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Theory of coupled differential equations

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Abstract. The problem of decoupling a system of linear coupled differential equations without changing the order of the equations will be considered. Starting from a theorem on the separation of the coupled equations, we continue the investigations in the general case, where the conditions set up by this theorem are not satisfied, in deriving a method of separation of the equations in the strong coupling case. An example on a system of two coupled Schrödinger equations will be taken up as an illustration of this method.

1. Introduction

In a previous paper (Cao 1981) it has already been shown that the separation of a system of coupled differential equations without increasing their order is governed by a theorem which sets up specific conditions on the coupling terms. These conditions, however, induce serious restrictions on the analytical form of these coupling functions, which in the case of Schrödinger equations may apply only to a very small number of real physical problems (Cao and Van Regemorter 1978).

It therefore seems appropriate to seek for an enlargement of the range of validity of this theorem in order to include more general types of problems which are frequently met in practice.

Within this scope, the present paper begins with a brief presentation of previous results where, for the sake of simplicity, we shall confine ourselves to the case of two coupled differential equations with strong coupling terms.

The essential points of the theory will be taken up in the next section where a formal derivation will be introduced to deal with the most general situations.

The discussion which follows selects two interesting cases, which in fact may cover almost all situations encountered in practice, and where it will be shown that the problem of strong coupling can be handled either with a decoupling approach at a given order of approximation, or with its transformation to a weak coupling problem which is generally easier to solve.

A concrete example will be discussed finally as an illustration of the above method.

2. Separation of a system of two coupled equations

As the weak coupling case presents in principle no substantial difficulties and may be handled by a number of conventional methods both analytically and numerically (Mott and Massey 1965), we shall consider in this work only the strong coupling case where

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these conventional methods become questionable and inadequate, mostly because of the very slow rate of convergence of the iterated solutions.

Consider, for example, the following system of coupled equations

$$[P+f_0(x)]y_0(x)=B(x)y_1(x), \qquad [P+f_1(x)]y_1(x)=B(x)y_0(x), \tag{1}$$

where as usual we shall keep the notations and conventions of earlier work (Cao 1981), i.e., $P=\Sigma_{n=1}\,\mathrm{d}^n/\mathrm{d}x^n$, $f_1(x)$, $f_0(x)$, $B(x)$ are assumed to be continuous and differentiable functions of x.

If $B(x)$ is of the same order as or larger than $f_1^0(x)$, we shall say by convention that the coupling is strong while weak coupling means the case $B(x)\ll f_1^0(x)$.

The theorem on the separation of the equations of this system states the following.

Theorem. System (1) may always be completely separated if and only if the quantity $B(x)/(f_1-f_0)$ is independent of x.

For the proof of this theorem, as well as its extension to the general case of a system of a finite number of coupled differential equations, we refer to Cao (1981). Furthermore, these results may also be applied to the case of non-identical terms of coupling, i.e. for systems such that

$$[P+f_0]y_0=By_1, \qquad [P+f_1]y_1=Cy_0, \qquad B\neq C,$$

and from this basis, a construction of the solution in the general case of three or more equations is also possible (Cao 1982).

The conditions set up by this theorem however give access only to a very narrow range of applications because the coupling functions $B(x)$ must be strictly fixed by the quantity $\Delta f=f_1-f_0$. For example, in the Schrödinger case if $f_i=k_0^2-l_i(l_i+1)/x^2$, $i=0$, 1, then $B(x)$ must be of the form A/x^2 etc.

In order to enlarge these results and make them more adapted to current situations, we shall have to re-examine system (1) in the case where the quantity $B/(f_1-f_0)$ is no longer independent of x as prescribed by the theorem. This means of course that the coupling term $B(x)$ may now take any analytical form regardless of the structure of the functions f_0 and f_1.

The basic idea which underlines the present work is that if in these conditions a complete separation of the equations in system (1) become impossible, we consider that a decisive improvement can nevertheless be achieved once the strong coupling problem with its inherent difficulties may be avoided and be transformed into a weak coupling one, for which we already have at our disposal a number of excellent techniques to obtain the solution.

As we shall see in the following, it turns out that the outcome of the discussion goes beyond this expectation, because it will be shown that not only is the transformation of a strong coupling problem into a weak coupling one possible, but furthermore in many cases, a decoupling of the equations at any given order of approximation may also be obtained.

3. The general case

Assume now that in system (1) the functions $B(x)$, $f_1(x)$, $f_0(x)$ may take any analytical form so that the condition $B/\Delta f$ independent of x is no longer satisfied. Introduce then an auxiliary function $C(x)$ which is subjected only to the condition $C/\Delta f$ independent of x, i.e.

$$C(x)=\alpha(f_1-f_0), \qquad \alpha \text{ constant}, \tag{2}$$

and rewrite (1) in the form

$$[P+f_0]y_0=Cy_1+(B-C)y_1, \qquad [P+f_1]y_1=Cy_0+(B-C)y_0. \tag{3}$$

We may now use the transformation

$$T(a)=\begin{pmatrix} 1-a & 1+a \\ -(1+a) & 1-a \end{pmatrix}, \tag{4}$$

in which a is the root of the equation

$$(f_1-f_0)a^2-4Ba-(f_1-f_0)=0, \tag{5}$$

to diagonalise the matrix equation

$$T(\mathscr{P}+\mathscr{F})T^{-1}TY=T\mathscr{C}T^{-1}TY+T\mathscr{D}T^{-1}TY, \qquad \mathscr{P}+\mathscr{F}=\begin{pmatrix} P+f_0 & 0 \\ 0 & P+f_1 \end{pmatrix}, \tag{6}$$

in which

$$\mathscr{C}=C\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \mathscr{D}=(B-C)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Define

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

and let $W=TY$; equation (6) becomes explicitly

$$\begin{aligned} &\left(P+\tfrac{1}{2}(f_1+f_0)+\frac{1}{2}\frac{\Delta f}{(1+4\alpha^2)^{1/2}}+\frac{2\alpha B}{(1+4\alpha^2)^{1/2}}\right)W_+=\left(-\frac{B}{(1+4\alpha^2)^{1/2}}+\frac{\alpha\Delta f}{(1+4\alpha^2)^{1/2}}\right)W_-, \\ &\left(P+\tfrac{1}{2}(f_1+f_0)-\frac{1}{2}\frac{\Delta f}{(1+4\alpha^2)^{1/2}}-\frac{2\alpha B}{(1+4\alpha^2)^{1/2}}\right)W_-=\left(-\frac{B}{(1+4\alpha^2)^{1/2}}+\frac{\alpha\Delta f}{(1+4\alpha^2)^{1/2}}\right)W_+. \end{aligned} \tag{7}$$

As the parameter α is arbitrary and still remains at our disposal its choice will reveal a number of interesting features which will be successively examined hereafter.

4. Discussion

As was said from the beginning, the strong coupling problem in the case of system (1) means that the function $B(x)$ must be larger than or of the same order as $f_1(x)$, $f_0(x)$, while the weak coupling one corresponds to the condition $B(x)\ll f_1, f_0$.

Consider first a special case where $\Delta f\ll B$, f_1, f_0 (for a system of two coupled Schrödinger equations this would correspond to a 'near resonance' situation) for which the use of the parameter α is unnecessary. In fact, if we let $\alpha\to\infty$ system (7) becomes

$$[P+\tfrac{1}{2}(f_1+f_0)+B]W_+=\tfrac{1}{2}\Delta fW_-, \qquad [P+\tfrac{1}{2}(f_1+f_0)-B]W_-=\tfrac{1}{2}\Delta fW_+, \tag{8}$$

which corresponds to the replacement of the transformation $T(a)$ by another one X_1,

$$X_1=\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}.$$

On the other hand, if $f_1=f_0$ we recover a well known result valid for any analytical form of $B(x)$ with the solution

$$W_\pm=\tfrac{1}{2}(y_0\pm y_1). \tag{9}$$

It is also known that in many fields of physics the coupling term $B(x)$ generally decreases at the same rate as or faster than the interaction involved in the functions f_1, f_0, at least at large distances so that it is conventionally admitted that the equations become asymptotically uncoupled (see for example Burke and Seaton 1971).

Returning to system (7), we see that it appears in a form similar to (1) and, keeping the notations as closely similar as possible between (1) and (7), we write

$$[P+F_+]W_+=NW_-, \qquad [P+F_-]W_-=NW_+ \tag{10}$$

in which

$$F_\pm=\tfrac{1}{2}(f_1+f_0)\pm\frac{1}{2}\frac{\Delta f}{(1+4\alpha^2)^{1/2}}\pm\frac{2\alpha B}{(1+4\alpha^2)^{1/2}},$$

$$N=-\frac{B}{(1+4\alpha^2)^{1/2}}+\frac{\alpha\Delta f}{(1+4\alpha^2)^{1/2}}.$$

From what was said above, we already know that system (10) cannot be separated because the quantity $N/\Delta F$, $\Delta F=F_+-F_-$ is not independent of x. However, if we introduce a new transformation $T(A)$ such that

$$T(A)=\begin{pmatrix}1-A & 1+A\\ -(1+A) & 1-A\end{pmatrix}, \tag{11}$$

A being the solution of the equation

$$\Delta FA^2-4NA-\Delta F=0, \tag{12}$$

and diagonalise the matrix equation

$$T(\mathscr{P}+\mathscr{F})T^{-1}TW=T\mathscr{N}T^{-1}TW,$$
$$\mathscr{P}+\mathscr{F}=\begin{pmatrix}P+F_+ & 0\\ 0 & P+F_-\end{pmatrix}, \qquad \mathscr{N}=N\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \tag{13}$$

the only cross term is given by

$$K(A)=[P,A]\tfrac{1}{2}(1+A^2)^{-1} \tag{14}$$

where

$$A=2N/\Delta F\pm[1+4(N/\Delta F)^2]^{1/2}$$

and [ ] means a commutator bracket.

In order to evaluate $K(A)$, note that the quantity $N/\Delta F$ is of the form

$$f(\gamma)=N/\Delta F=(\alpha-\gamma)/(1+4\alpha\gamma) \tag{15}$$

in which $\gamma = B/\Delta f$ and where the case most frequently met in practice is $\gamma < 1$. For completeness, we shall also discuss the case $\gamma > 1$; in fact, it will be seen that these two cases may be dealt with on the same footing.

Remarking that $f(\gamma)$ is an analytical function of γ in some region of the complex plane (γ) with a corresponding appropriate choice of the parameter α, we may always choose an arbitrary point γ_0 in this region and have a Taylor expansion of $f(\gamma)$ around γ_0

$$f(\gamma) = f(\gamma_0) + (\gamma - \gamma_0)f'(\gamma_0) + (1/2!)(\gamma - \gamma_0)^2 f''(\gamma_0) + \dots$$

or explicitly

$$f(\gamma) = \frac{1}{1 + r\alpha\gamma_0}\left[\alpha - \gamma_0 + \frac{1+4\alpha^2}{1+4\alpha\gamma_0}(\gamma - \gamma_0)\sum_{n=1}^{\infty}(-1)^n\left(\frac{4\alpha(\gamma-\gamma_0)}{1+4\alpha\gamma_0}\right)^{n-1}\right] \tag{16}$$

with a radius of convergence equal to $1/4\alpha + 2\gamma_0$.

From (16), the quantity A may now be evaluated and represented by a power series in terms of Γ,

$$A = \sum_{n=0}^{\infty} A_n \Gamma^n \qquad \text{with} \quad \Gamma = \gamma - \gamma_0 \tag{17}$$

and

$$1 + 4\left(\frac{\alpha - \gamma_0}{1 + 4\alpha\gamma_0}\right)^2 = I(\gamma_0), \qquad 1 + 4\alpha\gamma_0 = H(\gamma_0),$$

$$A_0 = 2\frac{\alpha - \gamma_0}{H} - I^{1/2}, \qquad A_1 = -2\frac{1+4\alpha^2}{H^2}\left(1 - 2\frac{\alpha - \gamma_0}{I^{1/2}}\right),$$

$$A_2 = -2\frac{1+4\alpha^2}{H^3}\left\{-4\alpha + \frac{\alpha - \gamma_0}{HI}\left[8\alpha + (1+4\alpha^2)\left(\frac{1}{\alpha - \gamma_0} - \frac{4(\alpha - \gamma_0)}{I}\right)\right]\right\}.$$

As γ_0 is still arbitrary, it may be shown that if we take $\gamma_0 = n/\alpha$, n being any parameter >0, there always exists a corresponding value α_n which makes $A_1 \equiv 0$.

The cross term will therefore be

$$K(A) = A_2 K(\Gamma^2) + A_3 K(\Gamma^3) + \dots. \tag{18}$$

If we are satisfied with the first order of approximation (i.e. neglecting terms with Γ^2 or more), system (10) can now be separated by use of the transformation $T(A)$:

$$[P + \tfrac{1}{2}(F_+ + F_-) + \tfrac{1}{2}(\Delta F^2 + 4N^2)^{1/2}]Z_+ = 0,$$
$$[P + \tfrac{1}{2}(F_+ + F_-) - \tfrac{1}{2}(\Delta F^2 + 4N^2)^{1/2}]Z_- = 0. \tag{19}$$

5. Remarks

This expansion is valid if γ lies in the region

$$n/\alpha < \gamma < (8n+1)/\alpha;$$

for example if we let $n = 1$, the acceptable values of γ will be

$$0.188 < \gamma < 1.696$$

etc. For larger values of γ, larger values of n must be chosen.

Consider now the case $\gamma_0 = 0$ which corresponds to the choice $n = 0$. It may be verified that the expansions (16) and (17) become

$$f_0(\gamma) = \alpha + (1+4\alpha^2)\gamma \sum_{n=0}^{\infty} (-1)^{n+1}(4\alpha\gamma)^n, \tag{16b}$$

$$A_0 = \sum_{n=0}^{\infty} A_{0n}\gamma^n,$$

$$A_{00} = 2\alpha - (1+4\alpha^2)^{1/2}, \qquad A_{01} = -2(1+4\alpha^2)^{1/2}[(1+4\alpha^2)^{1/2} - 2\alpha], \tag{17b}$$

$$A_{02} = 2(16\alpha^3 - 8\alpha^2 + 4\alpha - 1).$$

Expansion (16*b*) is valid if $\gamma < 1/4\alpha$ and the coefficient A_{01} is practically equal to zero if $\alpha > 5$. This means that γ must be <0.05. These results may be easily checked by a direct expansion of the quantity $f_0(\gamma) = (\alpha - \gamma)/(1+4\alpha\gamma)$.

If we are interested in the second order of approximation then the term $A_2K(\Gamma^2)$ must be taken into account in the second member of (19). But this does not present a real problem for us, because the above procedure may be repeated again to separate the equations as we did for the first approximation. This second separation operation necessitates however the introduction of a second parameter β etc.

Hence, at the cost of some algebraic manipulations, it is seen that the equations may always, in principle, be separated at any order of approximation.

Finally, the solution Y of system (1) can be recovered with the inverse transformation

$$Z = T(A)W, \qquad W = T(a)Y, \qquad Y = T^{-1}(a)T^{-1}(A)Z.$$

6. An example

Among the various types of problems which may be dealt with by the previous methods and which will be considered later, we select for the moment the case of two coupled differential equations with coupling terms such that the conditions prescribed by the theorem are not fulfilled. This problem originates from a work of Lane and Lin (1964) who investigated the dipole effect of an electron–atom interaction. In a schematic model of the two states approximation, they obtained from partial wave analysis two coupled Schrödinger equations in which they assumed that the diagonal terms of the potential function matrix (U_{00}, U_{11}) tend to zero exponentially (Seaton 1961) and that the cross terms (U_{01}, U_{10}) have the form A/x^2. The coupled equations are then

$$\left(\frac{d^2}{dx^2} + k_0^2 - \frac{l(l+1)}{x^2}\right)y_0 = \frac{A}{x^2}y_1, \qquad \left(\frac{d^2}{dx^2} + k_1^2 - \frac{l(l+1)}{x^2}\right)y_1 = \frac{A}{x^2}y_0. \tag{20}$$

They solved this system in the near resonance region ($k_0 \simeq k_1$) by use of the resonance distortion method (RDM) which consists of two steps. In the first step, exact resonance ($k_0 = k_1$) is assumed, making the separation of the equations possible,

$$\left(\frac{d^2}{dx^2} - k_0^2 - \frac{l(l+1) \pm A}{x^2}\right)Y_\pm = 0, \qquad Y_\pm = \tfrac{1}{2}(y_0 \pm y_1), \tag{21}$$

and the functions $Y_\pm$ may be expressed in terms of spherical Bessel functions.

In the second step, the functions y_0, y_1 on the right-hand sides of (20) will be replaced by y_0^0, y_1^0 of (21), and the approximation is expected to be good in the near resonance region $k_0 \simeq k_1$.

We wish now to enlarge the same problem by including in the coupling terms a quadrupole interaction f^2/x^4 (f^2 is a parameter) so that the system (20) becomes

$$\left(\frac{d^2}{dx^2}+k_0^2-\frac{l(l+1)}{x^2}\right)y_o=\left(\frac{A}{x^2}+\frac{f^2}{x^4}\right)y_1, \qquad \left(\frac{d^2}{dx^2}+k_1^2-\frac{l(l+1)}{x^2}\right)y_1=\left(\frac{A}{x^2}+\frac{f^2}{x^4}\right)y_0. \quad (22)$$

Clearly in this case, the RDM becomes inadequate because of the presence of the f^2/x^4 term which prevents any complete separation of the equations in the first step. To this end, for example in the near resonance region, results obtained in the case $k_0 \simeq k_1$ presented above appear to be most suitable. We have

$$B(x)=A/x^2+f^2/x^4, \qquad K^2=\tfrac{1}{2}(k_1^2+k_0^2)$$

$$f_1^0(x)=k_{\substack{0\\1}}^2-\frac{l(l+1)}{x^2}, \qquad L_\pm^2=\frac{l(l+1)\pm A}{x^2}, \qquad P=\frac{d^2}{dx^2}.$$

Equation (8) may be written as

$$\left(\frac{d^2}{dx^2}+K^2-\frac{L_\pm^2}{x^2}\pm\frac{f^2}{x^4}\right)W_\pm=-\tfrac{1}{2}\Delta k^2 W_\mp. \quad (23)$$

Consider for example the first equation of (23); in performing the three transformations

$$W_+=\sqrt{x}\psi_+, \qquad z=(K/f)^{1/2}x, \qquad z=e^r,$$

we have

$$d^2\psi_+/dr^2+[(L_+^2-\tfrac{1}{4})-2Kf\cosh 2r]\psi_+=\tfrac{1}{2}(f/K)\,e^{2r}\Delta k^2\psi_-. \quad (24)$$

The second equation ($-$sign) of (23) may be obtained in a similar form by replacing f by if'.

Therefore in the resonance condition, the conventional method for the weak coupling case may be applied. For example, if we use the iteration procedure, it may be remarked that the solution of the homogeneous equation

$$d^2\psi^+/dr^2+[(L_+^2-\tfrac{1}{4})+2Kf\cos 2r]\psi_+^0=0$$

can be expressed in terms of the Mathieu functions or Bessel series (see for example Holzwarth 1973) etc.

We close this section with two remarks. If it is true that the RDM is certainly suitable for a very small energy gap ($\Delta k^2 \simeq 0$, near resonance), its legitimacy may be questionable once this quantity grows larger. The present approach then appears more convenient because the solution of equation (24) can be evaluated directly without the intermediate assumption of exact resonance. Furthermore, as Δk^2 increases, one may appeal to the method of separation at first order with the appropriate parameter. The separated equations will be, after simplification,

$$\begin{aligned}&\{d^2/dx^2+K^2-l(l+1)/x^2+\tfrac{1}{2}[(Ak^2)^2+4B^2]^{1/2}\}Z_+=0,\\&\{d^2/dx^2+K^2-l(l+1)/x^2-\tfrac{1}{2}[(\Delta k^2)^2+4B^2]^{1/2}\}Z_-=0,\end{aligned} \quad (25)$$

which may be solved by the conventional Green function method, the Green function being simply expressed as a combination of spherical Bessel and Hankel functions. Note also that the parameter α can be eliminated from these equations but we shall need it in the inverse transformation to obtain the original solution Y ($Y = T^{-1}(a)T^{-1}(A)Z$).

7. Conclusion

A number of improvements in the theory of coupled differential equations have been obtained in this work and will be briefly summarised in the following.

Starting from the theorem which governs the separation of coupled equations, investigations are developed in order to achieve some release on the strictness of the conditions on the coupling functions prescribed by this theorem. In doing so, the range of applications of the theory is decisively enlarged, giving way to promising perspectives in the treatment of the many channel problem.

The discussion on the two cases which were selected and which already cover a large spectrum of situations in practice reveals that the strong coupling problem may indeed almost always be converted into a weak coupling one.

Moreover, a complete separation of the equations may also be performed in principle at any order of approximation.

More generally speaking, the results obtained here are useful in the sense that they can set up a more rational base to approach the problem of coupled differential equations, provide a means to examine this problem from a qualitative point of view, alleviating then the burden of the computational work.

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