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DETERMINATION OF THE TRANSITION MATRIX WITH N-COUPLED CHANNELS

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Résumé:
Nous appliquons les résultats obtenus auparavant dans le cadre de la théorie d'un système d'E.D.C. à la détermination des différences de phases qui interviennent dans les éléments de la matrice de transition. Quelques résultats numériques concernant les cas n=2 et n=3 seront présentés.

Abstract:
Previous results obtained in the frame of the theory system of C.D.F. are applied to the determination of the phase shifts corresponding to the element of the transition matrix. A number of numerical results for the cases n=2 and n=3 will be discussed.

INTRODUCTION/ In a transition from state i to state f of an atomic system, the amplitude of the transition matrix element is determined in computing integrals of the type

\[ \int_{0}^{\infty} F_i(r) R_{if}(r) F_f(r) dr \]

in which F_i(r) is the solution of a homogeneous differential equation of second order corresponding to the initial state i (in the Green's function technique) F_f(r), the exact solution on an inhomogeneous differential equation corresponding to the final state f and R_{if}(r) is the coupling function between these states. For example in a two states approximation the effect of all other states different from i and f are ignored so that F_f(r) is the solution of a system of two coupled equations.

This approximation may become insufficient however and the influence of a finite number of other states have to be taken into account so that the function F_f(r) is now a solution of a system of n coupled equations which is generally difficult to handle if the number n is large or if the coupling functions contain singularities or are slowly decreasing function with increasing distance r. This already may constitute a sufficient deterrent factor for a conventional iterative approach such as DWBA or R matrix etc.... chiefly because of the overgrowth of the time of computation.

Recently [1], it has been shown that this n equations system can be made tractable with the method of the decoupling operation which transform the original problem into a chain of subsystem of two coupled equations which are to be solved successively in a more convenient way. These partial solutions can then be recombined afterwards by inverse transformation to reconstruct the exact solution. It is seen therefore that in the present theory, the system of 2 coupled equations does play an essential role work will be organised as followed.

In the first paragraph we shall recall the essential points of the method and consider the n=4 case as an example in order to see more clearly how the transition matrix can be determined practically.
In the next one, we consider a modification of the method by introducing a second parameter in order to obtain further simplifications, making use of the concept of eigenphase shift.

The case of e-H collision with a transition from \(|1\rangle \rightarrow |1\pm 1\rangle\) is then taken up for which extensive numerical works are actually being performed. Finally, we summarize the numerical results obtained so far in the last paragraph.

**FORMULATION**

Using the same notations and conventions as in [1], we are concerned with a system of coupled differential (CD) equations of the form:

\[
\left[ P + f_p(r) \right] F_p(r) = \sum_q B_{pq}(r) F_q(r) \quad p,q = 0; 1; \ldots; n (1)
\]

and with a transition from the initial state \(|i\rangle\) to the final state \(|f\rangle\). There will be no loss of generality in relabelling the indices \(p,q\) such that the initial and final states correspond respectively to \(p = 0, 1\). The problem is then similar to the two equation case in which the effects of all other significant states are taken into account. To be more specific, consider with \(n = 4\) so that the transformation matrix is:

\[
T_4(\alpha_1) = \begin{pmatrix}
t_2(\alpha_1) & 0 \\
0 & 1
\end{pmatrix}
\]

where it was that an appropriate choice of the parameter \(\alpha_1\) lead to the partial decoupling of the subspace \((F_2, F_3)\), or in another words, the functions \(F_2, F_3\) can be determined by the equations

\[
\left[ P + f_k(r) \right] F_k(r) = B_{k1}(r) F_1(r) \quad k, l = 2, 3 (2)
\]

This a system of two (CD) equations which is now familiar to us. We solve it either by use of the usual Numerov's procedure or with semi analytical approach involving a supplementary parameter \(\alpha_2\) in the decoupling operation (see for example [2]).

Adopting now following notations:

\[
Z = \begin{pmatrix} z^{(1)} \\ z^{(2)} \end{pmatrix}, \quad \begin{pmatrix} z_0 \\ z_1 \end{pmatrix}, \quad \begin{pmatrix} z_2 \\ z_3 \end{pmatrix}, \quad \begin{pmatrix} F^{(1)} \\ F^{(2)} \end{pmatrix}, \quad \begin{pmatrix} F_0 \\ F_1 \end{pmatrix}, \quad \begin{pmatrix} F_2 \\ F_3 \end{pmatrix}
\]

with \(Z = T_4(\alpha_1)F\)

Noting that in the transformation \(T_4(\alpha_1)\), the subspace \(F^{(2)}\) remain unaffected i.e.

\(F_2 = z_2, \quad F_3 = z_3\)

it can be verified that \(z^{(1)}\) is the solution of the following system:

\[
\left[ \left[ P + f_k(F_0^2 + f_1) \right] z^{(1)} + \frac{2k_1 B_{11}}{(1 + 4\alpha_1^2)^2} J + \frac{\alpha_1 \Delta f}{(1 + 4\alpha_1^2)^2} K \right] z^{(1)} = t_2(\alpha_1) \begin{pmatrix} B_{21} + B_{33} \end{pmatrix} \ldots
\]
This is a system of 2 CD equations in which the r.h.s. is known and may be considered as a source term. As the solution obtained by solving this system is an exact one, we see that the original function \( F(1)(r) \) can be recovered by an inverse transformation.

\[
P(1) = t^1(\alpha_1)Z(1)
\]

More precisely:

\[
P_0(r) = \frac{1}{2(1+a^2)} \left[ (1-a)Z_0 - (1+a)Z_1 \right]
\]

Furthermore, the quantity \( I_{01} \) required in the determination of the transition matrix is given by:

\[
I_{01} = \int_0^\infty P_1(r') B_{01}(r') F_0(r') dr'
\]

in which \( P_1(r) \) is the regular component of the Green's function corresponding to the differential for \( F_0(r) \) and \( F_0(r) \) is given by (4). If the angular quantum number is \( 1 \), the total amplitude of the transition is

\[
f(\theta) = \frac{1}{(k_o k_1)^{1/2}} \sum_{l=1} (2l+1)\psi_{01}^{(1)} P_l(\cos \theta)
\]

with the usual notations.

In the above example we see that an exact solution can always be reached through two steps, in the first one a subroutine is set up for the Numerov method in order to determine \( Z_2 \), \( Z_3 \) which will then be incorporated into the second one where the same subroutine with of course the appropriate modifications can be used again. The time saving can be then improved substantially.

**THE EIGEN PHASE SCHIFT METHOD**

If instead of \( T_4(\alpha_1) \) we use another transformation defined by [3]:

\[
T_4(\alpha_1, A_1) = \begin{pmatrix} t_2(\alpha_1, A_1) & 0 \\ 0 & I \end{pmatrix}
\]

with

\[
t_2(\alpha_1, A_1) = \begin{pmatrix} c & d \\ -d & c \end{pmatrix}
\]

then the system (3) become, in matrix form:

\[
\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} P + \begin{pmatrix} F_+ & 0 \\ 0 & F_- \end{pmatrix} + (M + N) \begin{pmatrix} A_1 & -1 \\ 1 & A_1 \end{pmatrix} \begin{pmatrix} Z_0 \\ Z_1 \end{pmatrix} = \begin{pmatrix} c & d \\ -d & c \end{pmatrix} \begin{pmatrix} B_02 \\ B_12 \end{pmatrix} F_3 + \begin{pmatrix} B_03 \\ B_13 \end{pmatrix} F_3 \ldots
\]

The quantities \( M, N, c, d, A_1 \) are already derived in previous papers and

\[
P_\pm = \frac{1}{2}(f_0 + f_1) \pm \frac{1}{2} \left[ (\Delta f)^2 + 4B_0^2 \right]^{1/2}
\]
with 
\[ \gamma(r) = \frac{B_0 l Y(r)}{\Delta f} \]

it has been shown that if this quantity is monotonically decreasing with increasing \( r \), then it will always possible to choose the ± signs in the expression of \( A \) making its variation slowly and monotonically. This remark immediately interesting applications in atomic calculations: In fact, the equations in (5) become uncoupled at large distances \( (r > r_M) \) while for small distances \( (r < r_m) \) in the range of the exchange effects, (5) must be replaced by another system of coupled integrodifferential (CID) equations, the choice of \( r \) being dictated by the target wave function to be used. In our work, we are adopting however the Huck's model \([4]\) in which the effect of the integral terms is simulated by constants which are considered here as parameters.

In the intermediary region \( r_m < r < r_M \), the system (5) remains in principle coupled but however \( B \), because of the slowly varying character of \( A(\xi, \varphi) \), the effects of the quantities \( M, N \) can be neglected at first order of approximation (fig.2).

Therefor, after usual matching conditions at the boundary \( r = r_m \) it is possible \([5]\) to determine directly the eigenphase \( \xi \), from which the inelastic cross section will be inferred \([6]\) with the use of the mixing parameter defined in \([1]\).

**APPLICATIONS**

In order to have a test of the effectiveness of the present theory, we continue to take the simple example of e-H collision in a transition \( (n', l, m) \rightarrow (n, l', m') \); \( l' = l \pm 1 \) which lead to a system of \( 3 \) CD equations.

With our notations we have here:

\[ f_0 = k_0^2 - \frac{(l+1)}{r^2}; \quad f_1 = k_1^2 - \frac{(l-1)}{r^2}; \quad f_2 = k_1^2 - \frac{(l+1)(l+2)}{r^2} \]

\[ B_{ij} = \frac{C_{ij}}{r^2} \]

\( C_{ij} \) are constants of the same order of magnitude.

Correspondingly, we shall have to consider two quantities \( I_{1, l-1} \), \( I_{1, l+1} \), the second one obtained by interchanging the indices \( 1 \leftrightarrow 2 \) in system (1).

The function \( F \) are found to be respectively:

\[ \begin{align*}
1' = & l-1; \quad F_\pm = \frac{1}{2}(k_0^2 + k_1^2) - \frac{(l)}{r^2} \pm \frac{1}{2} \left( \frac{(\Delta k^2 - 2)}{r^2} \right) \pm \frac{1}{2} \left( \frac{(\Delta k^2 + 2(l+1))^2}{r^2} + \frac{c_{01}}{r^2} \right) \end{align*} \]

and

\[ \begin{align*}
1' = & l+1; \quad F_\pm = \frac{1}{2}(k_0^2 + k_1^2) - \frac{(l+1)}{r^2} \pm \frac{1}{2} \left( \frac{(\Delta k^2 + 2(l+1))^2}{r^2} + \frac{c_{02}}{r^2} \right) \end{align*} \]

Note also that for the non exact resonance case \( (\Delta k^2 = 0) \) we have \( M = N = 0 \) so that the equations become completely uncoupled with the solutions expressed in terms of Bessel functions. Therefore, a semi analytical approach similar to the resonance distortion method (RDM) \([5]\) is possible. However, in the non resonance case with non negligible energy gap \( \Delta k^2 \), we have noted that the RDM is no more justified and the present method would be more appropriate.

**NUMERICAL RESULTS**

Extensive computational work is actually
in progress and, although not yet complete, we wish nevertheless to comment briefly on some first results obtained so far which may give a hint on further developments of the method and in a sense, justify the general ideas presented above.

In fig.1 it can be seen the slowly varying character of the function $A(\alpha, \xi)$ which plays the crucial role in the theory.

The functions $M$ and $N$ are compared to $c, d$ in fig.2 where it may be noted that the effects of the coupling terms in relation (5) are sufficiently small to justify the use of first order of approximation while in the second one, the functions $M, N$ are taken into account.

To see this more clearly, we consider the $n=2$ system as in [2] and compare the 1st and 2nd approximation with the exact solution obtained by Numerov's approach in fig.3. The eigenphase shifts $S_1, S_2$ are determined directly from these solutions [7] and displayed in table 1 showing a quite acceptable agreement.

Calculations for the $n=3$ case are actually in progress.

We present in fig.4 the first numerical results represent the solutions $F_0, F_1, F_2$ of system [2] which are obtained by neglecting the effect of the factors $M, N$ where $F_3$ is represented by a wave Bessel function.

**CONCLUSION**

To summarize, we may consider the present method as a complementary tool with other existing techniques available for the $n$ coupled channels problem. As examples, we shall point out two salient features.

The use of first order approximation has enabled us to formulate an alternative to this problem with a direct determination of the eigen phase shift from the solutions of the coupled equations, a technique which become familiar to us from previous works.

It is apparent that to deal with a chain of subsystem of two coupled equations is much simpler than to handle the whole bulk of $n$ equations, a factor which useful from the practical point of view.

On a more general level, it can also be noted that the method presented in [1] may be understood as a special case of "forward-backward line of reasoning " in artificial intelligence methodology. This is the reason why it can be expected that its extension to system of large number $n$ will indeed not impossible to conceive in future works.
\[
\Delta k^2 = 0.5 \ (\varepsilon \nu) \quad \Delta k^2 = 1.0 \ (\varepsilon \nu)
\]

<table>
<thead>
<tr>
<th>(n^{th}) approximation</th>
<th>(S_1^{+}(\text{rad.}))</th>
<th>(S_1^{-}(\text{rad.}))</th>
<th>(S_1^{+}(\text{rad.}))</th>
<th>(S_1^{-}(\text{rad.}))</th>
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<td></td>
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<td>-0.447</td>
<td>0.444</td>
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<td></td>
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<td>-0.320</td>
<td>0.283</td>
<td>-0.255</td>
</tr>
<tr>
<td></td>
<td>5: 0.248</td>
<td>-0.233</td>
<td>0.188</td>
<td>-0.177</td>
</tr>
<tr>
<td></td>
<td>6: 0.184</td>
<td>-0.170</td>
<td>0.133</td>
<td>-0.122</td>
</tr>
<tr>
<td></td>
<td>7: 0.135</td>
<td>-0.130</td>
<td>0.094</td>
<td>-0.088</td>
</tr>
<tr>
<td>2nd approximation</td>
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</tr>
<tr>
<td></td>
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<td>-0.322</td>
<td>0.286</td>
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<td>7: 0.138</td>
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</table>

Tab-1

\(\ldots: 1^{st} \text{approximation}; \quad \ldots: 2^{nd} \text{approximation}; \quad \ldots: \text{Exact solution}\)
REFERENCES: