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1981 J. Phys. A: Math. Gen. 14 1069

(http://iopscience.iop.org/0305-4470/14/5/026)

J. Phys. A: Math. Gen. **14** (1981) 1069–1074. Printed in Great Britain

A theorem on the separation of a system of coupled differential equations

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Received 17 June 1980, in final form 27 October 1980

Abstract. We consider the separation of a system of finite, linear, coupled differential equations. We discuss first the conditions which govern this separation in the case of a system of two coupled equations. It is then shown how these results may be extended to the case of a system of a finite number of coupled equations for which a general theorem on the separability is formulated.

1. Introduction

In many-channel problems one must frequently deal with a finite system of coupled differential equations of the Schrödinger type from which the wavefunction for each channel can be extracted. Consider the following system:

$$[\Delta + k_\lambda^2 + U_{\lambda\lambda}(r)]y_\lambda(r) = \sum_{\mu\neq\lambda} U_{\lambda\mu}(r)y_\mu(r) \tag{1}$$

in which Δ is the usual Laplace operator, k_λ^2 the energy of channel λ and $y_\lambda(r)$ a function related in a simple way to the wavefunction of channel λ. $U_{\lambda\mu}(r)$ represents the interaction term connecting channel λ to the other channels μ.

In order to solve (1) one must proceed through the two following steps.

(a) The equations must be decoupled, i.e. one has to find a transformation R in order to diagonalise the interaction term such that

$$F_i = \sum_\lambda R_{\lambda i} y_\lambda \tag{2}$$

with

$$\mathscr{L}_i F_i = 0, \qquad \lambda, i = 1, 2, \ldots, n, \tag{3}$$

where $\mathscr{L}_i$ is an operator and system (3) results from the application of R on (1).

(b) The separated equations (3) must then be solved and the functions y_λ recovered by applying the inverse operator R^{-1} on (F_i). When the non-diagonal term $U_{\lambda\mu}(r)$, $\lambda \neq \mu$, may be regarded as small compared with the diagonal one $U_{\lambda\lambda}(r)$ (small coupling case), the problem is relatively easy to handle and a number of methods of approximation are available (Mott and Massey 1965) (Born approximation, DWBA etc).

These approaches nevertheless become inadequate when $U_{\lambda\lambda} \simeq U_{\lambda\mu}$ (strong coupling case) and the situation emerges with much more complexity. Generally speaking,

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numerical analysis is usually considered as the last recourse for this problem, although it does contain a number of inherent difficulties such as the question of convergence of the iterated solutions or the convergence in the summation over the orbital quantum number in the partial wave method (Lane 1980).

Note that when allowed, the decoupling operation can be performed using one of the following approaches.

(1) Decoupling with increase of the order of the differential equations. Consider, for example, the simplest system of two coupled equations such as

$$y_0'(r)=f_0(r)y_1(r), \qquad y_1'(r)=f_1(r)y_0(r). \tag{4}$$

$f_{0,1}(r)$ are assumed to be continuous and differentiable. The separated equations will be

$$y_\lambda''-(f_\lambda'/f_\lambda)y_\lambda'-f_0f_1y_\lambda=0, \qquad \lambda=0,1,$$

where the order of the equations has been doubled.

(2) Decoupling without increase of this order or diagonalisation of the interaction term.

The present work deals with this second point of view and will be organised in the following manner. For the sake of clarity we begin with a system of two coupled differential equations, and a number of results obtained previously will be recalled, with the proof of a theorem which governs the separation of this system of equations. These results will next be extended to the general case of a system containing a finite number of coupled differential equations.

2. System of two coupled equations

Consider the following system:

$$[P+f_0(r)]y_0=B(r)y_1, \qquad [P+f_1(r)]y_1=B(r)y_0, \tag{5}$$

in which P is an operator of differentiation of the form

$$P=\sum_m a_m\frac{\mathrm{d}^m}{\mathrm{d}r^m}, \qquad m=1,2,3,\ldots,$$

where a_m are constants, and $B(r)$, $f_0(r)$, $f_1(r)$ are assumed to be continuous and differentiable.

Theorem on the decoupling operation. For any functions $B(r)$, $f_0(r)$, $f_1(r)$ the system (5) can always be decoupled without increase of the order of the differential equations if and only if $B(r)$ is proportional to the difference $f_1(r)-f_0(r)$.

Proof. In matrix notation let us write

$$(\mathscr{P}+\mathscr{F})Y=\mathscr{B}Y, \tag{6}$$

where

$$Y=\begin{pmatrix} y_0 \\ y_1 \end{pmatrix}, \qquad \mathscr{B}=\begin{pmatrix} 0 & B(r) \\ B(r) & 0 \end{pmatrix},$$

$$\mathscr{P}+\mathscr{F}=\begin{pmatrix} P+f_0 & 0 \\ 0 & P+f_1 \end{pmatrix}.$$

Consider now a transformation T defined by

$$T=\begin{pmatrix} 1-a & 1+a \\ -(1+a) & 1-a \end{pmatrix} \tag{7}$$

where a may be any function of r. Note that

$$T=X_1X_2$$

where

$$X_1=\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \qquad X_2=\begin{pmatrix} 1 & a \\ -a & 1 \end{pmatrix}.$$

Using the form (7), it may be shown that the above equations are separated if and only if the following conditions are satisfied simultaneously:

(1) $[P, a]=0$ ([ ] is a commutator and a is considered here as an operator)

(2) $(f_1-f_0)a^2-4Ba-(f_1-f_0)=0$.

Condition (1) means that a must be independent of r, while (2) connects this quantity with $B(r)$, $f_0(r)$, $f_1(r)$.

Solving this last equation, we come to the conclusion that the ratio $B/(f_1-f_0)$ must be independent of r.

Note also that the matrices X_1, X_2 are not unitary in the sense that we do not have $X_iX_i^+=I$, where I is the unit matrix, $i=1, 2$, but $X_iX_i=m_iI$, where m_i is constant. Likewise it may be verified that

$$TT^+=2(1+a^2)I.$$

If we define

$$W=\begin{pmatrix} \omega_+ \\ \omega_- \end{pmatrix}$$

then

$$Y=TW$$

and (5) is now separated in the form

$$\{[P+\tfrac{1}{2}(f_1+f_0)]I+\tfrac{1}{2}[(f_1-f_0)^2+4B^2]^{1/2}D\}W=0 \tag{8}$$

with

$$D=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Remark. In order to enlarge the discussion on the choice of T, let

$$T=\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

in which α, β, γ, δ may in principle be any functions of r. We can write

$$T\mathscr{P}T^{-1}(TY)=T(\mathscr{B}-\mathscr{F})T^{-1}(TY).$$

Clearly the first member of this equation is diagonal only if T is independent of r, agreeing therefore with the above conclusion.

However, in solving this equation we are led to a system of three equations with four unknowns, meaning that some degree of liberty in the choice of the solution is possible. We find that only the form (7) is appropriate for the proof.

Example

In the Schrödinger case, if

$$P = \mathrm{d}^2/\mathrm{d}r^2, \qquad f_\lambda(r) = k_\lambda^2 - l(l+1)/r^2, \qquad \lambda = 0, 1,$$

then for the trivial case $k_0 = k_1$, $l_0 = l_1$, we have $a = 0$, which means that $T = X_1$ and

$$\omega_+ = \tfrac{1}{2}(y_0 - y_1), \qquad \omega_- = \tfrac{1}{2}(y_0 + y_1).$$

For the cases $k_0 = k_1$, $l_0 \neq l_1$ and $k_0 \neq k_1$, $l_0 = l_1$ this theorem indicates that the coupling term $B(r)$ must be subjected to specific restrictions: for instance, it must follow the 'inverse square law' for the first case and equal a constant in the second one in order to obtain complete separation. These are the cases which correspond to real physical situations, and it has been shown (Cao and van Regemorter 1978) that an exact analytical solution may be obtained and expressed in terms of Bessel and Neuman functions.

3. Extension to the general case

We shall first show how the previous results may be extended to the case of three coupled differential equations where a coupling of each channel to its nearest neighbours is assumed for the sake of clarity. In this case, the corresponding system of coupled equations will be

$$\begin{aligned} &[P + f_0(r)]y_0(r) = B(r)y_1(r), \\ &[P + f_1(r)]y_1(r) = B(r)y_0(r) + C(r)y_2(r), \\ &[P + f_2(r)]y_2(r) = C(r)y_1(r), \end{aligned} \tag{9}$$

where, as before, B, C, f_λ, $\lambda = 0, 1, 2$, are assumed to be continuous and differentiable.

Introduce now an auxiliary parameter ε_1 defined by $0 \leq \varepsilon_1 \leq 1$ and replace in (9) $C(r)$ by $\varepsilon_1 C(r)$. Assuming then the existence of the solutions of the differential equations at all values of ε_1 defined above, we may see that y_λ will be modified and depend now on ε_1:

$$y_\lambda = y_\lambda(r, \varepsilon_1).$$

Expanding these functions in terms of ε_1, we obtain

$$y_\lambda(r, \varepsilon_1) = y_\lambda(r, 0) + \varepsilon_1 y'_\lambda(r, 0) + \tfrac{1}{2}\varepsilon_1^2 y''_\lambda(r, 0) + \ldots \tag{10}$$

where y'_λ means differentiation in terms of ε_1 etc:

$$y'_\lambda(r, 0) = (\partial y_\lambda/\partial \varepsilon_1)_{\varepsilon_1 = 0} \text{ etc.}$$

Replacing (10) in (9) and subsequently by identification, the following sets of systems of equations are obtained:

$$
\begin{aligned}
&[P+f_0(r)]y_0(r,0)=B(r)y_1(r,0),\\
&[P+f_1(r)]y_1(r,0)=B(r)y_0(r,0),\\
&[P+f_2(r)]y_2(r,0)=0,
\end{aligned}
\tag{11}
$$

$$
\begin{aligned}
&[P+f_0(r)]y_0'(r,0)=B(r)y_1'(r,0),\\
&[P+f_1(r)]y_1'(r,0)=B(r)y_0'(r,0)+C(r)y_2(r,0),\\
&[P'+f_2(r)]y_2'(r,0)=C(r)y_1(r,0),
\end{aligned}
\tag{12}
$$

$$
\begin{aligned}
&[P+f_0(r)]y_0''(r,0)=B(r)y_1''(r,0),\\
&[P+f_1(r)]y_1''(r,0)=B(r)y_0''(r,0)+C(r)y_2'(r,0),\\
&[P+f_2(r)]y_2''(r,0)=C(r)y_1'(r,0),\\
&\quad\ldots.
\end{aligned}
\tag{13}
$$

It appears now clearly that, from what was stated in the case of two equations, system (11) may be decoupled if and only if the ratio $B/(f_1-f_0)$ is independent of r. Use of transformation T enables us then to obtain the solutions $y_0(r,0)$, $y_1(r,0)$, $y_2(r,0)$.

Replacing $y_1(r,0)$, $y_2(r,0)$ in (12) and using T again, we obtain the following system:

$$
\begin{aligned}
&\{P+\tfrac{1}{2}(f_1+f_0)+\tfrac{1}{2}[(f_1-f_0)^2+4B^2]^{1/2}\}W_+'(r,0)=(1+a)C(r)y_2(r,0),\\
&\{P+\tfrac{1}{2}(f_1+f_0)-\tfrac{1}{2}[(f_1-f_0)^2+4B^2]^{1/2}\}W_-'(r,0)=-(1-a)C(r)y_1(r,0),\\
&\{P+f_2(r)\}y_2'(r,0)=C(r)y_1(r,0),
\end{aligned}
$$

where $y_1(r,0)$, $y_2(r,0)$ are known from (11). These equations are separated, and after solving them we may recover the couple $y_0'(r,0)$, $y_1'(r,0)$ by

$$
Y'=TW',
$$

$$
Y'=\begin{pmatrix}y_0'(r,0)\\ y_1'(r,0)\end{pmatrix},\qquad W'=\begin{pmatrix}\omega_+'(r,0)\\ \omega_-'(r,0)\end{pmatrix}.
$$

Solving (12), we then obtain $y_0'(r,0)$, $y_1'(r,0)$, $y_2'(r,0)$ which will be replaced in (13) and so on.

Returning to (10), we may conclude that system (9) may be made soluble by expansion of the solution as a Taylor series in the parameter ε_1 and with $C(r)$ replaced by $\varepsilon_1 C(r)$.

Introduce now a second parameter ε_2; by replacing $B(r)$ by $\varepsilon_2 B(r)$ in (9) we obtain another set of functions $y_\lambda(r,\varepsilon_2)$, and use of the same reasoning leads to the conclusion that the ratio $C/(f_2-f_1)$ must be equal to a constant.

Combining these results and noting that the final solution is of the form

$$
y_\lambda(r)=\lim_{\varepsilon_1,\varepsilon_2\to 1}\tfrac{1}{2}[y_\lambda(r,\varepsilon_1)+y_\lambda(r,\varepsilon_2)],
$$

we may see that the condition for obtaining this solution is that $B/(f_1-f_0)$ and $C/(f_2-f_1)$ must be simultaneously independent of r.

Generally speaking, although the present approach does not yield a complete separation of system (9) similar to equation (7) in the two equations case, it may be noted however that a separation of the equations corresponding to different powers of ε_i ($i=1,2$) resulting from the Taylor series expansion is possible if and only if the ratio mentioned above is simultaneously independent of r. Whenever these last equations are soluble, the reconstruction of the final solution is then possible.

It is now relatively easy to extend this method to the general case and formulate the following statement.

Consider a system of coupled differential equations

$$[P+f_\lambda(r)]y_\lambda(r)=\sum_{\mu\neq\lambda} C_{\lambda\mu}(r)y_\mu(r), \qquad \lambda, \mu=0,1,2,\ldots.$$

For any $f_\lambda(r)$, $C_{\lambda\mu}(r)$ continuous and differentiable, this system can always be soluble in the above sense if and only if the ratio $C_{\lambda\mu}/(f_\mu-f_\lambda)$ is simultaneously independent of r.

4. Conclusion

For a system of coupled differential equations in the strong coupling case, it seems to us that one of the merits of this theorem is that it provides a set of conditions which governs the complete separation of the equations, thus putting the problem on a more rational basis. This is particularly transparent in the case of a system of two coupled differential equations, but even in the case where these conditions are only partially fulfilled, the use of this method in connection with physical arguments may sometimes give hints in the search for an appropriate method of approximation.

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