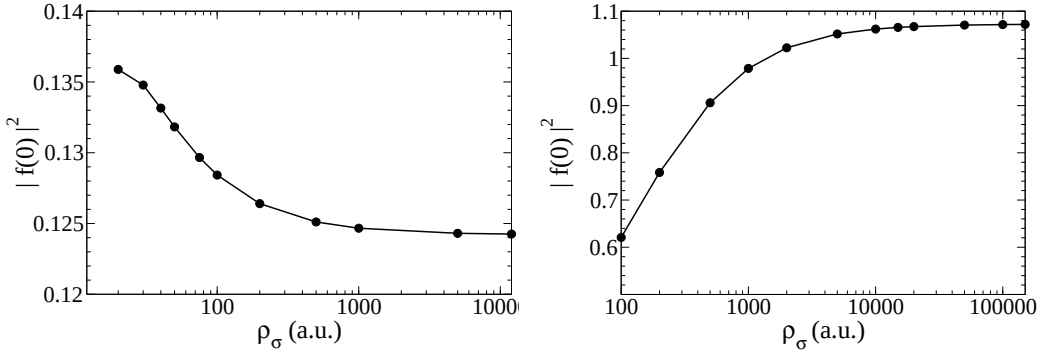

Figure 2. Squared amplitude versus the hyperradial distance ρ_σ at which the calculation is performed: (left) $K = 1$ a.u. ($E = 0.5$ a.u.) and (right) $K = 0.1$ a.u. ($E = 0.005$ a.u.)

4. Double Ionization of He: Temkin–Poet model

As a second test we consider a Temkin-Poet model of the double ionization of He by fast electrons [12]. As these may be described by plane waves, one ends up with a first order driven equation

$$[E - H]\,\Phi_{sc}^{(1)+}(\mathbf{r}_1, \mathbf{r}_2) = -\frac{1}{(2\pi)^3}\frac{4\pi}{q^2}\left(-Z + e^{i\mathbf{q}\cdot\mathbf{r}_1} + e^{i\mathbf{q}\cdot\mathbf{r}_2}\right)\Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2)\,, \tag{12}$$

where $\Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2)$ represents the initial He target ($Z = 2$), and $\mathbf{q}$ is the momentum transfer. Within a S–model approach, Eq. (12) becomes

$$\left[-\frac{1}{2r_1^2}\frac{\partial}{\partial r_1}\left(r_1^2\frac{\partial}{\partial r_1}\right) - \frac{1}{2r_2^2}\frac{\partial}{\partial r_2}\left(r_2^2\frac{\partial}{\partial r_2}\right) - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_>} - E_a\right]\Phi_{sc}^{+}(r_1, r_2) = \mathcal{F}(r_1, r_2)\,, \quad (13)$$

where the driven term reads

$$\mathcal{F}(r_1, r_2) = -\frac{1}{(2\pi)^3}\frac{4\pi}{q^2}\left[-Z + j_0(qr_1) + j_0(qr_2)\right]\Phi^{(0)}(r_1, r_2)\,. \quad (14)$$

To further simplify, in Ref. [12], the ground state of the S–wave model of He $\Phi^{(0)}(r_1, r_2)$ was chosen as the simple product of screened exponentials with variational charge $Z = 1.6875$.

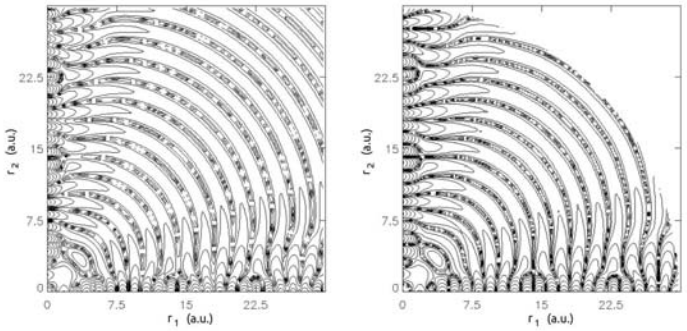

Figure 3. Left: real part of the scattering wave function $\Phi_{sc}^{(1)+}(r_1, r_2) \times \rho^{5/2}$ obtained with GSF as a function of the ejected electrons radial coordinates r_1 and r_2, for $E = 0.791$ a.u. and $q = 0.24$ a.u. Right: real part of $\Phi_{sc}^{(1)+}(\rho, \alpha) \times \rho^{5/2}$ obtained with GHSF.

The model equation (13) was numerically investigated [12] with both the spherical [5, 13] and the hyperspherical GSF method. For the latter, expansion (6) was used with basis functions with the desired asymptotic outgoing boundary condition (10) with charge Z. One of the kinematical situations studied in [12] is for a momentum transfer $q = 0.24$ a.u. which corresponds to the initial and final projectile energies of, respectively, $E_i = 5599$ eV and $E_f = 5500$ eV, and a deflection of 0.45^0, used in the $(e, 3e)$ Orsay experiment [14]. These values, together with the exact ground state energy of the bound initial state, define the final two–electrons energy equal to $\simeq 20$ eV. For an equal energy sharing situation, this corresponds to 10 eV per electron, as in the experiments [14]. It has to be noted that, no theoretical study of the full $(e, 3e)$ problem has yet managed to describe satisfactorily all the experimental data. What is more confusing and difficult to explain, is that several *ab initio* methods provide different answers both in cross sections shapes and magnitudes (see a review in Ref. [15]).

For the model $(e, 3e)$ problem, the real part of the scattering solution (actually $\Phi_{sc}^{(1)+} \times \rho^{5/2}$) is presented in Fig. 3 as a function of r_1 and r_2. The left panel shows that the coupling of products of spherical basis functions manage to generate, in the inner region, the appropriate solution with a hyperspherical outgoing front (this was shown also for the $(e, 2e)$ process [13]). With the hyperspherical expansion (right panel), the hyperspherical wave front is naturally generated by the basis. The two completely independent methods (and codes) are leading to the same answer, and the double ionization channel is obtained by enforcing outgoing type flux

conditions on the basis set. This agreement can be further appreciated through a more detailed and quantitative comparison between both numerical methods. Fig. 4 shows a comparison between both calculations for $r_1 = r_2$ (i.e., at $\alpha = \pi/4$), a region in which – although the amplitudes of the solutions are very low – the agreement between the results given by the two numerical approaches is excellent.

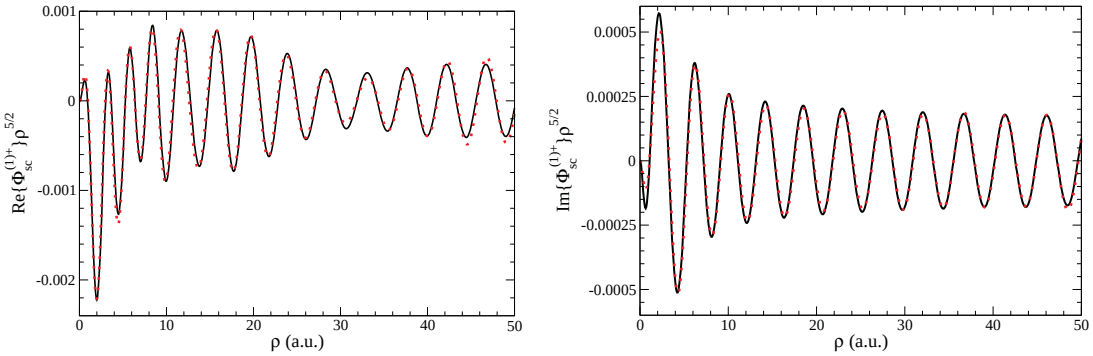

Figure 4. Real (left) and imaginary (right) part of the scattering wave function $\Phi_{sc}^{(1)+} \times \rho^{5/2}$ as a function of the ejected electrons hyperspherical coordinate ρ, obtained with the spherical (red, dotted) and hyperspherical (black, continuous) coordinates Sturmian expansions. $\alpha = \pi/4$, $E = 0.791$ a.u. and $q = 0.24$ a.u.

Within the same double ionization S–wave model, a detailed analysis of the scattering solution has been recently presented [16]. The single continuum (single ionization) channels populate the asymptotic domains Ω_i (with $i = 1, 2$) [17] which correspond to the situation in which one of the electrons is close to the nucleus, forming a bound state, and the other one is far away. Let us consider, for instance, the Ω_1 region, where the wave function should have the following asymptotic form:

$$\Phi^{+}_{sc,1}\left(\mathbf{q}, \mathbf{r}_1, \mathbf{r}_2\right) \underset{r_1 \to \infty}{\to} \frac{1}{2\pi} \sum_n F_n\left(k_n \hat{\mathbf{r}}_1, \mathbf{q}\right) \frac{e^{ik_n r_1 - i\eta_{1,n} \ln(2k_n r_1)}}{r_1} \phi_n(\mathbf{r}_2), \tag{15}$$

with $F_n\left(k_n \hat{\mathbf{r}}_1, \mathbf{q}\right)$ denoting the transition amplitude for that single ionization channel and the eikonal corresponds to the ejected electron asymptotic behavior. The extraction of the ejected electron functions is obtained by projecting the three–body $\Phi^{+}_{sc}(r_1, r_2)$ function onto each single electron He^+ bound state $\phi_n(\mathbf{r}_2)$. Within the GSF formulation there is a particular basis set which does contain those bound states, and makes the extraction of single continuum channels a trivial matter [16]. In Fig 5, we present separately the contributions of the wave function corresponding to the single ionization channels (up to $n = 5$) and the remainder of the function. Note that the double continuum with its hyperspherical front remains unaffected by this separation.

5. Double Ionization of He: full calculation

Although we are presently checking the convergence and agreement among the independent implementations, we show some preliminary GSF results for the full double ionization of He problem, going beyond the Temkin–Poet and $L = 0$ models.

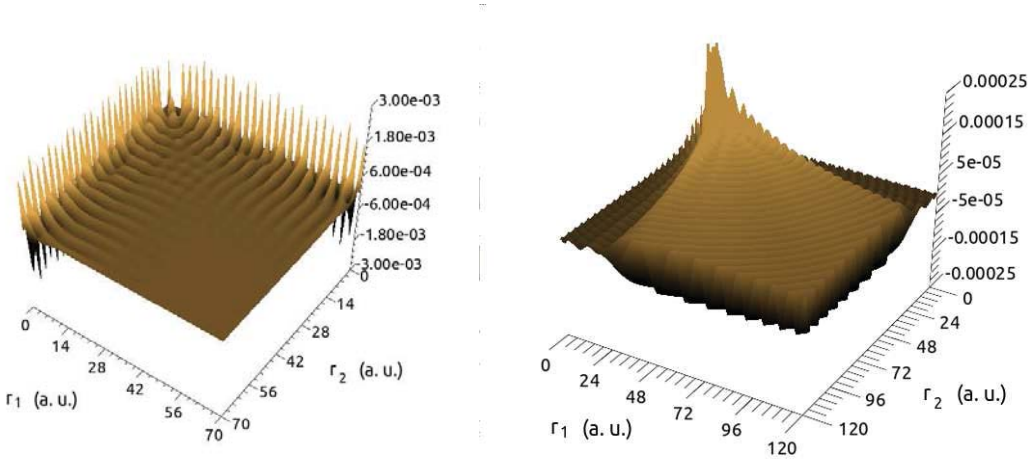

Figure 5. Separation of channels: single ionization (left) versus double ionization (right).

We have solved Eq. (12) again with $q = 0.24$ a.u.. In Fig. 6, we show the partial scattering wave functions corresponding to some of the dominant pairs contribution: $(l_1, l_2) = (0, 0)$ coupling to a total $L = 0$, $(l_1, l_2) = (0, 1)$ coupling to $L = 1$, $(l_1, l_2) = (0, 2)$ coupling to $L = 2$, and $(l_1, l_2) = (1, 2)$ coupling to $L = 1$. As for the $(e, 2e)$ or the model $(e, 3e)$ processes, the angular coupling of spherical GSF generates the outgoing Ω_0 hyperspherical front for the double continuum. It can be observed that the $L = 1$ waves produces the major contribution to double ionization process. This can be easily related to the fact that in the low momentum transfer limit this process has to resemble the double photoionization dipole limit, and within this regime there is a $\Delta L = 1$ selection rule. While for $(e, 3e)$ the same rule does not apply strictly, even at small q values, some trace can be found in the presented partial waves.

For the double ionization channel, in view of the Ω_0 region Peterkop asymptotic behavior in which hyperspherical coordinates appear naturally, an hyperspherical formulation is expected to be optimal. In the Ω_i $(i = 1, 2)$ regions, which correspond to single ionization channels, spherical coordinates are more natural and therefore the spherical formulation is presumably more adequate and efficient [16]. This said, both schemes can be used for either channel. Indeed, similarly to what observed for the $(e, 3e)$ S–wave model (See Fig. 3 and 4), we also found beautiful mutual agreement in both Ω_0 and Ω_i regions for the full physical problem. The two formulations (GSF and GHSF) are somehow complementary to understand the underlying physics of break–up problems. A comparison between them is presently being studied, and the advantages of each scheme being analyzed in separate spatial domains. Differential cross sections are also being tested within different numerical implementations and will be presented elsewhere.

6. Summary

The results presented in this contribution showed that the hyperspherical Sturmian approach is very efficient. First of all it provides a natural way to describe three–body break–up problems and in particular the Peterkop–type behavior (2) in the Ω_0 region. Second, the method has been tested successfully with two model problems, leading to indistinguishable results from those obtained with a spherical approach which is supposed to work better in the Ω_i regions. The same conclusions are obtained for the real double ionization problem.

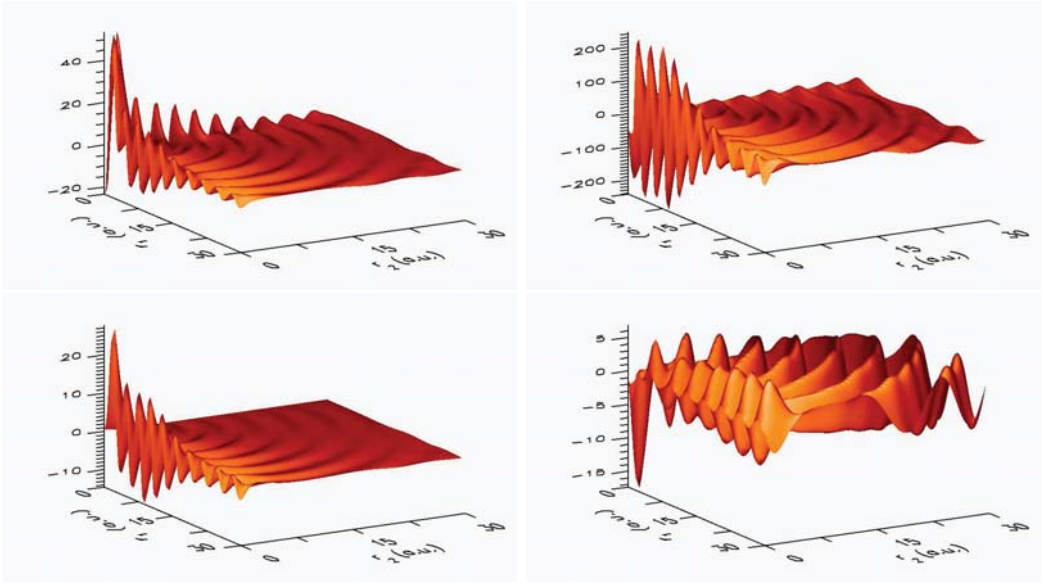

Figure 6. Partial wave contributions of the scattering wave function for double ionization of He (all multiplied by 10000). From left to right, first row: $(l_1, l_2) = (0, 0)$ coupling to a total $L = 0$, $(l_1, l_2) = (0, 1)$ coupling to $L = 1$. Second row: $(l_1, l_2) = (0, 2)$ coupling to $L = 2$, and $(l_1, l_2) = (1, 2)$ coupling to $L = 1$.

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