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Propagation in hyperspherical coordinates

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Summary. The R-matrix theory is used to discuss algorithms for the calculation of scattering amplitudes for chemical reactions. A formulation of the microscopic equations in terms of hyperspherical coordinates and the use of the hyperradius as the reaction coordinate requires a detailed specification of the multitude of available channels and particular emphasis is placed here on the treatment of the rotational manifold by means of a generator coordinate description. Examples are presented for atom-diatom systems

Key words: Quantum dynamics – Molecular dynamics

1. Introduction

Representations are developed here of the asymptotic channel states for reactive molecular collisions. Their aim is to simplify the treatment of a great number of partial waves by means of a localized description of the parameter space of the three-dimensional rotation group. Sparse matrix techniques offer efficient algorithms which compensate the loss of the partial wave block structure of the problem. Some suggestions for basis sets are presented and their efficiency is discussed.

Reaction rate theory at the microscopic level is developing rapidly with the help of new conceptual tools and, particularly, new computing equipment. Detailed determination of partial cross sections for reacting atom-diatom systems is now possible with the use of computer codes from several laboratories [1–8]. These capabilities can be expected to be extended to four-particle systems [9, 10]. The post-computing processing of the data will become an ever more demanding part of the work due to the great proliferation of channels and the incorporation of weighted averaging procedures while maintaining certain degrees of state specificity enters as a significant element in any study.

Miller [11] formulated a theory for rate constants in terms of the flux-flux autocorrelation function and the appropriate statistical distribution functions for a system where thermal equilibrium is maintained. More detailed, but not totally resolved, transition probabilities are being obtained in experimental laboratories

and it is a matter of concern to the theorist to find the most economic way to obtain as accurate results as possible with a prescribed resolution.

The motivation for the study presented here is that neither the conventional partial wave analysis [12] nor Born-type approximations [13] may be the optimal way towards the calculation of scattering amplitudes. Remarkable results by Regge [14] have demonstrated that the scattering amplitude may have an analytical extension to complex angular momentum which admits a simple representation in terms of a few residues and poles. Similarly there has been a great development in the theory of resonances from the study of dilatation transformations or complex scaling [15]. These developments point towards possibilities also in the numerical applications where "unconventional" basis sets may offer advantages. The long-range potentials which are important in low-energy molecular collisions give notoriously long series in partial wave expansions even though they may show relatively smooth differential cross sections.

A framework for the detailed classification of channels in a multidimensional scattering problem in quantum mechanics is offered in the next section and the hyperspherical picture is entered. Section 3 illustrates an alternative to the partial wave picture for potential scattering and Sect. 4 details a possible formulation of atom-diatom systems. Algorithmic considerations are given in the fifth part of the paper and a short discussion concludes this account.

2. The R-matrix on the hypersphere

Quantum mechanics is formulated, for a system of N particles in the time-independent, non-relativistic domain, as a variational problem. Thus we have a set of masses and configuration space coordinates:

$$\{m_j, \boldsymbol{R}_j; j = 1, 2, \ldots N\}$$

and an interaction potential:

$$W(\boldsymbol{R}_1, \boldsymbol{R}_2, \ldots \boldsymbol{R}_N)$$

which is assumed to be translationally and rotationally invariant. The standard transformation to center-of-gravity and internal coordinates is expressed through an orthogonal matrix as [16]:

$$\boldsymbol{r}_j = \sum_k \boldsymbol{R}_k \sqrt{m_k/M}\, O_{kj}, \qquad O_{kN} = \sqrt{m_k/M} \tag{1}$$

The total mass M will be the effective mass in the kinetic energy term and only the $N-1$ first transformed coordinates enter the potential. Accordingly we look for functions in a $3N-3$ dimensional space:

$$x = (\boldsymbol{r}_1, \boldsymbol{r}_1, \ldots \boldsymbol{r}_{N-1}), \quad x \in R^{3N-3} \tag{2}$$

Wigner–Eisenbud R-matrix theory [17] considers a subspace V with a suitably smooth boundary S [18]. The functional:

$$J(\Psi, \Phi) = \begin{cases} \displaystyle\int_v dx\{[E - W(x)]|\Psi(x)|^2 - |\nabla\Psi(x)|^2\} \\ \quad + \displaystyle\int_s dx[\Phi^*(x)\Psi(x) + \Psi^*(x)\Phi(x)] \\ \quad - \displaystyle\int_s dx\Phi^*(x) \int_s dx' R_s(x, x')\Phi(x') \end{cases} \tag{3}$$

is stationary for solutions of the Schrödinger equation with boundary conditions expressed through an integral kernel representing the R-matrix on the boundary S. The units of mass, length, and action are chosen so as to eliminate Planck's constant and the mass parameter from the expression.

Approximations to the integral kernel $R(x, x')$ on the boundary S can be constructed by means of matrix manipulations when a finite basis of functions on V is used to expand the wave function Ψ:

$$\Psi(x) = \sum u_j(x) c_j \tag{4}$$

The functional (3) is stationary and equals zero when:

$$R_s(x, x') = \Delta(x, x')/\Delta \tag{5}$$

for

$$\Delta(x, x') = \begin{vmatrix} A_{11} & A_{12} & \cdots & A_{1M} & u_1^*(x') \\ A_{21} & A_{22} & \cdots & A_{2M} & u_2^*(x') \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{MM} & u_M^*(x') \\ u_1(x) & u_2(x) & \cdots & u_M(x) & 0 \end{vmatrix} \tag{6}$$

and

$$\Delta = \begin{vmatrix} A_{11} & A_{12} & \cdots & A_{1M} \\ A_{21} & A_{22} & \cdots & A_{2M} \\ \vdots & \vdots & \ddots & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{MM} \end{vmatrix} \tag{7}$$

with

$$A_{jk} = \int_v dx \{[E - W(x)] u_j^*(x) u_k(x) - \nabla u_j^*(x) \cdot \nabla u_k(x)\} \tag{8}$$

More details are given in a recent publication [19].

Originally [17], it was assumed that the R-matrix should be calculated for the strong interaction domain and that its property of relating the amplitude and normal derivative at the boundary:

$$\Psi(x) = \int_s dx' R_s(x, x') \Psi_s(x') \tag{9}$$

be used to relate the amplitudes of the incoming and outgoing states. Alternatively, these states may be included in the basis and the boundary extended to the asymptotic region whereupon the scattering matrix may be extracted directly as Miller has shown recently [2, 20]. The main problem is in any case to cover the interaction region with a reasonable set of functions. The integral kernel is separable with the rank less than or equal to the number of basis functions M in the approximation and the question we will address in the following is whether the partial wave form can be replaced by another expansion with properties that are useful for the inversion of the matrix A.

The hyperspherical coordinate representation offers a convenient picture where the domain V and its boundary is given by:

$$V: \{x; |x| < Q\},\ S: \{x; |x| = Q\} \tag{10}$$

for a fixed value Q of the hyperradius. There remains to find an expedient characterization of the subspaces of S.

3. Potential scattering

Two-particle problems reduce to a situation where the integral kernel $R(x, x')$ connects two points on a sphere in three dimensions and the conventional partial analysis results in a diagonal representation when a basis of solid harmonics [21] is used and the potential is a function only of the hypperadius:

$$\{Y_{lm}(x); 0 \leqslant |m| \leqslant l \leqslant L\}, \qquad W(x) = W(|x|) \tag{11}$$

We assume that the units are chosen such that the hyperradius for the boundary equals unity so that the basis is orthonormal on S.

An integral kernel for the projection operator on the basis can be found in closed form [22]:

$$\begin{aligned} d_L(x, x') &= \sum_{l=0}^{L} \sum_{m=-l}^{m=l} Y_{lm}(x) Y^*_{lm}(x') \\ &= \frac{L+1}{4\pi(1-t)} \begin{vmatrix} P_{L+1}(1) & P_L(1) \\ P_{L+1}(t) & P_L(t) \end{vmatrix} \quad t = x_1 x'_1 + x_2 x'_2 + x_3 x'_3 \end{aligned} \tag{12}$$

and it is then clear that it should be possible to span the same space by means of a localized basis associated with points on the sphere:

$$\{d_L(x, a_j); |a_j| = 1, j = 1, 2, \ldots (L+1)^2\} \tag{13}$$

if the points are chosen judiciously. This basis is nonorthogonal with the metric matrix:

$$\{d_L(a_j, a_k)\}$$

and will give a point representation of the R-matrix kernel.

The basis (13) is of the kind considered in the discrete variable representation [23] but requires global integration techniques and offers no simple schemes for the selection of points [24].

A simpler basis obtains from a finite element discretization of the sphere. The set of points $\{a_j\}$ define a mesh of spherical triangles which may be mapped on a standard planar triangle. Baricentric coordinates for the standard triangle are defined from the solid angles of the spherical triangles. We denote the vertices of a spherical triangle as:

$$(a, b, c) \subset S \tag{14}$$

and its solid angle ε is obtained from the formula

$$\tan(\varepsilon/2) = \frac{|a, b, c|}{1 + b \cdot c + c \cdot a + a \cdot b} \tag{15}$$

where triple product of the three vectors is used. It will generally be assumed that the order of the vectors and their directions are such that the numerator and denominator both are positive so that the solid angle is positive and less than a quarter of the total space. The baricentric coordinate related to vertex a is given implicitly by the expression:

$$\tan[\varepsilon\lambda_a(x)/2] = \frac{|x, b, c|}{1 + b \cdot c + c \cdot x + x \cdot b} \tag{16}$$

and similar forms for the two additional coordinates. It is seen that small ε-values give the conventional results for a planar triangle.

The Jacobian for the transformation is readily worked out and the integration formula for the subset of S where all baricentric coordinates are positive, that is the interior of the triangle, is:

$$\int_s dx \to \int \frac{d\lambda_a \, d\lambda_b}{|x, \nabla\lambda_a, \nabla\lambda_b|} \tag{17}$$

Numerical cubature is conventionally used and high order rules are available [25]. An advantage in the finite element method is that basis functions are associated with certain nodal points in the set and that several schemes define functions only at vertices of the mesh. Only nodal points which occur together in at least one triangle give matrix elements for the associated functions which may be different from zero.

The considerations of a sphere in three dimension are concluded by an example of the matrix structure for a triangularization with icosahedral symmetry, 60 spherical triangles, and 32 vertices. A set of functions is defined at each vertex and the matrix A in the R-matrix formula will then have a block structure as indicated (see Fig. 1). A lower triangular profile form demonstrates that this particular arrangement of the nodes gives a moderate band width which permits considerable savings in storage and manipulation when equation systems should be solved.

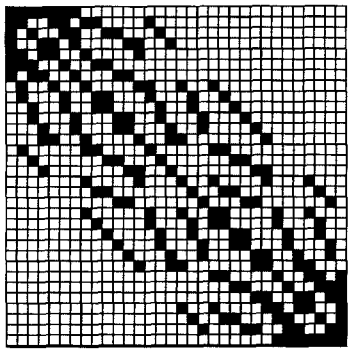

Fig. 1. Matrix pattern for a discretization of the unit three-sphere with 32 nodes and 60 spherical triangles

4. Three-particle systems

Wigner rotation matrices are the standard basis functions for representing the orientation of few-particle systems and nearly rigid structures. The associated projection kernel is most conveniently expressed in terms of the Euler–Rodrigues parameters [21, p. 18] which associate elements of the three-dimensional rotation group with points on the unit sphere in four dimensions. There seems to be no transformation in the literature that provides a direct route from the cartesian coordinates in six space to a form suitable for the finite element method on the hypersphere.

A formulation is given here which maps a subset of the unit sphere in six dimensions onto a direct product space of a unit circular disc and a standard tetrahedron. The circular disc has been used effectively for low angular momentum problems in connection with a generator coordinate formulation for the angular parts [26].

The basis parametrization of R^6 is the same as used previously [27]:

$$x = (\boldsymbol{r}_1, \boldsymbol{r}_2) = |x|(\boldsymbol{e}_1 \cos\chi \cos\vartheta - \boldsymbol{e}_2 \sin\chi \sin\vartheta, \boldsymbol{e}_1 \cos\chi \sin\vartheta + \boldsymbol{e}_2 \sin\chi \cos\vartheta) \tag{18}$$

and the concern will here be concentrated on the representation of the unit vectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ in terms of Euler–Rodrigues parameters and the subsequent discretization through a subdivision of the unit sphere in four dimensions into simplexes.

We consider unit vectors in four-space and choose two equivalent expressions:

$$\vec{\alpha} = (\alpha_0, \alpha_1, \alpha_2, \alpha_3) = (\cos\alpha, \boldsymbol{a} \sin\alpha), \quad |\boldsymbol{a}| = 1 \tag{19}$$

Two orthogonal unit vectors in three-space can then be formed [21, p. 19]:

$$\begin{aligned}(\boldsymbol{e}_1, \boldsymbol{e}_2) = (&\alpha_0^2 + \alpha_1^2 - \alpha_2^2 - \alpha_3^2, 2\alpha_1\alpha_2 + 2\alpha_0\alpha_3, 2\alpha_1\alpha_3 - 2\alpha_0\alpha_2, \\ &2\alpha_1\alpha_2 - 2\alpha_0\alpha_3, \alpha_0^2 - \alpha_1^2 + \alpha_2^2 - \alpha_3^2, 2\alpha_2\alpha_3 + 2\alpha_0\alpha_1)\end{aligned} \tag{20}$$

and we proceed to examine the nature of the basis functions we wish to find. The Wigner rotation matrices are homogeneous polynomials of the Euler–Rodrigues parameters and they have the degree $2J$ where we need only integer values of the angular momentum quantum number J. It is clear that the same function space may be represented as polynomials of the scalar products:

$$\boldsymbol{b} \cdot \boldsymbol{e}_1, \boldsymbol{b} \cdot \boldsymbol{e}_2, \boldsymbol{c} \cdot \boldsymbol{e}_1, \boldsymbol{c} \cdot \boldsymbol{e}_2, \boldsymbol{d} \cdot \boldsymbol{e}_1, \boldsymbol{d} \cdot \boldsymbol{e}_2 \tag{21}$$

provided the three vectors $\boldsymbol{b}$, $\boldsymbol{c}$, and $\boldsymbol{d}$ are linearly independent. This was used in a generator coordinate formulation [28]. Since there are three independent parameters in the form of Eq. (20) only three combinations of the scalar products are needed in order to solve for the basis vectors and then for the Euler–Rodrigues parameters [21, p. 19].

A particular choice of parameters is introduced in a mapping onto the unit sphere in four dimensions. Thus we define:

$$\boldsymbol{b} \cdot (\boldsymbol{e}_1 \cos\beta + \boldsymbol{e}_2 \sin\beta) \equiv e_b, \quad |\boldsymbol{b}| = 1 \tag{22}$$

and similar expressions for $\boldsymbol{c}$ and $\boldsymbol{d}$. The additional parameters β, γ, and δ serve to define four-vectors of the form of Eq. (19). An explicit inversion of Eq. (22) and its analogs is an exercise in matrix inversions which will not be given here

since there is no use for it. A different inversion relates to an expression for the vector $\vec{\alpha}$ in terms of $\vec{\beta}$, $\vec{\gamma}$, and $\vec{\delta}$. A fourth vector may be constructed as the orthogonal complement to these three. This construction is conveniently replaced by the definition of an additional vector in four-space, $\vec{\varphi} = (\cos\varphi, \boldsymbol{f}\sin\varphi)$, which is linearly independent to the others. Baricentric coordinates may again be defined in terms of the measure of the "volume" of the hyperspherical tetrahedra. There seems to be no expression available for this quantity in terms of elementary functions but quite accurate approximations are readily developed for "small" simplexes.

An analogous development is based on the tetrahedral volume in R^4 denoted as:

$$T(\vec{\beta}, \vec{\gamma}, \vec{\delta}, \vec{\varphi}) = \frac{1}{6}\begin{vmatrix} \beta_0 & \gamma_0 & \delta_0 & \varphi_0 \\ \beta_1 & \gamma_1 & \gamma_1 & \varphi_1 \\ \beta_2 & \gamma_2 & \delta_2 & \varphi_2 \\ \beta_3 & \gamma_3 & \delta_3 & \varphi_3 \end{vmatrix} \tag{23}$$

and the corresponding hyperspherical volume:

$$\Omega(\vec{\beta}, \vec{\gamma}, \vec{\delta}, \vec{\varphi}) = \int_{\Gamma} d\vec{\alpha} \tag{24}$$

where the set Γ is defined as all unit vectors in four-space for which the tetrahedral volumes $T(\vec{\alpha}, \vec{\gamma}, \vec{\delta}, \vec{\varphi})$, $T(\vec{\beta}, \vec{\alpha}, \vec{\delta}, \vec{\varphi})$, $T(\vec{\beta}, \vec{\gamma}, \vec{\alpha}, \vec{\varphi})$, and $T(\vec{\beta}, \vec{\gamma}, \vec{\delta}, \vec{\alpha})$ all are positive. The baricentric coordinates are thus:

$$\lambda_b = \Omega(\vec{\alpha}, \vec{\gamma}, \vec{\delta}, \vec{\varphi})/\Omega(\vec{\beta}, \vec{\gamma}, \vec{\delta}, \vec{\varphi}) \tag{25}$$

and they provide a suitable vehicle for the use of numerical integration rules over a standard tetrahedron [29]. Polynomials or other simple functions of the baricentric coordinates can be used to represent the wave function locally. The evaluation of matrix elements involves the calculation of α-coordinates for the appropriate λ-values as well as the six-space gradients $\nabla\lambda$. Expressions for the gradients are structurally simple but involve the solution of a system of seven equations for the four gradients $\nabla\lambda$. This is most efficiently done by numerical matrix inversion since no compact analytical form is immediately available.

The previous development demonstrates a feasible way towards a discretization of the space relating to the rotational degrees of freedom for a three-particle system. Earlier it has been shown that the remaining two hyperangles, χ and θ, relate to points on the unit circular disc [27, 28] and an appropriate triangularization is easily achieved there. The intricacies of inversion symmetry and the restriction to the upper half of the unit four-sphere will be dealt with in another context.

Organization of the distinct simplexes and their vertices in a three-dimensional structure such as the one discussed above becomes an important issue for achieving an optimal matrix structure. The unit four-sphere can be mapped on the solid three-sphere by disregarding α_0 and a more easily studied spatial structure with its connections helps the matter. Thus we may consider as a simple discretization the previously devised dodecahedron together with an inscribed icosahedron and its center as defining 45 nodes and 100 tetrahedra. An example of a connection matrix is:

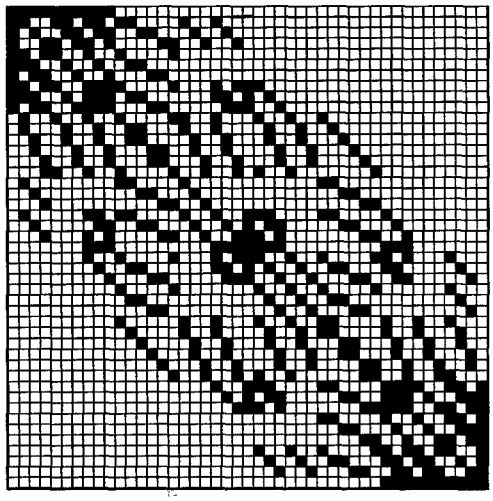

Fig. 2. Matrix pattern for a discretization of the unit four-sphere (or the solid three-sphere) with 45 nodes and 100 tetrahedra

which ends the present analysis.

5. Matrix structures and algorithms

The basis functions for a full finite element method approach to the R-matrix as conceived above would be direct product functions for the rotational, the hyperradial, and the internal hyperangular or shape coordinates. A sparse matrix will result with a block structure corresponding to each set of functions. The one-dimensional, hyperradial block structure can readily be arranged in a block tri-diagonal form, while a more scattered structure can be expected for higher dimensions where the connectivity in a lattice of nodal points becomes more complex. Algorithms for the determination of optimal numbering are available but there may be reasons originating in the physical problem at hand to design particular structures.

It has been common practice in the hyperspherical formulation to determine a suitable angular basis, admirably accomplished by Launay [8] and by Kuppermann [1], and to propagate the total wave function solution from small hyperradii towards the asymptotic region. This is equivalent to a finite element formulation with the radial functions as determining the coarse structure of the matrix A. An alternative solution procedure of the same problem has been used effectively [30] to propagate the solutions from the asymptotic region towards a hyperradius which effectively terminates the solution. Both methods involve an intermediate truncation of an angular basis to a smaller and more manageable one by means of a diagonalization to adiabatic surface functions. This is a time consuming step in the process.

Three-particle problems require a detailed description of the internal rovibrational states for bound two-particle clusters in the asymptotic region and consequently a large basis. This becomes a concern when the total angular momentum is large. It appears that the description of the radial factor of the wave function can be well described by relatively few basis functions for a given direction in hyperspace and that it is advantageous to permute the order in

which to arrange the matrix computation. Preliminary results have shown that savings in computer time result from this simple rearrangement [31].

Additional benefits are derived from the fact that a large number of the hyperangular channels are closed even at moderately large hyperradii and that consequently several nodes may be shut out totally and that others require only few matrix elements. Similar considerations apply towards a truncation of the space for the total angular momentum treatment. Launay [8] has shown how the basis of Wigner functions can be reduced and the treatment by Parker and Pack [6] serves a similar purpose. The finite element basis for the angular parts offers an alternative. All diagonal blocks for a given node on the four-sphere will be identical since the potential is assumed to be invariant under rotations. Thus it will be advantageous to reduce such blocks to a diagonal form and to truncate the basis for shape and size variables. This development is under way.

The various orders of treatment are illustrated in Figs. 3 and 4. The first one depicts a reduction of the angular space to surface functions on the different hyperspheres which is followed by a radial propagation. The alternative suggested here is that the "breeding mode" motion described by the hyperradius is adapted to the particular shape specified by the internal hyperangles. This should then be followed by the construction of a suitable basis for a fixed orientation of the system. The final step relates to the different orientations and the R-matrix describes the propagation of the system from one shape and direction to all other shapes and directions admitted by the basis set employed. It is here that we see the effect of a limited resolution in the angular states and only the practice will show whether the "smudging" of the pure angular momentum states will be

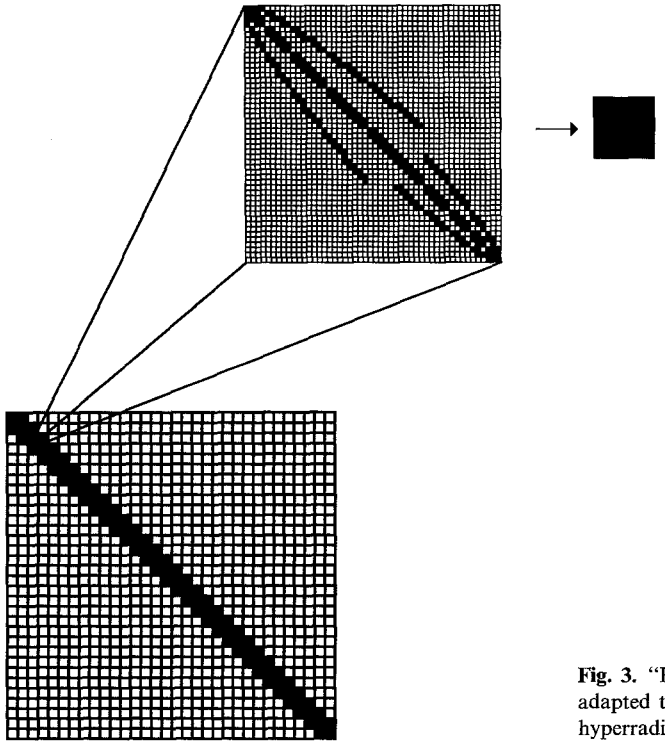

Fig. 3. "Propagation" structure adapted to dealing with the hyperradial dimension

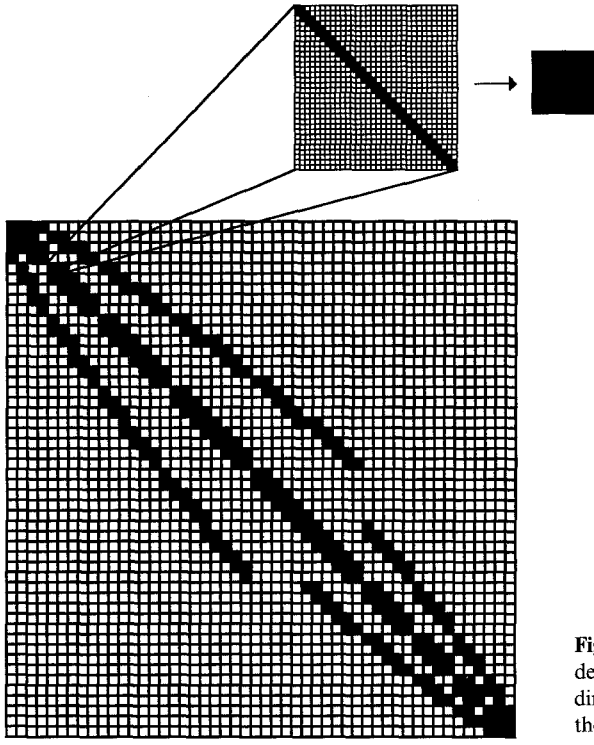

Fig. 4. Matrix structure adapted to dealing with the hyperradial dimension in the innermost part of the algorithm

detrimental to the detailed analysis of differential cross sections, resonances and other features.

Matrix structures of the kind exhibited here indicate by themselves the possibilities for concurrent processing. Nodal points couple only to neighbors and matrix elements for one point requires little information. Information can be generated independently by massive parallelization. Basis set truncation procedures require matrix manipulations relating subsets of nodal points but different subsets are dealt with separately and may be subjected to concurrent processing. The final matrix inversion or linear system solving deals with large structures where block methods apply which admit some concurrency in the processing. Iterative methods such as relaxation might come into play here since it allows a considerable degree of parallelization.

6. Remarks

Systems with more than three particles give greater complexities and for molecular systems with three atoms there is often a need of going beyond the Born–Oppenheimer formulation and to include some electronic degrees of freedom. Two elements of the preceding analysis would seem to apply also in these cases. The total angular momentum treatment may be simplified through the use of a discrete representation and the "breeding mode" will be possible to consider in a simple basis. Detailed descriptions of the possibilities for asymptotic states will probably require sophisticated management of the possibilities for basis functions where localization will be an important element [16].

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