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Generalisation of the theory of coupled differential equations

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Abstract. We generalise a method derived from the theorem on the separation of coupled equations which was stated previously to solve the case of two equations. It will be shown that this generalisation is always possible with a sequence of special transformation in terms of scaling parameters. The case of a system of three coupled differential equations is considered in some detail including a discussion on the search and use of these parameters.

1. Introduction

Consider the following system of coupled differential equations

$$[P+f_i]y_i = \sum_j B_{ij} y_j \qquad i,j=1,\ldots,n \tag{1}$$

in which P may be any linear differential operator and $f_i(r)$ and $B_{ij}(r)$ are assumed to be analytic functions of the variable r. For instance, in the many-channels problem (1) would correspond to n coupled Schrödinger equations with

$$P = \mathrm{d}^2/\mathrm{d}r^2 \qquad f_i(r) = k_i^2 - \frac{l_i(l_i+1)}{r^2} - B_{ii}(r)$$

where $B_{ij}(r)$ are expressed in terms of some integrals and usually are symmetric in the sense $B_{ij} = B_{ji}$.

The motivation of the present work is twofold.

(i) A general method for separation (decoupling) of (1) is still not available at present and this obviously constitutes an interesting challenge for further investigations from the mathematical point of view.

(ii) In applications to physical problems (for instance the Schrödinger case) the conventional numerical iteration procedure or variational approach which in most cases requires a considerable amount of computational work particularly when strong coupling and long-range coupling interactions are involved because of the slow rate of convergence or even divergence of the iterated solutions. It is hoped that one of the remedies to this situation may lie in the present approach in which a new representation is set up such that system (1) can be completely or partially decoupled and transforming the strong coupling problem into a weak coupling one for which the conventional iteration methods can be handled more conveniently. We refer to Cao (1981, 1982, 1984 and references therein, hereafter referred to as I, II and III, respectively) for a more general introduction to this subject.

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2. The transformation matrix

Let $\eta > 2$ and write (1) in a more convenient matrix notation:

$$[\bar{P}+\bar{F}]Y=\bar{B}Y \tag{2}$$

where Y is a column matrix (y_l); $m, l=1,2,\dots,n$; $\bar{P}=PI_n$; I_n is an $n\times n$ unit matrix; $\bar{F}$ is a diagonal matrix (f_{ll}) and $\bar{B}$ is an $n\times n$ symmetric matrix $(B_{l,m})$.

Consider now an $n\times n$ matrix T_n defined by

$$T_n=\begin{pmatrix} T_2 & 0 \\ 0 & I_{n-2} \end{pmatrix}$$

where

$$T_2=\begin{pmatrix} 1-a & 1+a \\ -(1+a) & 1-a \end{pmatrix}$$

is a 2×2 matrix defined in I. On the other hand, we have already introduced an arbitrary parameter α related to a by:

$$a=2\alpha+(1+4\alpha^2)^{1/2}.$$

It is useful to note that

$$\Delta=2(1+a^2) \qquad \det(T_n)=\Delta \qquad T_n^{-1}=\begin{pmatrix} T_2^{-1} & 0 \\ 0 & I_{n-2} \end{pmatrix}$$

T_n^{-1} being the inverse of T_n.

Note that if we had defined the transformation matrix by

$$\bar{T}_n=\begin{pmatrix} \bar{T}_2 & 0 \\ 0 & I_{n-2} \end{pmatrix} \qquad \text{with} \qquad \bar{T}_2=\frac{1}{\Delta^{1/2}}T_2$$

then it can be verified that $\bar{T}_n$ is unitary and unimodular, i.e. belongs to SU(n). However we find it more convenient to use T_n instead of $\bar{T}_n$ for reasons to be seen shortly below.

We introduce another column matrix Z defined by (Z_l):

$$Z=T_nY.$$

Then system (2) can be written as

$$[P+T_n(\bar{F}-\bar{B})T_n^{-1}]Z=0 \tag{3}$$

where the term $T_n(\bar{F}-\bar{B})T_n^{-1}$ can be cast in the form

$$T_n(\bar{F}-\bar{B})T_n^{-1}=\frac{1}{\Delta}L^+ + J+K+L \tag{4}$$

where L, J, K are the $n\times n$ matrices:

$$L=\begin{pmatrix} 0 & m \\ 0 & 0 \end{pmatrix} \qquad J=\begin{pmatrix} g & 0 \\ 0 & 0 \end{pmatrix}$$

$$K=\begin{pmatrix} 0 & 0 \\ 0 & h \end{pmatrix} \qquad L^+=\begin{pmatrix} 0 & 0 \\ m^+ & 0 \end{pmatrix}.$$

Here, h is an $(n-2)\times(n-2)$ matrix obtained by truncating $\bar{F}-\bar{B}$ of the first two rows and columns; m is a rectangular $2\times(n-2)$ matrix and m^{+} its adjoint; g is a 2×2 matrix

$$g=(g_{ij}) \qquad i,j=1,2.$$

More precisely $(k=3,4,\ldots,n)$:

$$g_{11}=\tfrac{1}{2}(f_1+f_2)+\frac{\frac{1}{2}\Delta f+2\alpha B_{12}}{(1+4\alpha^2)^{1/2}} \qquad g_{22}=\tfrac{1}{2}(f_1+f_2)-\frac{\frac{1}{2}\Delta f+2\alpha B_{12}}{(1+4\alpha^2)^{1/2}}$$

$$g_{12}=g_{21}=-\frac{B_{12}-\alpha\Delta f}{(1+4\alpha^2)^{1/2}} \qquad \Delta f=f_2-f_1$$

$$m=(m_{ik}) \qquad m_{ik}=\sum_j (T_2)_{ij}B_{jk}.$$

Consider now sufficiently large values of α such that $(1+4\alpha^2)^{1/2}\gg 1$. After some simple algebra, it can verified that:

$$\frac{|1\pm a|}{\Delta}<\frac{1}{(1+4\alpha^2)^{1/2}}<\frac{\alpha}{(1+4\alpha^2)^{1/2}}<|1\pm a|. \tag{5}$$

From relation (4) this means that the effect on the coupling of the matrix L^{+} is negligible compared to the effect of J, K and L†. The space spanned by Z may consequently split into two subspaces

$$Z^{(2)}=(Z_i) \qquad Z^{(n-2)}=(Z_k)$$

and system (3) can be rewritten as:

$$[PI_2+\bar{g}]Z_1^{(2)}=mZ^{(n-2)}$$

$$[PI_{n-2}+h]Z^{(n-2)}=0.$$

More precisely we have:

$$\left.\begin{aligned}&[P+\bar{g}_{11}]Z_1=\bar{g}_{12}Z_2+\sum_k m_{1k}Z_k\\ &[P+\bar{g}_{22}]Z_i=\bar{g}_{21}Z_1+\sum_k m_{2k}Z_k\end{aligned}\right. \tag{6}$$

$$[P+f_k]Z_k=\sum_l B_{kl}Z_l \qquad k\neq l \qquad k,l=3,4,\ldots,n. \tag{7}$$

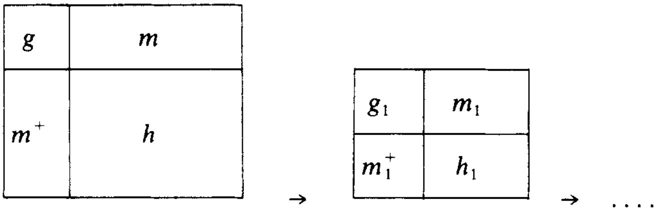
This means that, if $Z^{(n-2)}$ can be obtained as a solution of (7), its elements may be replaced in (6) which is then reduced to a system of two coupled differential equations. It has already been shown in II that this type of equation can, with some supplementary constraints on the choice of α, become completely or partially decoupled. The choice as well as the use of this parameter will be discussed in the next paragraph.

On the other hand, we may note that (7) is formally exactly the same as (1) but with the dimension reduced by two units. Repeating then the above procedure once again with the choice of another parameter we see that the space $Z^{(n-2)}$ in turn can be decomposed into $Z_1^{(2)}$, $Z_1^{(n-1)}$ with the corresponding $(n-4)\times(n-4)$ matrix h_1, as well as g_1, m_1.

† See appendix 1.

As each step reduces the original dimension by two units, at the end of the process we shall reach the smallest system of coupled equations with two or three equations depending on the even or odd character of n, i.e. $n=2t$ or $n=2t+1$ $(t=0,1,\ldots)$. Both cases require t parameters α_p. Each one is closely related to the specific analytic behaviour of the quantity $B_{2p+1,2p+2}/f_{2p+2}-f_{2p+1}$ together with the condition $(t+4\alpha^2)^{1/2}\gg 1$†.

The following diagram summarises the method:



3. The system of three equations

As $n=3$, we have $t=1$ so that only one parameter is needed. In (8) we obtain three equations in which the third one is uncoupled. Consider another representation

$$W=(W_l) \qquad l=1,2,3 \qquad W=T(A)Z$$

where $T(A)$ is defined in II as

$$T(A)=\begin{pmatrix} 1-A & 1+A \\ -(1+A) & 1-A \end{pmatrix}$$

with

$$A=2f+(1+4f^2)^{1/2} \qquad \gamma=\frac{B_{12}}{\Delta f} \qquad \Delta f=f_2-f_1 \qquad f=\frac{\alpha+\gamma}{1+4\alpha\gamma}.$$

Neglecting only the first term in (5), in this new representation, the exact form of (1) is

$$\left[P+\tfrac{1}{2}(f_1+f_2)+\tfrac{1}{2}(\bar{\Delta}f^2+4B_{12}^2)^{1/2}+\frac{1}{1+A^2}[P,A]\right]W_1$$
$$=\frac{1}{1+A^2}[P,A]W_2+(cB_{13}+dB_{23})W_3$$
$$\left[P+\tfrac{1}{2}(f_1+f_2)-\tfrac{1}{2}(\bar{\Delta}f^2+4B_{12}^2)^{1/2}+\frac{1}{1+A^2}[P,A]\right]W_2$$
$$=-\frac{1}{1+A^2}[P,A]W_1+(-dB_{13}+cB_{23})W_3 \qquad (8)$$
$$[P+f_3]W_3=0$$

in which

$$c=-2(a+A) \qquad d=2(1-aA)$$

and [,] means the commutator bracket.

† See below and appendix 2.

In order to obtain the original solution Y of I we must consider the inverse transformation

$$Y = V_3^{-1} W \tag{9}$$

where

$$V_3 = T_3(\alpha) T_3(A). \tag{10}$$

We find

$$V_3 = \begin{pmatrix} c & d & 0 \\ -d & c & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Note also that if we had used $\bar{V}_3$ instead of V_3 with

$$\bar{V}_3 = \begin{pmatrix} c/e & d/e & 0 \\ -d/e & c/e & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where $e = [c^2 + d^2]^{1/2} = 2[(1+A^2)(1+a^2)]^{1/2}$ then it can be verified that $\bar{V}_3$ is unitary and unimodular (SU(3)) and can be written as

$$\bar{V}_3 = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where $\tan\varphi = d/c$ which clearly is equivalent to a rotation around the third axis.

4. The scaling and mixing parameters

As the problem is now reduced to a sequence of systems of two coupled differential equations, it is interesting to investigate further this special case and point out a number of remarks which will be useful in the choice of the parameter α and the role of the conventional mixing parameter. Consider, for instance, the Schrödinger case ($P = \mathrm{d}^2/\mathrm{d}r^2$) so that

$$[P, A] = \frac{\mathrm{d}^2 A}{\mathrm{d}r^2} + 2\frac{\mathrm{d}A}{\mathrm{d}r}\frac{\mathrm{d}}{\mathrm{d}r}.$$

This means that the RHS of the first two equations in (9) involves three coupling terms

$$N\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} Z_{11} \\ Z_2 \end{pmatrix} + M\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\frac{\mathrm{d}}{\mathrm{d}r}\begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} cB_{13} + dB_{23} \\ -dB_{13} + cB_{23} \end{pmatrix} Z_3$$

where

$$M = \frac{2}{1+A^2}\frac{\mathrm{d}A}{\mathrm{d}r} \qquad N = \frac{1}{1+A^2}\frac{\mathrm{d}^2 A}{\mathrm{d}r^2}$$

and the third term is known.

If the quantity $\gamma = B_{12}/\Delta f$ is independent of the variable α, we always have $N = 0$, $M = 0$ so that the two equations are completely separated as stated by the theorem in I.

If this is not the case, we also expect that an appropriate choice of the parameter α will minimise the effect of the terms M and N compared to the effect of the third term which involves the coefficients c and d.

More precisely, after some algebra, we find that M and N are given by

$$M=\frac{2}{1+4\gamma^2}\frac{\mathrm{d}\gamma}{\mathrm{d}r}$$
$$N=\frac{\mathrm{d}M}{\mathrm{d}r}+2AM^2 \tag{11}$$

which shows that M is always independent of the choice of α but is strongly related to the analytic behaviour of $\gamma(r)$. To see this more clearly, let us now be more specific by assuming (as is usually the case in many-channel problems) that $\gamma(r)$ is a monotonic decreasing function with increasing values of r, i.e. $\gamma(r)=C/r^p$ (C is a constant, $p\geqslant 2$). Then $(1+4\gamma^2)^{-1}$ is essentially an increasing function (from $0\to 1$) while $\mathrm{d}\gamma/\mathrm{d}r$ is a decreasing one. There exists a position $r=r_0$ where $M=M_0$ reaches a maximum (in absolute value). We find for this case

$$M_0=\frac{p+1}{2^{(3p+1)/p}}\frac{1}{C^{(2p+1)/p}}\left(\frac{8p}{p+1}C^2-1\right)^{(p+1)/2p} \tag{12}$$

which shows that, for fixed p, M_0 is decreasing with increasing coupling strength C. We are thus led to an interesting situation in which the original difficulty pertaining to the strong and long-range coupling can be avoided and the problem transformed into another one with weak and shorter-range coupling (due to the effect of $\mathrm{d}\gamma/\mathrm{d}r$) to be dealt with more conveniently with conventional iteration methods. The quantity N is dependent on α so that this parameter may be chosen graphically such that

$$N, M \ll c, d$$

(see appendix 2).

Therefore, for strong coupling problems, the effect of the operator $(1+A^2)^{-1}[P, A]$ on the coupling terms is expected to be negligible compared to the effect of terms involving the quantities C and d which generally increases with α.

As an example, consider the case where $p=2$, $C=6$ so that $\gamma(r)=6/r^2$. For $\alpha=7.0$ we find $M_0=0.24\ (1+4\alpha^2)^{-1/2}=0.072$ and (in absolute values)

$$N, M<0.20 \qquad c, d>10$$

everywhere. Consequently, as a first stage, we may consider these two equations as separated and the effects of the commutator can be re-injected in a second stage as a perturbation in the equations if more accuracy is needed. For the physical aspects of this special case and comparison with other methods see, e.g., Cao and Bougouffa (1987).

The quantity α plays the role of the scaling parameter for obvious reasons and leads to the definition of the mixing parameter. In fact, in the present theory, we may discern two cases.

(i) If γ is independent of r then

$$\chi=\frac{1-a}{1+a}.$$

(ii) If this is not the case, we must consider first a mixing function

$$\chi(r)=\frac{d}{c}=\frac{1-aA}{a+A}$$

which will be useful in the construction of the 'trial function' in conventional variational approaches. The mixing parameter for this case will be

$$\chi=\lim_{r\to\infty}\chi(r).$$

As a check of consistency, consider the following cases.

(i) If $B_{12}=0$ (no coupling), then $\alpha=0$, $a\to 1$, $\chi\to 0$ (no mixing).

(ii) If $\Delta f=0$ (exact resonance), then $\gamma\to\infty$, α large so that $A\to 1$, $\chi\to 1$ (maximum coupling).

5. Conclusion

The present work completes the series of papers dealing with the theory of separation of a system of coupled differential equations. It is shown that, with an extension of the use of the special transformation matrix T_n, the system of n coupled equations can always be broken into $n/2$ partial systems of two coupled equations. Each of these systems can be made tractable by use of a second transformation of the type $T_2(A)$ corresponding to the scaling parameters α which are related to the analytic behaviour of the coupling functions. The theory finally leads to a logical definition of the mixing function and mixing parameter for each of these subsystems.

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Appendix 1

Note that the elements of the matrices h and m defined in K, L are respectively (B_{kl}); $k, l=3,4,\ldots,n$ and $(I\pm a)B_{ik}$; $i=1,2$. Therefore in (5), if we neglect the first two terms, h and m will be unaffected by the approximation while the matrix g must be replaced by $\bar{g}$ with:

$$\bar{g}_{11}=\tfrac{1}{2}(f_1+f_2)+\frac{2\alpha}{(1+4\alpha^2)^{1/2}}B_{12} \qquad \bar{g}_{22}=\tfrac{1}{2}(f_1+f_2)-\frac{2\alpha}{(1+4\alpha^2)^{1/2}}B_{12}$$

$$\bar{g}_{12}=\bar{g}_{21}=-\frac{\alpha}{(1+4\alpha^2)^{1/2}}\Delta f.$$

On the other hand, if we neglect only the first term then g will also remain unaffected.

Appendix 2

In order to determine the parameter in question, consider for example the function $A(\alpha,\gamma)$ defined in equation (8) and above. This parameter must obviously comply to the following conditions.

(i) $(1+4\alpha^2)^{1/2} \gg 1$.

(ii) It must be chosen such that the effect of the operator $(1+A^2)^{-1}[P, A]$ is as small as possible.

The function A has the following mathematical properties.

(i) It is always analytic even when the coupling function have singularities.

(ii) If $\gamma(r)$ is a monotonic decreasing function, A is also monotonic (i.e. $\mathrm{d}A/\mathrm{d}r$ does not change sign).

(iii) It can be verified that:

$$\frac{\mathrm{d}A}{\mathrm{d}r} \leqslant \left|\frac{\mathrm{d}\gamma}{\mathrm{d}r}\right| \qquad \lim_{r\to\alpha} \frac{\mathrm{d}A}{\mathrm{d}r} = 0.$$

These properties are helpful as a guideline and suggest various alternatives for the determination of α, for example resulting in the numerical or graphical solution. As explained in the text, the operator $(1+A^2)^{-1}[P, A]$ consists of two parts, M which is independent and N which does depend on the parameter α. The problem is to determine α such that $N, M \ll c, d$. In order to show the existence of such a solution, note that the quantities c and d are functions of α and r. For fixed r their absolute values increase almost linearly with increasing values of α while the rate of increase of the function $A(\alpha, r)$ in the expression of N is less rapid. Therefore, if $M_0 < 1$, $M^2 \ll 1$ and there always exists values of α such that the above condition is satisfied.

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