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# A variational correction procedure for solving coupled differential equations

M R H Rudge

Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast BT7 1NN, Northern Ireland

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**Abstract.** A variational correction procedure is derived for evaluating the solutions of sets of coupled differential equations. The procedure is compared and contrasted with the Kohn correction method and with perturbation theory; and illustrated by considering a simple exactly soluble problem. The procedure has particular applications in scattering theory.

## 1. Introduction

In a previous paper (Rudge 1980a) a variational procedure for determining multichannel scattering parameters was described, and in a subsequent paper (Rudge 1980b) a variational technique was used to develop asymptotic solutions. Using these methods high accuracy can be achieved by systematically increasing the size of the basis set. For some applications, however, it is more convenient to fix the basis set and to use a variational correction technique to optimise the results that can be obtained with this established basis. One conventional procedure for determining a variational correction is due to Kohn (1948) but, as pointed out by Kato (1950), any asymptotic normalisation of the trial function can be used and there is a different correction belonging to each such arbitrary choice of normalisation. The fact that there are infinitely many 'corrections' and no basis for choosing the best one is a great drawback of the Kohn method. The purpose of the present paper is to derive a correction formula for the solutions of coupled differential equations which does not have this deficiency. The method can be used either to determine the solutions themselves or the scattering parameters directly. It is shown that there is an ambiguity in perturbation theory which is somewhat similar to that of the Kohn variational correction and the three methods, the conventional correction technique, the correction technique derived here and the perturbation results are compared for the case of a simple soluble potential.

The technique described has a number of applications in scattering theory and in particular may be used to find asymptotic solutions.

## 2. Theory

### 2.1. The variational method

Let us consider for example an  $N$ -channel scattering problem and define

$$D_q = \frac{d^2}{dr^2} + k_q^2 - \frac{l_q(l_q + 1)}{r^2} \quad 1 \leq q \leq N \quad (1)$$

and

$$\mathcal{L}_0 = \text{diag}(D_q). \tag{2}$$

A wide variety of scattering processes are described by equations of the form

$$\mathcal{L}_0 \mathcal{F}_\lambda = -\mathbf{V} \mathcal{F}_\lambda = \sum_{p=1}^P r^{-p} \mathbf{v}_p \mathcal{F}_\lambda \tag{3}$$

for large values of the variable  $r$ , where  $\mathcal{F}_\lambda$  is an  $N \times N$  solution matrix, the constant matrices  $\mathbf{v}_p$  are symmetric and  $\mathbf{v}_1 = \text{diag}(-2Z)$ . There are two linearly independent matrices  $\mathcal{F}_\lambda$  and it is convenient to group these and their derivatives into a single matrix  $\mathcal{F}$  defined by

$$\mathcal{F} = \left( \begin{array}{c|c} \mathcal{F}_1 & \mathcal{F}_2 \\ \hline \mathcal{F}'_1 & \mathcal{F}'_2 \end{array} \right). \tag{4}$$

We may normalise the solutions to have a unit Wronskian by choosing the asymptotic forms of  $\mathcal{F}_1$  and  $\mathcal{F}_2$  in the open channels, ( $k_q^2 > 0$ ), to be

$$\mathcal{F}_2 + i\mathcal{F}_1 \underset{r \rightarrow \infty}{\sim} \text{diag}(k_q^{-1/2} \exp i\theta_q) \tag{5}$$

where

$$\theta_q = k_q r - \frac{1}{2} l_q \pi + \eta_q \ln(2k_q r) + \arg \Gamma(l_q + 1 - i\eta_q) \tag{6}$$

and  $\eta_q = Zk_q^{-1}$ . If some channels are closed then, for these values of  $q$ , we can write  $k_q^2 = -K_q^2$  and

$$\begin{aligned} (\mathcal{F}_1)_{qq} &\underset{r \rightarrow \infty}{\sim} N_q (2K_q)^{-1/2} \exp(K_q r - \eta_q \ln r) \\ (\mathcal{F}_2)_{qq} &\underset{r \rightarrow \infty}{\sim} N_q^{-1} (2K_q)^{-1/2} \exp[-(K_q r - \eta_q \ln r)] \end{aligned} \tag{7}$$

where  $\eta_q = ZK_q^{-1}$  and  $N_q$  is arbitrary. If we define

$$\epsilon = \left( \begin{array}{c|c} \mathbf{0} & \mathbf{1} \\ \hline -\mathbf{1} & \mathbf{0} \end{array} \right) \tag{8}$$

then the Wronskian condition can be written

$$\tilde{\mathcal{F}} \epsilon \mathcal{F} = -\epsilon \tag{9}$$

at all values of  $r$ . We may note that, given any  $\mathcal{F}$  which satisfies (9)

$$\mathbf{G} = \mathcal{F} \mathbf{Z} \tag{10}$$

also satisfies (9) provided that

$$\tilde{\mathbf{Z}} \epsilon \mathbf{Z} = \epsilon. \tag{11}$$

Now let

$$\mathcal{F}'_\lambda = \mathcal{F}_\lambda + \delta \mathcal{F}_\lambda \quad \lambda = 1, 2 \tag{12}$$

be trial solution matrices where

$$\delta \mathcal{F}_\lambda(r = R_1) = 0. \tag{13}$$

On defining

$$\mathbf{L}_{\lambda\mu} = \int_{R_0}^{R_1} \tilde{\mathcal{F}}'_\lambda(\mathbf{L}_0 + \mathbf{V}) \mathcal{F}'_\mu \, dr \tag{14}$$

we find, on integrating by parts, that

$$\mathbf{L}_{\lambda\mu} = (\tilde{\mathcal{F}}'_\lambda \delta \mathcal{F}_\mu - \tilde{\mathcal{F}}_\lambda \delta \mathcal{F}'_\mu)_{r=R_0} + \langle \delta \tilde{\mathcal{F}}_\lambda(\mathbf{L}_0 + \mathbf{V}) \delta \mathcal{F}_\mu \rangle \tag{15}$$

where the condition (13) has been used and where the integration of equation (14) is denoted in (15) by brackets.

If we now define

$$\mathbf{L} = \begin{pmatrix} \mathbf{L}_{11} & \mathbf{L}_{12} \\ \mathbf{L}_{21} & \mathbf{L}_{22} \end{pmatrix} \tag{16}$$

then the four results of equation (15) can be combined to give the variational principle

$$\mathbf{L} = -(\tilde{\mathcal{F}} \boldsymbol{\varepsilon} \delta \mathcal{F})_{r=R_0} + \langle \delta \tilde{\mathcal{F}}(\mathbf{L}_0 + \mathbf{V}) \delta F \rangle. \tag{17}$$

where  $F$  comprises the first  $N$  rows of  $\mathcal{F}$ . The importance of (17) is that if a value is assigned to the second-order term then it is possible to solve for  $\mathcal{F}$ . In the Kohn method, wherein one uses a variational principle for only one of the solutions, this is not possible. If we assign the value zero to the second-order term and use a trial matrix which satisfies

$$\tilde{\mathcal{F}}^t \boldsymbol{\varepsilon} \mathcal{F}^t = -\boldsymbol{\varepsilon} \tag{18}$$

then on writing at  $r = R_0$ ,

$$\mathcal{F} = \mathcal{F}^t \mathbf{X} \tag{19}$$

we find from (17) that

$$\mathbf{X} = \mathbf{I} + \boldsymbol{\varepsilon} \mathbf{L}. \tag{20}$$

Reference to equation (11), however, shows that the result (20) is not quite good enough because the Wronskian relation is not satisfied by it; this arises because the proper value of second-order term in (17) is not zero. Equation (11) is satisfied by any matrix  $\mathbf{Z}$  of the form

$$\mathbf{Z} = (\mathbf{I} + \boldsymbol{\varepsilon} \mathbf{Y})(\mathbf{I} - \boldsymbol{\varepsilon} \mathbf{Y})^{-1} \tag{21}$$

provided that

$$\mathbf{Y} = \tilde{\mathbf{Y}}. \tag{22}$$

We therefore obtain a better variational correction if we write  $\mathbf{X}$  in the form (21) and allow it to have the approximate value (20). Since  $\mathbf{L} = \tilde{\mathbf{L}}$  one simple procedure is to replace (20) by

$$\mathbf{X} = (\mathbf{I} + \frac{1}{2} \boldsymbol{\varepsilon} \mathbf{L})(\mathbf{I} - \frac{1}{2} \boldsymbol{\varepsilon} \mathbf{L})^{-1}. \tag{23}$$

A second possibility is to choose

$$\mathbf{X} = (\mathbf{I} + \tanh \frac{1}{2} \boldsymbol{\varepsilon} \mathbf{L})(\mathbf{I} - \tanh \frac{1}{2} \boldsymbol{\varepsilon} \mathbf{L})^{-1} = \exp(\boldsymbol{\varepsilon} \mathbf{L}). \tag{24}$$

If  $|\mathbf{L}|$  is small then there is little difference between (23) and (24) but the latter is more reliable if  $|\mathbf{L}|$  is large and can be approximated by writing

$$\tanh(\frac{1}{2} \boldsymbol{\varepsilon} \mathbf{L}) \approx \frac{1}{4} \boldsymbol{\varepsilon} [(\mathbf{I} + \frac{1}{2} \boldsymbol{\varepsilon} \mathbf{L})^{-1} + (\mathbf{I} - \frac{1}{2} \boldsymbol{\varepsilon} \mathbf{L})^{-1} \mathbf{L}]. \tag{25}$$

Suppose that at  $r = R_0$   $N$  solution vectors  $\mathcal{F}_0$  have been calculated which satisfy the boundary condition that they are regular at the origin. Then at  $r = R_0$  there exist matrices  $\mathbf{A}_i$  such that

$$\mathcal{F}_0 \mathbf{A}_0 = \mathcal{F} \begin{pmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \end{pmatrix}. \tag{26}$$

If there are  $N_0$  open channels we may choose  $\mathbf{A}_1$  to be

$$\mathbf{A}_1 = \begin{pmatrix} N_0 \mathbf{I}_{N_0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \tag{27}$$

and the leading  $N_0 \times N_0$  block of  $\mathbf{A}_2$  is the  $\mathbf{K}$  matrix of scattering theory.

The accuracy of the calculation can be systematically improved without changing the basis size by using intermediate values of  $r$ , say  $r_j$ , where  $R_0 \leq r_j \leq R_1$ . The  $\mathbf{K}$  matrix can then be compared with its previous value and the number of intermediate steps increased until the desired accuracy is attained. The variational correction method can thus be made as accurate as is needed without changing the basis size.

The choice of trial functions can be made in a variety of ways. If we define  $\phi_\lambda$  by

$$\mathcal{L}_0 \phi_\lambda = 0 \tag{28}$$

and

$$\Phi = \begin{pmatrix} \phi_1 & \phi_2 \\ \phi_1' & \phi_2' \end{pmatrix} \tag{29}$$

where  $\tilde{\Phi} \epsilon \Phi = -\epsilon$ , then perhaps the simplest choice is to write

$$\mathcal{F}^t = \Phi \alpha \tag{30}$$

and  $\alpha$  is chosen to satisfy the boundary conditions at  $r = R_1$ .

### 2.2. Perturbation theory

It is interesting to compare the variational procedure with a perturbation approach to the problem. Let

$$\mathbf{F} = (\mathcal{F}_1 \vdots \mathcal{F}_2) \tag{31}$$

and write equation (3) in the form

$$\mathcal{L}_0 \mathbf{F} = -\mu \mathbf{V} \mathbf{F} \tag{32}$$

where  $\mu$  is a parameter. If we write

$$\mathbf{F} = \sum_n \mu^n \mathbf{F}^{(n)} \tag{33}$$

then, on equating the coefficients of all powers of  $\mu$  zero, it is found that

$$\begin{aligned} \mathcal{L}_0 \mathbf{F}^{(0)} &= 0 \\ \mathcal{L}_0 \mathbf{F}^{(n)} &= -\mathbf{V} \mathbf{F}^{(n-1)}. \end{aligned} \tag{34}$$

If  $\phi = (\phi_1 \vdots \phi_2)$  then a Green matrix for the operator  $\mathcal{L}_0$  is given by

$$\mathbf{g}(r, r') = \phi(r) \epsilon \tilde{\phi}(r') u(r' - r) \tag{35}$$

where  $u$  is the unit step function. The solutions of (34) then become

$$\mathbf{F}^{(0)} = \phi \mathbf{X}_0 \tag{36}$$

$$\mathbf{F}^{(n)} = \phi \epsilon \int_r^{R_1} \tilde{\phi}(r') \mathbf{V}(r') \mathbf{F}^{(n-1)}(r') dr' + \phi \mathbf{X}_n \tag{37}$$

where the  $\mathbf{X}_n$  are constant matrices. If the order of approximation is  $N$  and

$$\mathbf{F}_N = \sum_{n=0}^N \mu^n \mathbf{F}^{(n)} \tag{38}$$

then the boundary conditions at  $r = R_1$  are satisfied by  $\mathbf{F}_N$  if

$$\sum_{n=0}^N \mu^n \mathbf{X}_n = \alpha. \tag{39}$$

This does not determine the  $\mathbf{X}_n$  and the usual practice is to make an arbitrary selection, for example,

$$\mathbf{X}_n = \delta_{n0} \alpha. \tag{40}$$

If this choice is adopted then from (37) we get

$$\begin{aligned} \mathbf{F}_1 &= \phi \alpha + \phi \epsilon (\tilde{\alpha})^{-1} \mathbf{L} \\ &= \phi \alpha (\mathbf{I} + \epsilon \mathbf{L}) \end{aligned} \tag{41}$$

and the the first-order perturbation result is identical with that of equation (20).

A more satisfactory choice of the  $\mathbf{X}_n$  can be made by examining

$$\begin{aligned} \mathbf{L}_N &= \langle \tilde{\mathbf{F}}_N (\mathcal{L}_0 + \mu \mathbf{V}) \mathbf{F}_N \rangle \\ &= \mu^{N+1} \langle \tilde{\mathbf{F}}_N \mathbf{V} \mathbf{F}^{(N)} \rangle \\ &= \mu^{2N+1} \langle \tilde{\mathbf{F}}^{(N)} \mathbf{V} \mathbf{F}^{(N)} \rangle + \mu^{N+1} \langle \tilde{\mathbf{F}}_{N-1} \mathbf{V} \mathbf{F}^{(N)} \rangle. \end{aligned} \tag{42}$$

The structure of (42) suggests that  $\mathbf{L}_N$ , the matrix which appears in the variational correction, can be made of order  $\mu^{2N+1}$ , by choosing

$$\langle \tilde{\mathbf{F}}_{N-1} \mathbf{V} \mathbf{F}^{(N)} \rangle = 0. \tag{43}$$

Equation (43) then effects a choice of  $\mathbf{X}_N$ . For example, if  $N = 1$ , it is found that

$$\mathbf{X}_1 = \mathbf{L}_0^{-1} \langle \mathbf{L}'_0 \epsilon \mathbf{L}_0 \rangle \mathbf{X}_0 \tag{44}$$

where

$$\mathbf{L}'_0 = -\tilde{\phi} \mathbf{V} \phi. \tag{45}$$

However, the computation (44) involves a quadrature over  $\mathbf{L}_0(r)$  and, although the accuracy can be much enhanced in this way, this feature is unattractive from the standpoint of rapid computation.

### 3. An illustrative example

The difference between the correction procedure described above, the Kohn correction procedure and conventional perturbation theory can be illustrated by considering an exactly soluble problem.

Let

$$\left(\frac{d^2}{dr^2} + k^2 + \mu\delta(r-R)\right)F(r) = 0. \quad (46)$$

Then the regular solution is

$$F(r) = A\left(\sin kr - \frac{\mu}{k}\sin kR \sin k(r-R)u(r-R)\right) \quad (47)$$

where  $A$  is any constant. The  $K$  matrix is

$$K = \frac{\mu \sin^2 kR}{k - \mu \sin kR \cos kR}. \quad (48)$$

Using conventional perturbation theory we can obtain

$$F(r) = \sum_n \mu^n F^{(n)}(r) \quad (49)$$

where

$$F^{(n)}(r) = k^{-1}[\cos kr \sin kRu(r-R) + \sin kr \cos kRu(R-r)]F^{(n-1)}(R) + X_n \sin kr \quad (50)$$

$$F^{(0)} = X_0 \sin kr.$$

If one makes the choice  $X_n = \delta_{n0}$ , then the  $K$  matrix is

$$K = \frac{\mu \sin^2 kR}{k} \sum_{n=0}^{\infty} \left(\frac{\mu \sin 2kR}{2k}\right)^n. \quad (51)$$

The Born perturbation series then diverges for  $\mu > 2k \operatorname{cosec}(2kR)$ . If on the other hand we chose

$$X_1 = -k^{-1}X_0 \cos kR \sin kR \quad (52)$$

then we obtain the exact wavefunction and exact value of  $K$  in first order.

The essential difficulty of the perturbation theory approach is that one is iterating with a particular choice of Green function and the results depend very significantly on the choice adopted. A similar difficulty occurs in the usual variational correction methods (Kohn 1948, Kato 1950). In these methods let  $F^t$  be a function which satisfies

$$F^t(0) = 0$$

$$F^t \sim \sin(kr + \theta) + \lambda_t \cos(kr + \theta) \quad (53)$$

where  $\theta$  is arbitrary and  $K$  is related to  $\lambda$  by

$$K = \frac{\lambda \cos \theta + \sin \theta}{\cos \theta - \lambda \sin \theta}. \quad (54)$$

The Kohn procedure then gives the result that

$$\lambda \approx \lambda_t + k^{-1} \int_0^{\infty} F^t \mathcal{L} F^t dr. \quad (55)$$

Let us choose for example

$$F^t = \sec \theta \sin kr \quad (56)$$

then (55) becomes

$$\lambda \approx -\tan \theta + \mu k^{-1} \sec^2 \theta \sin^2 kR \quad (57)$$

$$K \approx \frac{\mu k^{-1} \sin^2 kR}{1 - \mu k^{-1} \sin^2 kR \tan \theta}. \quad (58)$$

The normal form of the Kohn correction is the one obtained by choosing  $\theta = 0$  (Kato 1950) and (58) then becomes identical with the first-order perturbation result in (51). Of all the other possible and equally valid choices of  $\theta$ , the value  $\theta = (\frac{1}{2}\pi - kR)$  gives the exact result.

The matrix  $\mathbf{L}$  for this problem using the trial function (30) and  $R_1 = 0$ ,  $R_0 > R$  is

$$\mathbf{L} = -\mu k^{-1} \begin{pmatrix} \sin^2 kR & \frac{1}{2} \sin 2kR \\ \frac{1}{2} \sin 2kR & \cos^2 kR \end{pmatrix}. \quad (59)$$

In this case,  $\exp(\epsilon \mathbf{L}) \equiv \mathbf{I} + \epsilon \mathbf{L}$  and it follows using (19) and (20) that

$$K = \frac{\mu k^{-1} \sin^2 kR}{1 - \mu (2k)^{-1} \sin 2kR}$$

which is the exact result.

#### 4. Concluding remarks

The problem of solving sets of coupled differential equations has been solved by a variational method. The principal result is contained in equation (19) where  $\mathbf{X}$  may be chosen to be given either by (23) or by (24). Which of these is used may affect the rate of convergence but not the final result. The  $\mathbf{K}$  matrix can be determined to within a given accuracy by splitting the range of the calculation.

The method has similarities to that of Kohn (1948) but by solving simultaneously for all the solutions of the set of equations the principal difficulty of the Kohn method—that any asymptotic normalisation can be used—is overcome.

There is also an analogy with perturbation theory, wherein there is a problem closely akin to that of the Kohn variational method in that any Green function can be used and the iteration may converge or diverge according to the choice made.

One problem in which the correction procedure is likely to be useful is that of finding asymptotic solutions of coupled differential equations (Rudge 1984).

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