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A new method to approximate coupled equations for scattering

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Abstract. A method is formulated to extend the field of application of the energy sudden (adiabatic) and centrifugal sudden approximations in scattering calculations. The method consists in applying the approximations in limited radial intervals and only to the coefficients of linearly independent solutions of uncoupled equations. This gives rise to a transformation on each of the channel wavefunctions at the points separating the intervals. We have tested the method in a two-channel model with good results.

In the past few decades the theories of nuclear and molecular scattering have shown a number of parallel developments, such as the common application of the Feshbach theory of resonances and the semiclassical theory for molecular scattering as compared with the scattering of heavy ions in nuclear physics. The present paper is devoted to another common field of interest: the development of methods to reduce the computational effort in coupled-channel calculations†. The coupled-channel theory of (in)elastic scattering and reactions is based on the expansion of the wavefunction, describing the total system of the collision partners, in a set of states for the internal degrees of freedom and the relative angular motion. The expansion coefficients depend on the relative distance r . For each r they give the relative probability amplitudes for the various states of internal degrees of freedom and angular motion. They satisfy Schrödinger's equation, here in the form of a set of coupled radial differential equations.

Until some years ago, the DWBA (distorted wave Born approximation) was a common method to simplify this set of equations. The coupling terms are then treated as a first-order perturbation. More recently, the interest has shifted to a more exact treatment, able to deal with stronger transitions and more-step processes. Solving the full coupled equations, subject only to an inevitable truncation of the set of internal and angular states, is now a widely adopted procedure. Such calculations are often very cumbersome, especially due to the rapid increase of the computational effort with the number of channels included. From this point of view it is desirable to introduce, besides new numerical methods, physical approximations which are more justified than the DWBA.

† One of the difficulties which stand in the way of easy communication between the two fields is the different terminology. The coupled-channel method for nuclear reactions is commonly referred to as the close-coupling method in molecular scattering.

In the following we shall consider two of these. We start with the coupled-channel (cc) equations. In matrix notation these equations have the form

$$\mathbf{R}''(r) = \mathbf{A}(r)\mathbf{R}(r), \quad (1)$$

where a prime denotes differentiation with respect to the radial distance r , \mathbf{R} is an N -dimensional vector and \mathbf{A} is an $N \times N$ matrix. The problem of finding solutions to these equations is simplified considerably if there exist r -independent Hermitian commutators of \mathbf{A} : $[\mathbf{C}, \mathbf{A}] = 0$. As is well known this gives rise to a partial decoupling of the problem.

In the situation that we consider, the matrix \mathbf{A} itself does not have such commutators, but it has after subtraction of a constant diagonal matrix \mathbf{D} : $\mathbf{A} = \mathbf{D} + (\mathbf{A} - \mathbf{D})$. In the adiabatic or energy sudden (ES) approximation (Verhaar and Schulte 1977, Schulte 1978, Khare 1978), the elements of this matrix \mathbf{D} are essentially differences of excitation energies of the scatterer. In the ES approximation these are assumed to be so small that the matrix \mathbf{A} can be replaced by $(\mathbf{A} - \mathbf{D})$. Usually this is interpreted classically to correspond to slow internal motion of the scatterer.

In another approximation, which is referred to as centrifugal sudden (CS) approximation in molecular scattering theory (Inopin 1966, McGuire and Kouri 1974), the matrix \mathbf{D} has a simple $1/r^2$ radial dependence. The angular-momentum-dependent centrifugal barrier is replaced by a constant one. The matrix \mathbf{D} contains the differences between these barriers and thus is r -dependent. Again, the matrix \mathbf{D} is neglected.

Essentially due to the introduction of additional commutators the ES and CS approximations have been shown to give rise to a considerable simplification of the scattering problems to which they are applicable. In this paper we propose a method by which the field of application of the approximations can be extended. Let us first look at the ES approximation from a classical point of view. If the internal motion of the scatterer is not slow enough to permit it to be considered as 'frozen' during the entire collision, it may still be slow enough to permit frozen internal coordinates for shorter time intervals.

Inspired by this observation, in the stationary quantum-mechanical description we correspondingly subdivide the r axis in a number of limited radial intervals. In each interval we neglect the matrix \mathbf{D} . As mentioned above, this is advantageous for finding solutions \mathbf{R} . At the interval boundaries we apply a certain transformation on the solution to correct for neglecting the matrix \mathbf{D} . Thus each component of the solution \mathbf{R} has discontinuities at the points separating the intervals. The kind of transformation to be applied is suggested by a second observation.

Over larger radial intervals outside the interaction region the ES wavefunction \mathbf{R} provides a bad approximation: differences in channel wavenumbers, determined by the elements of the matrix \mathbf{D} , no matter how small, give rise to arbitrarily large phase changes in ingoing and outgoing waves at large distances. A better approximation is obtained if the ES approximation is only used to calculate the coefficients of ingoing and outgoing waves, i.e. the S matrix. Classically this procedure means that the internal degrees of freedom need to be frozen only during the interaction process. Outside this interval the exact evolution of the system is trivial.

This leads us to define in the interaction region for each of the channels i , a pair of basis waves together with their adiabatic counterparts and to determine for each of the radial intervals the matrix transforming the coefficients of the waves on one side of the interval into those on the other side, using the ES approximation. This matrix is then taken over in the exact case but to transform the coefficients of non-adiabatic waves.

The latter are then defined so as to take into account correctly the amplitude and the phase changes due to ‘diagonal propagation’ within the channels. To ensure this we take them to be (easily obtainable) linearly independent solutions f_i and g_i of equation (1), including only the diagonal part of \mathbf{A} . We write

$$R_i = a_i f_i + b_i g_i \quad R'_i = a_i f'_i + b_i g'_i$$

the coefficients being r -dependent in general. The adiabatic basis waves are similarly defined by equation (1) with \mathbf{A} replaced by the diagonal part of $\mathbf{A} - \mathbf{D}$. The above-mentioned transformation is unique as soon as a correspondence between adiabatic and non-adiabatic waves f_i and g_i is defined. We make use of the freedom in choosing f_i and g_i to make the adiabatic and non-adiabatic transformations from r_1 to r_2 as closely identical as possible, in the following sense: the matrices are to be identical to the highest possible order in $h = r_2 - r_1$. This requirement can be handled by expanding the transformation matrix following from the differential equations:

$$\begin{aligned} a'_i &= g_i \sum_{j \neq i} A_{ij} (a_j f_j + b_j g_j) \\ b'_i &= -f_i \sum_{j \neq i} A_{ij} (a_j f_j + b_j g_j) \end{aligned} \tag{2}$$

in a Taylor series around r_1 and identifying for each of the matrix elements adiabatic and non-adiabatic terms of equal order in h . The differential equations are derived by (a) differentiating the previous expression for R_i and equating it to the expression for R'_i , (b) differentiating the latter and relating it to the functions R_i through equation (1), and (c) making use of the uncoupled equations for f_i and g_i .

We find that the adiabatic and non-adiabatic basis waves (\bar{f}_i, \bar{g}_i and f_i, g_i , respectively) shall be equal in r_1 , together with their first derivatives. As a consequence the corresponding coefficients too are identical in r_1 and the procedure of taking over the adiabatic transformation matrix from r_1 to r_2 reduces to taking over the adiabatic coefficients in the non-adiabatic case, i.e. combining them with a pair of non-adiabatic basis waves. Distinguishing also other adiabatic quantities with a bar, the transformation at r_2 thus takes the form:

$$\left. \begin{aligned} \bar{R}_i &= \bar{a}_i \bar{f}_i + \bar{b}_i \bar{g}_i \\ \bar{R}'_i &= \bar{a}'_i \bar{f}'_i + \bar{b}'_i \bar{g}'_i \end{aligned} \right\}_{r=r_2} \rightarrow \left. \begin{aligned} \tilde{R}_i &= \tilde{a}_i f_i + \tilde{b}_i g_i \\ \tilde{R}'_i &= \tilde{a}'_i f'_i + \tilde{b}'_i g'_i \end{aligned} \right\}_{r=r_2} \tag{3}$$

where a tilde denotes our corrected solution. From the differential equations (2) we find that in r_1 :

$$\begin{aligned} \bar{a}'_i &= a'_i & \bar{b}'_i &= b'_i, \\ \bar{a}''_i &= a''_i, & \bar{b}''_i &= b''_i. \end{aligned}$$

As a consequence the corrected solution at r_2 has a value and a derivative correct to order h^2 . The coefficients start to differ in the order h^3 , so one would expect a discrepancy in our corrected solution in this order. It turns out, however, that the corrected value is correct to one order higher, due to compensation of h^3 errors in the coefficients \bar{a}_i and \bar{b}_i . This compensation does not take place in the case of the first derivatives. It follows that our corrected solution is better by two orders in h , compared with the adiabatic solution, both with respect to value and to first derivative. Because in many cases the adiabatic approximation is not so badly satisfied, it is expected that our method will then give good results with subdivision in only a small number of intervals.

It should be noted that the results obtained with our method converge to the CC result with increasing number of intervals.

Note furthermore that the linear transformation (3), i.e.

$$\begin{pmatrix} \bar{R}_i \\ \bar{R}'_i \end{pmatrix}_{r_2} = \begin{pmatrix} f_i & g_i \\ f'_i & g'_i \end{pmatrix}_{r_2} \begin{pmatrix} \bar{f}_i & \bar{g}_i \\ \bar{f}'_i & \bar{g}'_i \end{pmatrix}_{r_2}^{-1} \begin{pmatrix} \bar{R}_i \\ \bar{R}'_i \end{pmatrix}_{r_2} \quad (4)$$

has the convenient property that its determinant equals 1. As a consequence the generalised Wronskians for the coupled channels are conserved. The corrected solutions therefore share this feature with the exact CC solutions.

With this our method is fully described. We want to make some additional remarks, which are of practical use when applying the method. The first one concerns alternative formulations of the method. In the given formulation a Taylor series expansion around r_1 is used to obtain the optimal correspondence between exact and adiabatic basis waves. It is also possible, however, to make that expansion around r_2 , which results in equal function values and first derivatives in r_2 , and in a transformation, similar to (4), of the adiabatic wavefunction at the beginning of the interval r_1 . Therefore, in this case we start with a transformation at the beginning of the interval and after that we integrate adiabatically from r_1 to r_2 . The order of convergence in this formulation is the same as in the previous one. Which formulation is preferred depends on the variation of the coupling strength in the interval.

Secondly, we point out that essentially the same method as described above can be applied if the CS approximation is considered, by itself or in combination with the ES approximation.

We have tested our method in a two-channel scattering model. The two channels have different internal states and different orbital angular momentum l . The potential is characteristic for nuclear scattering: 40 MeV nucleon scattering by a target nucleus with mass number $A = 60$. The diagonal elements of the potential matrix have a Woods-Saxon form, and the non-diagonal elements are proportional to the first derivative of this form. The depth of the potential well is 50 MeV and the strength of the coupling potential corresponds to a deformation parameter $\beta_2 = 0.2$. A Coulomb potential does not influence our conclusions essentially and is not taken into account.

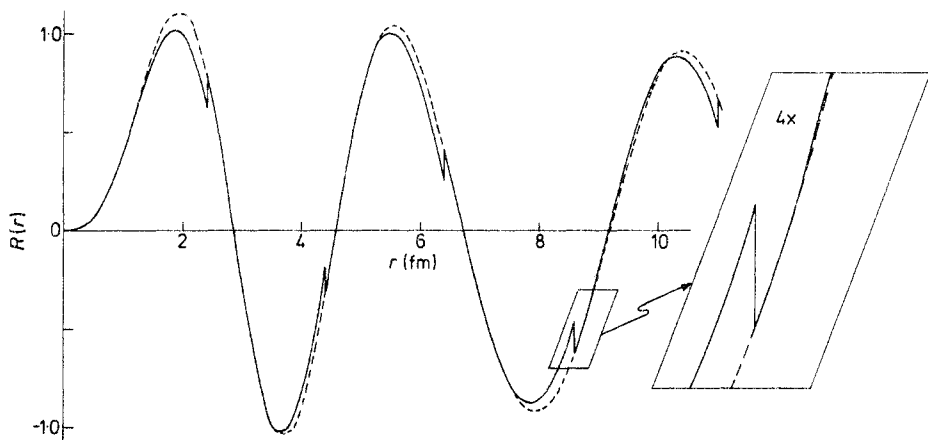


Figure 1. Approximate wavefunction —, compared with coupled-channel result ---. Note the discontinuities at the interval separation points, where the adiabatic wavefunction is 'jacked up' almost to the coupled-channel function. Vertical axis in arbitrary units.

We first consider the ES approximation. In figure 1 we show an example of a CC wavefunction, together with the wavefunction obtained with our method. Note the discontinuities between the intervals. Apparently the CC wavefunction is reproduced very well after correction. In figure 2 we show resulting S-matrix elements for a set of

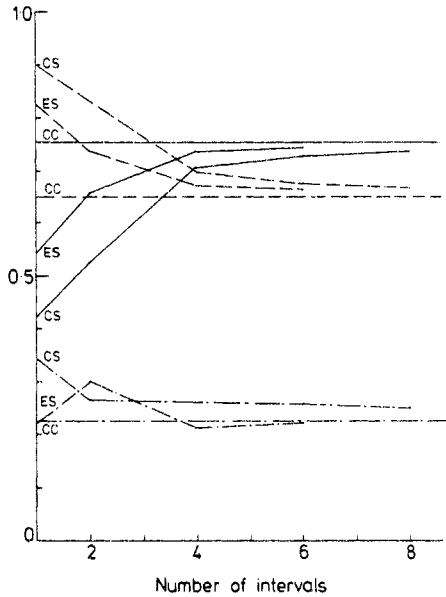


Figure 2. Typical S-matrix elements in the ES and CS approximations, as a function of the number of intervals, compared with CC. The curves are guides to the eye. Given are $\text{Re}(S_{2 \rightarrow 2}) \rightarrow$, $\text{Im}(S_{2 \rightarrow 4}) \text{ ---}$ and $\text{Im}(S_{4 \rightarrow 4}) \text{ - \cdot -}$.

$l = 2$ and $l = 4$ channels, with excitation energies of 5 and 0 MeV, respectively, as a function of the number of intervals. In the same figure the horizontal lines give the corresponding CC results, with which we should compare our results. The intervals are chosen to be shortest in the coupling region (i.e. around the nuclear surface). Figure 3 shows similar results for a second set of channels with the l values replaced by 6 and 8, respectively. The convergence to the CC results is shown clearly. In table 1 some full S matrices are given for the first set of channels. The agreement of the ordinary ES approximation with the CC calculations is poor. Our method, however, gives already satisfactory results with subdivision into six intervals even for the large energy separation of 5 MeV between the internal states. The accuracy is expected to be sufficient relative to the accuracy normally required for coupled-channel calculations in view of experimental errors. The results for other strongly coupled channels are comparable.

The remaining curves in figures 2 and 3 give corresponding CS results. Table 2 again gives full S matrices relative to the CS approximation for the second set of channels. The figures illustrate the general tendency of the CS values to be somewhat worse than ES values. This tendency is confirmed by S matrices based on the ordinary ES and CS approximations. In the CS case too we obtain satisfactory results, here with subdivision into eight intervals. Results for other strongly coupled channels are again similar.

We conclude that the accuracy of our method is comparable with that of coupled-channel calculations. From the number of intervals needed in our calculations, it is

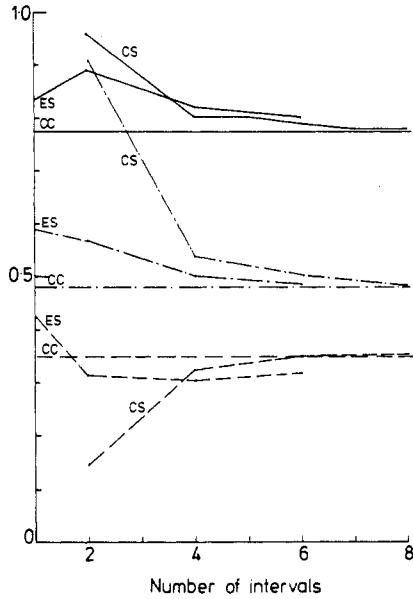


Figure 3. Same as figure 2 for second set of channels. $\text{Im}(S_{6 \rightarrow 6})$ —, $\text{Im}(S_{6 \rightarrow 8})$ --- and $\text{Im}(S_{8 \rightarrow 8})$ - · -.

Table 1. Two-channel S matrix in two approximations: energy sudden plus corrections in six intervals and ordinary energy sudden approximation, compared with the coupled-channel result (for channel quantum numbers see text).

$\begin{pmatrix} 0.75 - 0.00i & 0.09 - 0.65i \\ 0.09 - 0.65i & 0.72 + 0.22i \end{pmatrix}$	Coupled channel
$\begin{pmatrix} 0.74 - 0.00i & 0.10 - 0.66i \\ 0.10 - 0.66i & 0.70 + 0.22i \end{pmatrix}$	Energy sudden approximation in six intervals
$\begin{pmatrix} 0.45 - 0.25i & -0.01 - 0.85i \\ -0.01 - 0.85i & 0.46 + 0.24i \end{pmatrix}$	Ordinary energy sudden approximation

Table 2. S matrix in centrifugal sudden approximation plus corrections with subdivision into eight intervals, compared with coupled-channel result and ordinary CS result.

$\begin{pmatrix} 0.51 - 0.78i & 0.08 + 0.35i \\ 0.08 + 0.35i & 0.80 + 0.48i \end{pmatrix}$	Coupled channel
$\begin{pmatrix} 0.51 - 0.78i & 0.08 + 0.35i \\ 0.08 + 0.35i & 0.80 + 0.49i \end{pmatrix}$	Centrifugal sudden approximation in eight intervals
$\begin{pmatrix} 0.99 - 0.07i & -0.04 - 0.12i \\ -0.04 - 0.12i & 0.82 - 0.56i \end{pmatrix}$	Ordinary centrifugal sudden approximation

expected that in actual calculations with our method a considerable reduction of computation time can be obtained with respect to coupled-channel calculations. It should be noted that in the foregoing illustrations of the principle and correctness of our

method we solved the ES and CS radial equations relative to the basis set of the more exact CC equations. The approximations, however, are advantageous only if we transform to a basis adapted to the above-mentioned commutators \mathcal{C} . Calculations in this sense, comprising proton and alpha scattering by spherical nuclei in the ES+CS approximation are in progress.

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