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On the use of the finite-element method with Lagrange multipliers in scattering theory

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Abstract. It is shown that the use of the finite-element method with Lagrange multipliers in scattering theory is equivalent to the Kohn variational principle. For simple test problems, the convergence of the reactance matrix is found to agree with the predicted behaviour, that is, the error in K_{ij} is proportional to the square of the error of the Lagrange multiplier.

1. Introduction

In recent years there has been some interest in the application of the finite-element method (FEM) to solve scattering problems, see e.g. Shore (1974), Nordholm and Bacskay (1978) or Hendry (1979). The underlying variational principle for FEM requires the boundary conditions to be in the form

$$au(R_1)+b\left.\frac{\mathrm{d}u}{\mathrm{d}r}\right|_{r=R_1}=0$$

where a and b are constants and R_1 is the matching point. This is the form of the boundary conditions in the R-matrix method, and it is thus natural to use FEM to solve the eigenvalue equations in the R-matrix method, as has been done by Shore (1974).

Hendry and Hennell (1977, 1978) modified the Kohn variational principle by adding surface terms to the variational principle, to allow different basis elements to be used in each subregion, which greatly improves the convergence. However, they have to consider the whole space, forcing them to cope with long-range free–free integrals. Further, in order to obtain a Kohn corrected result for the scattering matrix, they need to perform further integrals.

The present method incorporates features from both the above approaches. As in R-matrix theory the space is divided into an outer region where the solution is known and an inner region where it is not. In contrast to the R-matrix method, which solves an eigenvalue problem, here the equations on the inner region are solved using the finite-element method with Lagrangian multipliers (FEML) described by Babuska (1973). When the dimension of the equations is 2 or more (Pitkäranta 1980a, b), detailed error analyses are available, and the K matrix is expected to converge to the optimal value, limited in accuracy only by the accuracy of the asymptotic solution.

The formulation is presented in detail in § 2, where the connection to the Kohn variational principle is shown.

The goal of this project is to solve the partial differential equations obtained by projecting out the angular part of the Schrödinger equation for the scattering of electrons on hydrogenic systems. In order to test the ability of FEML to handle scattering problems, the method was applied to simple one-dimensional potential scattering; this work is described in § 3. Some concluding remarks are in § 4. As results for only ordinary differential equations (ODE's) are presented we restrict the theory to the one-dimensional case. The generalisation will be presented along with results in a subsequent paper.

2. Theory

2.1. The scattering problem

The close-coupling equations for the scattering of an electron on a one-electron target can be written as

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+k_i^2\right)\psi_{ik}(r)=\sum_{j=1}^{N_\mathrm{T}} V_{ij}(r)\psi_{jk}(r)$$

$$i=nl_1l_2LM \qquad i,j=1,\ldots,N_\mathrm{T} \qquad k=1,\ldots,N_1 \tag{2.1a}$$

subject to the boundary conditions

$$\psi_{ik}(0)=0 \tag{2.1b}$$

$$\psi_{ik}(r)\to\begin{cases} k_i^{-1/2}(\delta_{ik}\sin\eta_i+K_{ik}\cos\eta_i) & i=1,\ldots,N_1 \\ k_i^{-1/2}\exp(-|k_i|r)K_{ik} & i=N_1+1,\ldots,N_\mathrm{T}\end{cases} \tag{2.1c}$$

where $V_{ij}(r)$ is the potential, N_1 is the number of open channels ($\varepsilon_i=k_i^2>0$), N_T the total number of channels and

$$\eta_i=k_ir-\tfrac{1}{2}l_i\Pi+\sigma_i$$

is the phase.

Let us define the outer region II by the requirement that the potential $V_{ij}(r)$ can be expanded in powers of r^{-1}. A program to obtain solutions F_{ij} and I_{ij} to (2.1a) in region II subject to asymptotic boundary conditions

$$F_{ji}(r)\to\delta_{ij}k_j^{-1/2}\begin{cases}\sin\eta_j & \varepsilon_j>0\\ \exp(-|k_j|r) & \varepsilon_j<0\end{cases}$$

and

$$I_{ji}(r)\to\delta_{ij}k_j^{-1/2}\begin{cases}\cos\eta_j & \varepsilon_j>0\\ \exp(-|k_j|r) & \varepsilon_j<0\end{cases}$$

has been written by Norcross (1969). Therefore the original problem is reduced to solving (2.1a) on I, the inner region, subject to boundary conditions (2.1b) at $r=0$ and

$$\psi_{ik}(R_1)=\sum_j F_{ij}(R_1)\delta_{jk}+I_{ij}(R_1)K_{jk} \tag{2.1d}$$

at $r=R_1$.

2.2. *Kohn's variational principle* (KVP)

Let the solution $\psi_{ij}(r)$ to (2.1*a*, *b*) be composed of two different functions $u_{ij}(r)$ and $v_{ij}(r)$ such that

$$\psi_{ij}=\begin{cases} v_{ij}(r) & r\leqslant R_1 \\ u_{ij}(r) & r\geqslant R_1 \end{cases}.$$

A possible way to generalise KVP for this type of wavefunction is, as pointed out by Oberoi and Nesbet (1973), to introduce Lagrange multipliers. Their argument, needed in a variational derivation of the R-matrix method, is briefly addressed below.

Consider the functional $\Xi^{(s)}_{mn}=\frac{1}{2}(\Xi_{mn}+\Xi_{nm})$, where Ξ_{mn} is defined as

$$\Xi_{mn}=\sum_{pq}\int \psi_{pm}(r)H_{pq}\psi_{qn}\,\mathrm{d}r-2\sum_{p}(u(r_1)_{pm}-v(r_1)_{pm})\lambda_{pn} \tag{2.2}$$

$$H_{pq}=(\mathrm{d}^2/\mathrm{d}r^2+k_p^2)\delta_{pq}-V_{pq}$$

and λ_{pm} is a Lagrange multiplier introduced to assure continuity across R_1. As the first derivative of ψ_{ij} may be discontinuous, the integral over the first term of H_{pq} reads

$$\int_0^\infty \psi_{pm}\frac{\mathrm{d}^2}{\mathrm{d}r^2}\psi_{pn}\,\mathrm{d}r=\int_0^{R_1} v_{pm}(r)\frac{\mathrm{d}^2}{\mathrm{d}r^2}v_{pn}\,\mathrm{d}r+\int_{R_1}^\infty u_{pm}\frac{\mathrm{d}^2}{\mathrm{d}r^2}u_{pn}\,\mathrm{d}r$$
$$-(v_{pm}(R_1)v'_{pn}(R_1)-u_{pm}(R_1)u'_{pn}(R_1)).$$

On using this and the symmetry of K_{mn} we obtain for small variations of $(\Xi^{(s)}_{mn}-K_{mn})$

$$\delta(\Xi^{(s)}_{mn}-K_{mn})=\sum_{pq}\left(\int_0^{R_1}\delta v_{pm}H_{pq}v_{qn}\,\mathrm{d}r+\int_{R_1}^\infty \delta u_{pm}H_{pq}u_{qn}\,\mathrm{d}r\right)$$
$$+\sum_p \delta v_{pm}(R_1)(\lambda_{pn}-v'_{pn}(R_1))-\sum_p \delta u_{pm}(R_1)(\lambda_{pn}-u'_{pn}(R_1))$$
$$+(m\leftrightarrow n)+\mathrm{O}(\delta\lambda^2+\delta\psi^2+\delta\lambda\delta\psi). \tag{2.3}$$

Choosing u_{pn} to be the exact solution in the outer region and taking $\lambda_{pn}=u'_{pn}(R_1)$, we find the following set of equations must be satisfied for all p in order to obtain a stationary point for $\Xi^{(s)}_{mn}-K_{mn}$:

$$\int_0^{R_1}\delta v_{pm}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+k_p^2\right)v_{pn}\,\mathrm{d}r-\int_0^{R_1}\delta v_{pm}\left(\sum_q V_{pq}v_{qn}\right)\mathrm{d}r+\delta v_{pm}(R_1)(u'_{pn}(R_1)-v'_{pn}(R_1))=0$$
$$\delta v'_{pm}(v_{pn}(r_1)-u_{pn}(r_1))=0. \tag{2.4}$$

It is easily seen that $\Xi^{(s)}_{mn}$ vanishes at the stationary point which implies that K_{mn} is stationary.

2.3. *Finite-element method including Lagrange multipliers* (FEML)

The aim here is to show that Kohn's variational principle as formulated in the previous section arises in a natural way in FEML. If the coefficients K_{jk} in (2.1*d*) were known, FEML, as formulated by Babuska (1973), could be applied directly. For the moment assume K_{jk} to be known and call the boundary function $g(s)$ where s is either R_1 or R_0. Babuska's results, specialised for ODE's, would then read as follows.

The weak solutions ω_i to

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+k^2\right) v_{ik}(r)=\sum_j V_{ij}v_{jk}(r) \qquad r\in[R_0, R_1]$$

$$v_{ik}(r)=g_{ik}(r) \qquad \text{for} \quad r=R_0, R_1$$

create a stationary point for

$$I(v_{ik}, \lambda_{ik})=\int_{R_0}^{R_1}\left[\left(\frac{\mathrm{d}}{\mathrm{d}r}v_{ik}\right)^2-\sum_j V_{ij}v_{ik}v_{jk}+k^2v_{ik}^2\right]\mathrm{d}r$$
$$+2\lambda_{ik}^1(v_{ik}(R_1)-g_{ik}(R_1))-2\lambda_{ik}^0(v_{ik}(R_0)-g_{ik}(R_0)) \tag{2.5}$$

where

$$\lambda_{ik}^1=\left.\frac{\mathrm{d}\omega_{ik}}{\mathrm{d}n}\right|_{R_1}.$$

The above is a trivial result of Green's theorem, while the main point of Babuska's work is to show that the converse is true for certain classes of functions, especially for Hermite cubics (to be defined later). In these cases, the stationary point $(\bar{v}_i, \bar{\lambda}_i)$ satisfies

$$\bar{v}_{ik}\to\omega_{ik}, \qquad \bar{\lambda}_{ik}^0\to -\left.\frac{\mathrm{d}\omega_{ik}}{\mathrm{d}x}\right|_{R_0}, \qquad \bar{\lambda}_{ik}^1\to\left.\frac{\mathrm{d}\omega_{ik}}{\mathrm{d}x}\right|_{R_1}$$

as $M\to\infty$, where M is the size of the basis set (e.g., twice the number of mesh intervals in the Hermite cubic representation discussed below). The Lagrange multiplier λ_{ik} introduced to assure correct boundary behaviour does, in general, depend on the matching point.

For simplicity we assume the trial solutions to be exact at R_0. In this case the term containing the Lagrange multiplier λ_0 disappears and the treatment is equivalent to the normal finite-element method. A treatment at R_0 similar to the one introduced below for R_1 will be discussed in example 3. The functional (2.5) now reads

$$I(v, \lambda)=\int_{R_0}^{R_1}\left[\left(\frac{\mathrm{d}v_{ik}}{\mathrm{d}r}\right)^2-\sum_j V_{ij}v_{ik}v_{jk}+k^2v_{ik}v_{jk}\right]+2\lambda_{ik}(v_{ik}(R_1)-g_{ik}(R_1)).$$

We can make use of the known functional behaviour of v_{ik} (and $\mathrm{d}v_{ik}/\mathrm{d}r$) in the asymptotic region to expand λ_{ik} in such a way that the variational coefficients are independent of R_1. If the function had continuous first derivatives at R_1, we would have

$$\lambda_{ik}^1\to\left.\frac{\mathrm{d}\omega_{ik}}{\mathrm{d}r}\right|_{r=R}=\sum_j\left.\frac{\mathrm{d}S_{ij}}{\mathrm{d}r}\right|_{r=R_1}\delta_{jk}+K_{jk}\left.\frac{\mathrm{d}C_{ij}}{\mathrm{d}r}\right|_{r=R_1} \qquad \text{as } M\to\infty$$

where S_{ij}, C_{ij} are the asymptotic functions. As we can assume the first derivative to be known it seems natural to try for λ_{ik}^1 the form (see (2.1d))

$$\lambda_{ik}^1=\sum_j\left.\frac{\mathrm{d}F_{ij}}{\mathrm{d}r}\right|_{r=R_1}\delta_{jk}+\left.\frac{\mathrm{d}I_{ij}}{\mathrm{d}r}\right|_{r=R_1}a_{jk}.$$

As will be demonstrated in example 3, a_{jk} is nearly independent of R_1.

In order to give up the assumption that K_{ik} is known, we have to introduce N additional conditions, for each k. From (2.4) we see that with the choice

$$a_{ik} = K_{ij}$$

the variational principle is identical to Kohn's variational principle. The importance of this link is that an error analysis is available for FEML, which assures convergence (at least in a statistical sense as is seen in example 3, figure 4(a, b)).

Another possible application of FEML is in connection with the variable phase method of Le Dourneuf and Vo Ky Lan (1977). As this is the subject of a subsequent paper, the method is only briefly outlined. The functions F and I in (2.1d) are now solutions of the asymptotic equations leading to an r-dependent K-matrix $\tilde{K}(r)$. Through the matching between the interior and exterior regions we obtain an initial value for $\tilde{K}$ which is to be integrated outwards until it becomes constant ($\tilde{k}_{ij}(\infty) = K_{ij}$). In practice the trial function for λ^1_{ik} has to be changed to

$$\lambda^1_{ik} = \sum_j \left.\frac{\mathrm{d}S_{ij}}{\mathrm{d}r}\right|_{R_1} \delta_{jk} + K_{jk}(R_1) \left.\frac{\mathrm{d}C_{ij}}{\mathrm{d}r}\right|_{R_1} + \left.\frac{\mathrm{d}K}{\mathrm{d}r}\right|_{R_1} C_{ij}(R_1)$$

where K_{ij} and $\mathrm{d}K_{ij}/\mathrm{d}r$ are variational parameters.

3. Numerical examples

After we have introduced the basis elements we consider three numerical examples, the first two being 'standard' test problems for variational methods. In the first example we see that the resonance behaviour is reproduced well. The second example is included mainly because of the number of papers devoted to this problem, but also because R_1 is well defined and a unique relation exists between step size and number of elements. The third problem has more in common with a realistic scattering problem, in particular the r^{-2} singularity which allows us to test different ways of treating the inner boundary.

3.1. Basis elements

As basis functions we will use the Hermite cubics (see Strang and Fix 1973) defined as follows. Let the region $[0, R_1]$ be covered by a mesh $x_1, x_2, \ldots, x_N$ and define the basis functions $\{\psi_i(x), \omega_i(x)\}$ as piecewise third-order polynomials which are non-zero only on $]x_{i-1}, x_{i+1}[$ and which satisfy

$$\psi_i(x_n) = \delta_{in}, \qquad \left.\frac{\mathrm{d}\psi_i}{\mathrm{d}x}\right|_{x=x_n} = 0 \qquad \omega_i(x_n) = 0, \qquad \left.\frac{\mathrm{d}\omega_i}{\mathrm{d}x}\right|_{x=x_n} = \delta_{in}. \tag{3.1}$$

(The use of the symbol ψ_i for one of the basis functions is standard in finite-element theory. As it is always clear whether a basis function or a wavefunction is in question, we will keep this notation.) Using the same mesh for all channels, we can write the channel function v_{ik} as

$$v_{ik}(x) = \sum_{j=1}^{N} q^{ik}_{2j-1}\psi_j(x) + q^{ik}_{2j}\omega_j(x) \equiv \sum_{\alpha=1}^{2N} q^{ik}_{\alpha}\varphi^{\alpha}(x) \tag{3.2}$$

where $q^{ik}_{2j-1} \to v_{ik}(x_j)$ and $q^{ik}_{2j} \to (\mathrm{d}v_{ik}/\mathrm{d}x)|_{x=x_j}$.

The advantages of using Hermite cubics are that they are very compact, being non-zero over only two intervals (leading to a narrow banded matrix); they exhibit the minimum continuity for a solution to a second-order differential equation, namely C^1; and finally they seem to interpolate bound, as well as free wavefunctions very well. From the error analysis by Babuska (1973) we would expect the solution to converge as h^4, and the first derivative as h^3, where h is the step size. As an estimate of the error in the Lagrange multiplier, we can use the discontinuity in the first derivative at R_1. From (2.3) we see that the expected convergence rate for K is h^6.

3.2. *The Bethe–Bacher (1936) model problem*

Choosing $N_T = 1$ and $V_{11}(r) = 2\,e^{-r}$ we are left with the problem

$$\begin{aligned} &(d^2/dr^2 - 2\,e^{-r} + k^2)u = 0 \\ &u(0) = 0 \\ &u(R_1) = \sin(kR_1) + K_{11}\cos(kR_1) \end{aligned} \tag{3.3}$$

which has the exact solution (in the limit $R_1 \to \infty$)

$$K_{11}^{ex} = -\mathrm{Im}(Q)/\mathrm{Re}(Q)$$

where

$$Q = J_{-2ki}(2\sqrt{2})\frac{(2\sqrt{2})^{2ki}}{\Gamma(1+2ki)},$$

J being a Bessel function. It is well known (see e.g. Truhlar *et al* 1974) that the above problem exhibits pseudoresonances when the Kohn or Rubinov variational methods are used in the energy range [0.1, 1] (Ryd). The solution K_{11}, the relative error $(K_{11} - K_{11}^{ex})/K_{11}^{ex}$ and the determinant are shown in figure 1, and it is seen that no pseudoresonances occur. The true resonance is reproduced reasonably well, with the energy of the resonance in error by ~0.00002 Ryd.

In order to test the convergence a variety of values for N and R_1 was chosen. A typical curve of the error of the K-matrix as a function of the step size is shown in figure 2. The slope of the line is 5.2, somewhat less than the expected value of 6. As expected, when R_1 is too small the converged value of K is erroneous. Truhlar *et al* (1974) also give detailed Kohn-principle results for $k^2 = 0.55$, obtaining much better convergence rates than found here; however the occurrence of pseudoresonances makes their method doubtful at arbitrary energies.

3.3. *Huck (1957) model*

Here we have

$$N_T = 2, \qquad V_{ii} = 0, \qquad V_{ij} = \begin{cases} C, & r<1 \\ 0, & r>0 \end{cases}$$

leading to the coupled equations

$$\left(\frac{d^2}{dr^2} + k_i^2\right)u_{ik} = \begin{cases} Cu_{jk} & r<1 \\ 0 & r>1 \end{cases} \tag{3.4}$$

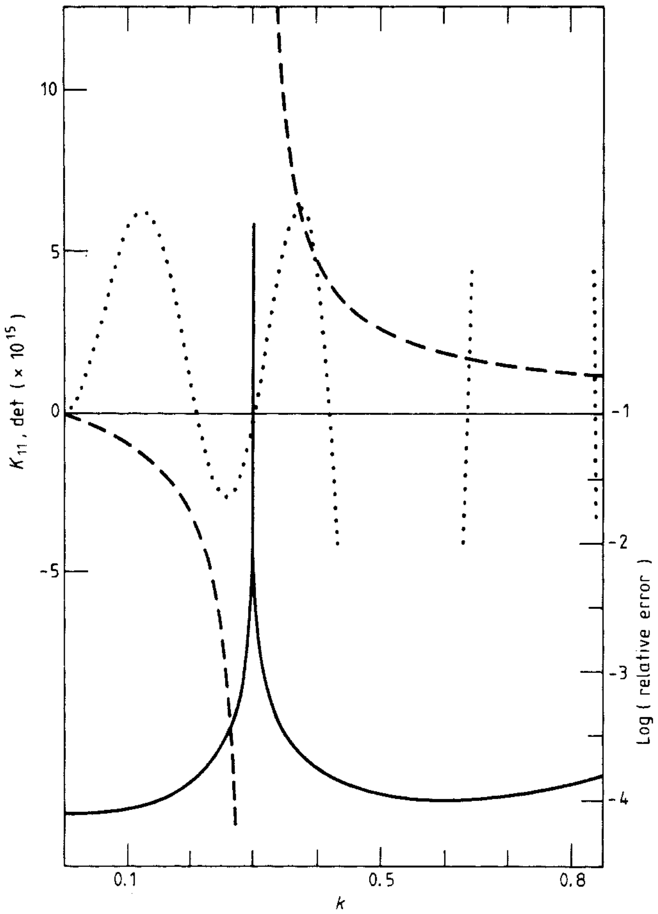

Figure 1. Bethe–Bacher model: – – –, K_{11}; ——, log (relative error of K_{11}); $\cdot\cdot\cdot\cdot$ determinant of matrix to be inverted.

described in detail by Huck (1957). For $C^2 = 10$ the error curve which is plotted in figure 3 as a function of step size shows a slope $\alpha = 5.8$. Because of the well defined values of the domain, inste ₐd of the step size we can use the total number of basis functions as the x axis. Nє bet's (1969, 1978) results using the OAF method are also shown. Recent results by Rudge (1980) using a consistent Kohn method are considerably better than those obtained here, although, in comparing the two methods, it should be noted that a nonlinear parameter had to be determined before the variation procedure was performed.

3.4. Seaton model

We obtain the Seaton model (Seaton 1961) choosing

$$V_{ij} = A/r^2, \qquad V_{ii} = l(l+1)/r^2, \qquad N_{\mathrm{T}} = 2$$

and assuming the same energy in both channels, i.e. we get

$$(\mathrm{d}^2/\mathrm{d}r^2 - l(l+1)/r^2 + k^2)u_{ik} = (A/r^2)u_{jk}. \tag{3.5}$$

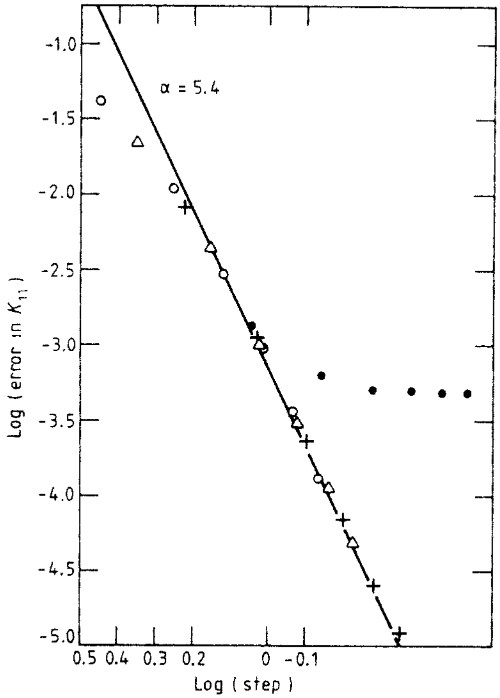

Figure 2. Bethe–Bacher model. Log (relative error in K_{11}) as a function of step size for $R_1 = : 10$, (●); 15, (+); 20, (△) and 25, (○). The slope of the plotted line is 5.4.

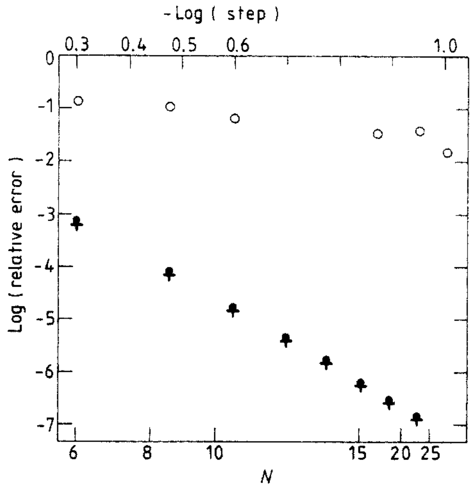

Figure 3. Huck model with $C^2 = 10$: (○), OAF result of Nesbet (1978); (+), present elastic (inelastic) results. The rate of convergence is 5.8.

The exact solution can be written as

$$K_{11} = \tfrac{1}{2}(K_+ + K_-) \qquad K_{21} = \tfrac{1}{2}(K_+ - K_-)$$

where $K_\pm$ is defined as

$$K_\pm = \tan [\![\tfrac{1}{4}\pi\{2l + 1 - [(2l+1)^2 \pm 4A]^{1/2}\}]\!].$$

It is easily seen that exterior solutions $S_{ij}(r)$, $C_{ij}(r)$ can be constructed from $J_{\mu^++1/2}$, $J_{\mu^-+1/2}$, $Y_{\mu^++1/2}$ and $Y_{\mu^-+1/2}$ where

$$\mu^{\pm}=-0.5+[(l+\tfrac{1}{2})^2\pm A]^{1/2}.$$

It is the singularity at $r=0$ which makes this model interesting. There are two ways of treating this singularity: one is to impose zero boundary conditions at some small value R_0; the other is to use Lagrange multipliers as is done at R_1. Inserting a power expansion in (3.3) and using the regularity at zero we obtain a series solution for $u_i(r)$ of the form

$$u_i(r)=A_0r^{q_1}\left(\sum_{j=0}^{\infty}a_jr^j\right)\pm B_0r^{q_2}\left(\sum b_jr^j\right) \tag{3.6}$$

where a_j and b_j are known coefficients. Proceeding as at R_1 we can write the Lagrange multiplier as

$$\lambda_i=\alpha\left(r^{q_1-1}\sum_j (q_1+j)a_jr^j\right)+\beta\left(r^{q_2-1}\sum_j (q_2+j)b_jr^j\right).$$

A third approach is used only for comparison, that is to impose the exact boundary condition at R_0.

The error in the K matrix, the L_2 error of the wavefunction and the discontinuity of the first derivative at R_1 for $l=1$, $A=1.50$ and $R_1=10$ are shown in figure 4(a) for three different values of R_0. The discontinuity of the first derivative approximates the error in the Lagrange multiplier, and it is seen from figure 4(a) that, as expected, the rate of convergence of the K matrix equals the square of the rate of convergence of the Lagrange multiplier. In figure 4(b) are shown the relative error of K_{il} and the L_2 error of u_{il} for $l=1$, $A=1.5$, $R_1=10$ and $N=20$ as continuous functions of R_0. We see that the lack of convergence observed in figure 4(a) for $R_0=10^{-5}$ is associated with the general increase in the error for small R_0. The size of the increase $\Delta\equiv$ error ($R_0=10^{-4}$)-error ($R_0=1$) can be related to the behaviour of the solution at $r=0$ as follows. When the first derivative is singular Δ is fairly large and the convergence for small R_0 therefore poor, whereas Δ is somewhat smaller when the first derivative is regular but the second derivative is singular. In realistic scattering problems, where the solution behaves as r^{l+1}, we expect Δ to vanish, and therefore the results obtained by imposing zero boundary conditions at R_0 should converge. When the exact value is imposed at R_0, the error oscillates around zero implying that the logarithm of the error approaches minus infinity giving rise to the dominant structure in figure 4(b). The same feature is observed for $R_0=0.1$ as N is increased (figure 4(a)).

The procedure is fairly insensitive to the zeros of the outer matching functions, as is seen from figure 5, where the error for $R_0=0.5$ is shown as a function of R_1. The only appreciable effect is found in K_{21}, where a correlation between zeros of $S(x)$ and $C(x)$ and extrema in the error of K_{21} is found.

The convergence for higher l was better than for $l=1$ in the sense that, over a wide range of A values, one could come very close ($<10^{-10}$) to the singularity without any levelling off of the error curve. In particular, this means that one can impose zero boundary conditions at R_0 and obtain results indistinguishable from those obtained imposing the exact boundary conditions or obtained using Lagrange multipliers near the origin.

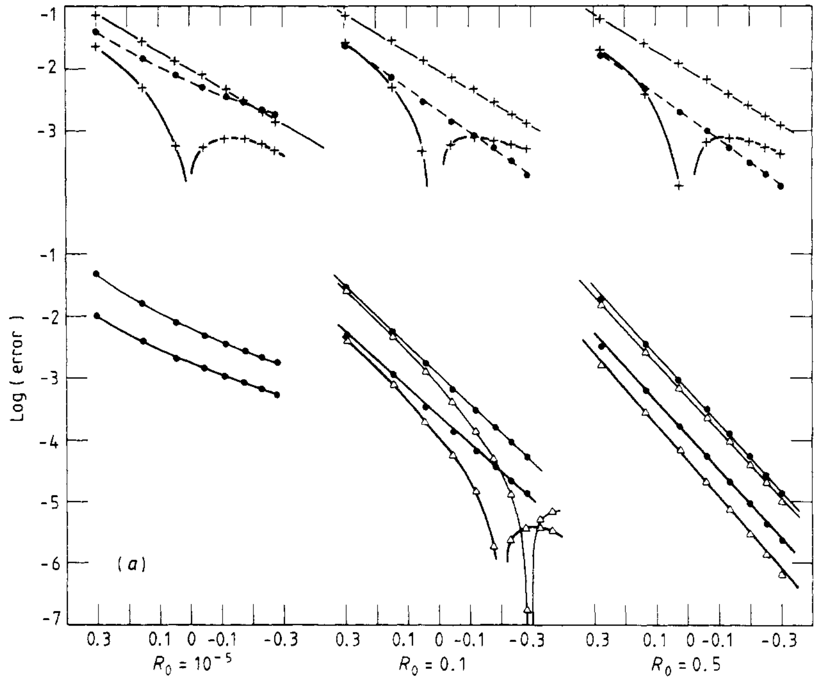

Figure 4(*a*). Seaton model as a function of step size with $l = 1$, $A = 1.5$, $R_1 = 10$ for three different values of R_0. The L_2 error (– · –) and the discontinuity of the first derivative at R_1(– × –), shown on the upper part of the figure, are independent of the treatment of R_0 (zero boundary condition only imposed for $R_0 = 10^{-5}$), therefore only one curve is shown. The lower of the two discontinuity curves corresponds to the inelastic channel, as is also the case for the error in the K matrix shown on the lower part of the figure. Imposing exact boundary conditions at R_0 (△) and using Lagrange multipliers (●) yield nearly identical results for the K matrix for $R_0 = 10^{-5}$; only one curve is shown. The slopes are approximately: 3 (discontinuity); 4 (L_2 error) and 5.6 (error in K matrix).

4. Conclusion

Calculations of the reactance matrix for simple potential scattering problems using FEML yield very encouraging results. The result for a given problem is rather dependent on parameters such as the accuracy of the basis functions at the matching point (figure 2), and treatment of inner boundary (figure 4(*b*)). Nevertheless, we are sure, for a given set of parameters, to obtain good convergence when the mesh is refined, in the sense that although the error may oscillate around zero its amplitude will decrease as h^a, $a \simeq 6$.

Two different ways of treating the singular region were tried. In the test case here the Lagrange multiplier method was superior. Since the lack of convergence for zero boundary conditions results from the irregularity of the second and third derivatives, one may expect this method to work for realistic scattering problems.

There are two important features of the method. First it combines a well-established numerical method with a variational method, resulting in an increase in the rate of convergence for the scattering matrix. Because of the link to FEML we can be sure that the method will converge. Second, one is allowed to treat the asymptotic region separately.

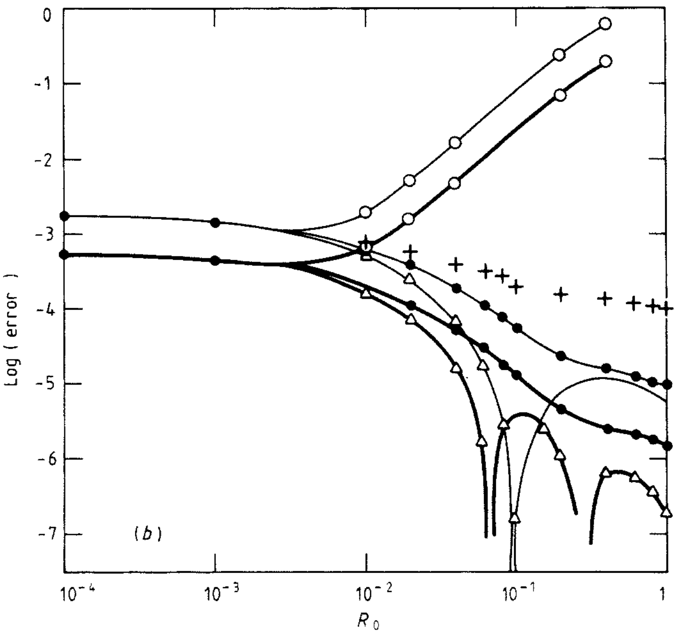

Figure 4(*b*). Seaton model as a function of R_0 with $l = 1$, $A = 1.5$, $R_1 = 10$ and $N = 20$. The symbols are the same as in figure 4(*a*). (○) indicate results obtained on imposing zero boundary conditions at R_0.

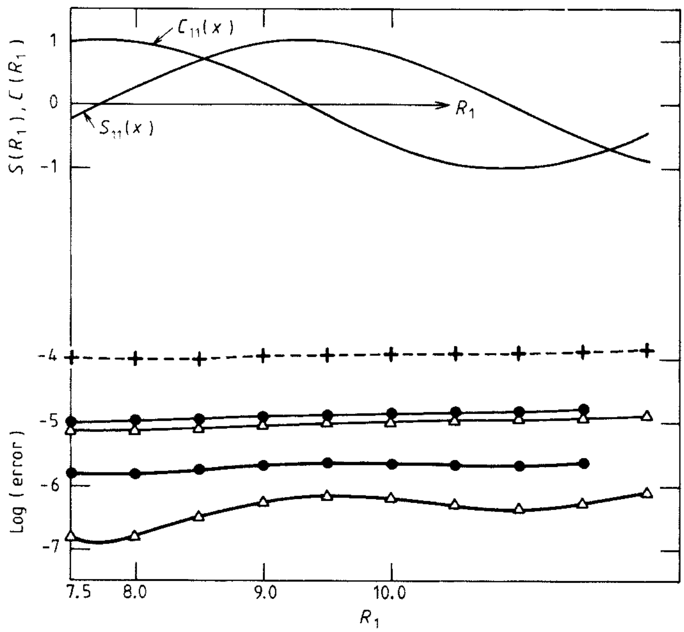

Figure 5. Seaton model with constant step size for $l = 1$, $A = 1.5$, $R_0 = 0.5$, $N = 20, 22, \ldots$. Symbols are the same as in figure 4. The values of the asymptotic basis functions at R_1 are shown on top. The values of $S_{21}(x)$ and $C_{21}(x)$ never exceed 0.1 and are therefore not shown.

At the moment the generalisation of the procedure to two dimensions is under way. It should however be noted that one can also apply this procedure to the close-coupling method; the advantage of the present method being that the integral operator can be included directly instead of being treated by means of an extra equation, as in the non-iterative treatment of *C–C* equations.

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