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1979 J. Phys. A: Math. Gen. 12 771

(http://iopscience.iop.org/0305-4470/12/6/007)

J. Phys. A: Math. Gen., Vol. 12, No. 6, 1979. Printed in Great Britain

A mixed local–global variational approach and its application to a discontinuous potential

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Received 9 August 1978

Abstract. A recently proposed regional variational method is used with a mixture of local and global trial functions to solve the Schrödinger equation for a discontinuous potential. Good results are obtained. In addition, it is illustrated how known features of the solution may be included in a conventional finite-element method, and the resulting equations solved efficiently.

1. Introduction

Variational methods have become popular for the numerical solution of differential equations. Two implementations have been developed, based on a global (global variational method, GVM; see Mikhlin 1971) or a local (finite-element method, FEM; see Strang and Fix 1973) approach to the trial function choice. In practice, both methods provide satisfactory results for suitably smooth problems, the GVM having the distinct advantage of a fast convergence rate (provided a 'good' choice of trial function is made) while the FEM is well suited for irregular shaped regions. Both methods, however, lead to poor results for problems containing non-smooth behaviour. In such situations it is usual to augment the systematic expansion set (typically orthogonal polynomials in a GVM or piece-wise continuous low-degree polynomials in a FEM) by specially constructed core terms incorporating the features of the non-smooth behaviour. This approach, while apparently attractive, is not without numerical problems due to the presence of two types of term close to the singularity (see Fix *et al* 1973).

Recently, a new variational approach, the global element method, GEM, has been proposed (Delves and Hall, 1976). The GEM tries to retain the good features of both the FEM and GVM. In the GEM, the region under consideration is subdivided into a small number of subregions and a suitable trial function chosen in each subregion. This choice of trial function is simplified by the implicit (rather than explicit, as in the FEM) imposition of suitable continuity conditions across the subregion interfaces. If desired, the boundary conditions may also be treated in an implicit manner.

When a conventional GVM or FEM is used to solve the Schrödinger equation with a discontinuous potential (e.g. square well), a slow convergence rate is obtained (due to the presence of a second-derivative discontinuity in the wavefunction). The convergence rate can be improved by incorporating specially constructed core terms in the trial function as in Hendry and Hennell (1976, referred to as HH1) and Hendry and Hennell (1977). The GEM has also been applied to such a system, using orthogonal

0305-4470/79/060771+09$01.00

polynomials in each subregion, with good results and a very fast (approximately exponential) convergence rate (see Hendry and Hennell 1978, referred to as HH2).

As originally proposed, it was anticipated that a global choice of trial function would be made in each subregion of the GEM. However, this is not necessary. In this paper, a GEM calculation is described with a localised choice of trial functions in one subregion together with a global choice of trial function in subregions where the solution behaviour is known. The linear equations which arise in this case reflect the trial function choice in each subregion and can be solved efficiently by a modification of the scheme proposed by Delves and Phillips (1976).

2. Problem and global element method

2.1. The problem

The s-wave scattering of a two-body system is described by (k^2 is the energy)

$$\mathscr{L}u \equiv \left(-\frac{d^2}{dr^2} + V(r) - k^2\right)u = 0, \qquad r \in [0, \infty]. \tag{2.1a}$$

Asymptotically ($r \to \infty$),

$$u \to F + qG$$

where

$$F = (\sin kr)/k \qquad G = \cos kr \qquad q = (\tan \delta)/k$$

and δ is the scattering phase-shift. Near $r = 0$,

$$u(r) \sim r. \tag{2.1b}$$

In this paper it is assumed that the potential $V(r)$ has a discontinuity at $r = r_c$ and, in particular, use is made of the $^1S_0$ potential of Bressel *et al* (1969), referred to as BKR (see HH1 for a detailed description of this potential). The BKR potential is constant and repulsive for $0 \leqslant r < r_c$ and attractive for $r > r_c$.

2.2. The GEM approach

From the form of the potential V, it is natural to identify three subregions for equation (2.1):

(i) a core region, c, $0 \leqslant r \leqslant r_c$;

(ii) a middle region, m, $r_c \leqslant r \leqslant r_b$;

(iii) a background region, b, where the effects of V are negligible, $r \geqslant r_b$.

In the GEM, equation (2.1) is replaced by the coupled problems

$$\mathscr{L}u_l = 0 \qquad l = \text{c, m, b} \tag{2.2a}$$

subject to the boundary conditions

$$\begin{aligned} u_c &\sim r & r &\to 0 \\ u_b &\sim F + qG & r &\to \infty \end{aligned} \tag{2.2b}$$

and the interface conditions

$$u_c(r_c-)=u_m(r_c+) \qquad u_m(r_b-)=u_b(r_b+)$$
$$u'_c(r_c-)=u'_m(r_c+) \qquad u'_m(r_b-)=u'_b(r_b+) \qquad u'=\mathrm{d}u/\mathrm{d}r. \tag{2.2c}$$

Note that the interface conditions at r_c are exactly the physical conditions for the solution of the Schrödinger equation with a discontinuous potential. It can then be shown (see HH2 for details) that the functional

$$[q_t^{(2)}]=q_t-\int_0^{r_c} w_c\mathscr{L}w_c\,\mathrm{d}r-\int_{r_c}^{r_b} w_m\mathscr{L}w_m\,\mathrm{d}r-\int_{r_b}^{\infty} w_b\mathscr{L}w_b\,\mathrm{d}r$$
$$-(w_cw'_c)_{r=0}-(w_mw'_c-w'_mw_c)_{r=r_c}-(w_bw'_m-w'_bw_m)_{r=r_b} \tag{2.3}$$

is stationary about the solution of equation (2.2*a*) for arbitrary variations in the trial functions w_l without these trial functions satisfying explicitly either the boundary conditions (2.2*b*) or the interface conditions (2.2*c*), but with

$$w_b=F+q_tG+w \qquad w\to 0,\ r\to\infty.$$

Functional (2.3) gives a second-order estimate $q_t^{(2)}$ of the scattering parameter q and is very similar to the conventional Kohn variational principle (referred to as CKVP; see Delves 1973) for equations like (2.1).

Introducing suitable expansion sets $\{h_{l,i}\}$ in each subregion l

$$w_l=\sum_{i=1}^{N_l}\alpha_{l,i}h_{l,i} \qquad l=\mathrm{c},\mathrm{m}$$
$$w_b=F+q_tG+\sum_{i=1}^{N_b}\alpha_{b,i}h_{b,i} \tag{2.4}$$

and finding the stationary value of (2.3) leads to the 4×4 block symmetric matrix equation for the parameters $\alpha_{l,i}$:

$$\begin{bmatrix} \mathbf{L}_{cc} & \mathbf{B}_{cm} & \mathbf{0} & \mathbf{0} \\ \mathbf{B}_{cm}^{T} & \mathbf{L}_{mm} & \mathbf{B}_{mb} & \boldsymbol{B}_{mG} \\ \mathbf{0} & \mathbf{B}_{mb}^{T} & \mathbf{L}_{bb} & \boldsymbol{L}_{bG} \\ \mathbf{0} & \boldsymbol{B}_{mG}^{T} & \boldsymbol{L}_{bG}^{T} & L_{GG} \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha}_c \\ \boldsymbol{\alpha}_m \\ \boldsymbol{\alpha}_b \\ q_t \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ -\boldsymbol{B}_{mF} \\ -\boldsymbol{L}_{bF} \\ \tfrac{1}{2}(1-2L_{GF}) \end{bmatrix}. \tag{2.5}$$

Some typical matrix elements in (2.5) are

$$\mathbf{L}_{bb}\equiv\tfrac{1}{2}\int_{r_b}^{\infty}(h_{b,i}\mathscr{L}h_{b,j}+h_{b,j}\mathscr{L}h_{b,i})\,\mathrm{d}r \qquad i,j=1,\ldots,N_b$$
$$\mathbf{B}_{mb}\equiv\tfrac{1}{2}(h'_{m,i}h_{b,j}-h_{m,i}h'_{b,j})_{r=r_b} \qquad \begin{cases} i=1,\ldots,N_m \\ j=1,\ldots,N_b \end{cases}$$
$$\boldsymbol{L}_{bF}\equiv\tfrac{1}{2}\int_{r_b}^{\infty}(h_{b,i}\mathscr{L}F+F\mathscr{L}h_{b,i})\,\mathrm{d}r \qquad i=1,\ldots,N_b \tag{2.6}$$
$$\boldsymbol{B}_{mF}\equiv\tfrac{1}{2}(Fh'_{m,i}-F'h_{m,i})_{r=r_b} \qquad i=1,\ldots,N_m$$
$$\boldsymbol{\alpha}_l\equiv\alpha_{l,i} \qquad i=1,\ldots,N_l \qquad l=\mathrm{c},\mathrm{m},\mathrm{b}.$$

Similar definitions apply for the remaining quantities in (2.5).

2.3. Choice of trial functions

In subregions c, b, the trial functions are as previously used in HH2:

$$h_c = \begin{cases} \sinh(|p|r) & p^2 > 0 \\ \sin(|p|r) & p^2 < 0 \end{cases} \qquad p^2 = V(\tfrac{1}{2}r_c) - k^2$$
$$h_{b,i} = L_{i-1}(2\beta(r - r_b))\, e^{-\beta r} \qquad i = 1, \ldots, N_b \tag{2.7a}$$

where L_i is a Laguerre polynomial. Note that there is only one trial function in subregion c, the known exact solution. Thus in equation (2.5), L_{cc}, α_c are scalar and $\boldsymbol{B}_{cm}$ is a vector.

In subregion m, a local form of trial function is used. The subregion was first mapped to $x \in [0, M]$, for some suitable integer M, and the trial function written as

$$w_m = \sum_{j=-1}^{M+1} \alpha_{m,j} B_j(x) \tag{2.7b}$$

where B_j is the cubic B-spline centred at $x = j$ and only these portions of the spline lying in $x \in [0, M]$ are relevant (see HH1 for details). In the notation of equation (2.4),

$$N_m = M + 3.$$

2.4. Solution of linear equations

As in the CKVP, equation (2.5) is first reduced to a pair of equations

$$\begin{bmatrix} \mathbf{L}_{cc} & \mathbf{B}_{cm} & \mathbf{0} \\ \mathbf{B}_{cm}^T & \mathbf{L}_{mm} & \mathbf{B}_{mb} \\ \mathbf{0} & \mathbf{B}_{mb}^T & \mathbf{L}_{bb} \end{bmatrix} \begin{bmatrix} a_c & b_c \\ \boldsymbol{a}_m & \boldsymbol{b}_m \\ \boldsymbol{a}_b & \boldsymbol{b}_b \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \boldsymbol{B}_{mF} & \boldsymbol{B}_{mG} \\ \boldsymbol{L}_{bF} & \boldsymbol{L}_{bG} \end{bmatrix} \tag{2.8}$$

where

$$\boldsymbol{\alpha}_l = -(\boldsymbol{a}_l + q_l \boldsymbol{b}_l) \qquad l = c, m, b$$

and

$$q_l = \tfrac{1}{2}(1 - 2L_{GF} + 2\boldsymbol{B}_{mG}^T \cdot \boldsymbol{a}_m + 2\boldsymbol{L}_{bG}^T \cdot \boldsymbol{a}_b)/(L_{GG} - \boldsymbol{B}_{mG}^T \cdot \boldsymbol{b}_m - \boldsymbol{L}_{bG}^T \cdot \boldsymbol{b}_b).$$

For the choice of trial functions (2.7), L_{cc} is scalar and zero, while $\boldsymbol{B}_{cm}$ is a row vector. Thus the solution of (2.8) can be further reduced to

$$\begin{bmatrix} \mathbf{L}_{mm} & \mathbf{B}_{mb} \\ \mathbf{B}_{mb}^T & \mathbf{L}_{bb} \end{bmatrix} \begin{bmatrix} \boldsymbol{a}_{1m} & \boldsymbol{a}_{2m} \\ \boldsymbol{a}_{1b} & \boldsymbol{a}_{2b} \end{bmatrix} = \begin{bmatrix} \boldsymbol{B}_{mF} & \boldsymbol{B}_{cm}^T \\ \boldsymbol{L}_{bF} & \mathbf{0} \end{bmatrix} \tag{2.9a}$$

where

$$\boldsymbol{a}_l = \boldsymbol{a}_{1l} - a_c \boldsymbol{a}_{2l} \qquad l = m, b$$
$$a_c = \boldsymbol{B}_{cm} \cdot \boldsymbol{a}_{1m} / \boldsymbol{B}_{cm} \cdot \boldsymbol{a}_{2m}.$$

(A similar result holds for the equations corresponding to b_c, $\boldsymbol{b}_m$, $\boldsymbol{b}_b$ in (2.8).)

The structure of $\mathbf{B}_{mb}$ can now be exploited to solve efficiently a system of equations like (2.9a). For simplicity, the discussion here is restricted to the single equation

$$\begin{bmatrix} \mathbf{L}_{mm} & \mathbf{B}_{mb} \\ \mathbf{B}_{mb}^T & \mathbf{L}_{bb} \end{bmatrix} \begin{bmatrix} \boldsymbol{d}_m \\ \boldsymbol{d}_b \end{bmatrix} = \begin{bmatrix} \boldsymbol{e}_m \\ \boldsymbol{e}_b \end{bmatrix}. \tag{2.9b}$$

From equation (2.6),

$$\mathbf{B}_{mb} = \tfrac{1}{2}(\mathscr{M}'^{T}\mathscr{B} - \mathscr{M}^{T}\mathscr{B}')$$

where $\mathscr{M}$ and $\mathscr{B}$ are row vectors:

$$\mathscr{M} = \{h_{m,1}, \ldots, h_{m,N_m}\}_{r=r_b} \qquad \mathscr{M}' = \{h'_{m1}, \ldots, h'_{m,N_m}\}_{r=r_b}$$

$$\mathscr{B} = \{h_{b,1}, \ldots, h_{b,N_b}\}_{r=r_b} \qquad \mathscr{B}' = \{h'_{b,1}, \ldots, h'_{b,N_b}\}_{r=r_b}.$$

Hence

$$\begin{bmatrix} \mathbf{0} & \mathbf{B}_{mb} \\ \mathbf{B}_{mb}^{T} & \mathbf{0} \end{bmatrix} = \sum_{i=1}^{4} \sigma_i \boldsymbol{\alpha}_i^{T} \boldsymbol{\beta}_i$$

where

$$\boldsymbol{\alpha}_1 = (\mathscr{M}' \; \mathbf{0}) = \boldsymbol{\beta}_3 \qquad \sigma_1 = \sigma_3 = \tfrac{1}{2}$$

$$\boldsymbol{\alpha}_2 = (\mathscr{M} \; \mathbf{0}) = \boldsymbol{\beta}_4 \qquad \sigma_2 = \sigma_4 = -\tfrac{1}{2}.$$

$$\boldsymbol{\alpha}_3 = (\mathbf{0} \; \mathscr{B}) = \boldsymbol{\beta}_1$$

$$\boldsymbol{\alpha}_4 = (\mathbf{0} \; \mathscr{B}') = \boldsymbol{\beta}_2$$

Thus (2.9*b*) can be rewritten as

$$\begin{bmatrix} \mathbf{L}_{mm} & \mathbf{0} \\ \mathbf{0} & \mathbf{L}_{bb} \end{bmatrix} \begin{bmatrix} \boldsymbol{d}_m \\ \boldsymbol{d}_b \end{bmatrix} = \begin{bmatrix} \boldsymbol{e}_m \\ \boldsymbol{e}_b \end{bmatrix} - \sum_{i=1}^{4} \sigma_i \gamma_i \boldsymbol{\alpha}_i^{T} \tag{2.10}$$

where

$$\gamma_i = \boldsymbol{\beta}_i \cdot \begin{pmatrix} \boldsymbol{d}_m \\ \boldsymbol{d}_b \end{pmatrix}$$

and each γ_i is a scalar.

Provided that the γ_i are known, (2.10) can easily be solved as

$$\begin{aligned} \boldsymbol{d}_m &= \boldsymbol{x}_m - \sigma_1\gamma_1\boldsymbol{y}_m - \sigma_2\gamma_2\boldsymbol{z}_m \\ \boldsymbol{d}_b &= \boldsymbol{x}_b - \sigma_3\gamma_3\boldsymbol{y}_b - \sigma_4\gamma_4\boldsymbol{z}_b \end{aligned} \tag{2.11a}$$

with

$$\begin{aligned} \mathbf{L}_{mm}(\boldsymbol{x}_m\boldsymbol{y}_m\boldsymbol{z}_m) &= (\boldsymbol{e}_m\mathscr{M}'^{T}\mathscr{M}^{T}) \\ \mathbf{L}_{bb}(\boldsymbol{x}_b\boldsymbol{y}_b\boldsymbol{z}_b) &= (\boldsymbol{e}_b\mathscr{B}^{T}\mathscr{B}'^{T}). \end{aligned} \tag{2.11b}$$

The γ_i are found by premultiplying (2.11*a*) by $\mathscr{B}$, etc, to get a 4×4 set of equations

$$\begin{bmatrix} 1 & 0 & \sigma_3\mathscr{B}\cdot\boldsymbol{y}_b & \sigma_4\mathscr{B}\cdot\boldsymbol{z}_b \\ 0 & 1 & \sigma_3\mathscr{B}'\cdot\boldsymbol{y}_b & \sigma_4\mathscr{B}'\cdot\boldsymbol{z}_b \\ \sigma_1\mathscr{M}'\cdot\boldsymbol{y}_m & \sigma_2\mathscr{M}'\cdot\boldsymbol{z}_m & 1 & 0 \\ \sigma_1\mathscr{M}\cdot\boldsymbol{y}_m & \sigma_2\mathscr{M}\cdot\boldsymbol{z}_m & 0 & 1 \end{bmatrix} \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \gamma_4 \end{bmatrix} = \begin{bmatrix} \mathscr{B}\cdot\boldsymbol{x}_b \\ \mathscr{B}'\cdot\boldsymbol{x}_b \\ \mathscr{M}'\cdot\boldsymbol{x}_m \\ \mathscr{M}\cdot\boldsymbol{x}_m \end{bmatrix}. \tag{2.12}$$

Thus the solution of (2.9) can be found by first solving (2.11*b*) for the x, y, z (which merely requires the solution of matrices on the diagonal blocks), and then constructing and solving (2.12) for γ_i to enable the solution to be found using (2.11*a*).

Note that in the present work $\mathbf{L}_{mm}$ is banded while $\mathbf{L}_{bb}$ is full, and hence the solution of (2.11*b*) can be performed with a suitable equation solver for each subregion.

The procedure outlined here is based on that given by Delves and Phillips (1976). For the more general case when $\mathbf{L}_{cc}$ and $\mathbf{B}_{cm}$ are matrices, an analogous procedure can be carried out on $\mathbf{B}_{cm}$, resulting in the inversion of matrices only on the diagonal blocks.

3. Results and discussion

3.1. Present results

The results from the method outlined in §§ 2.2 and 2.3 are shown in figure 1. The subregion m was linearly mapped,

$$r = \left(\frac{r_b - r_c}{M}\right)x + r_c,$$

and a suitable choice for r_b was found to be $r_b = 3r_c$. For convenience $M = 2N_b$, there

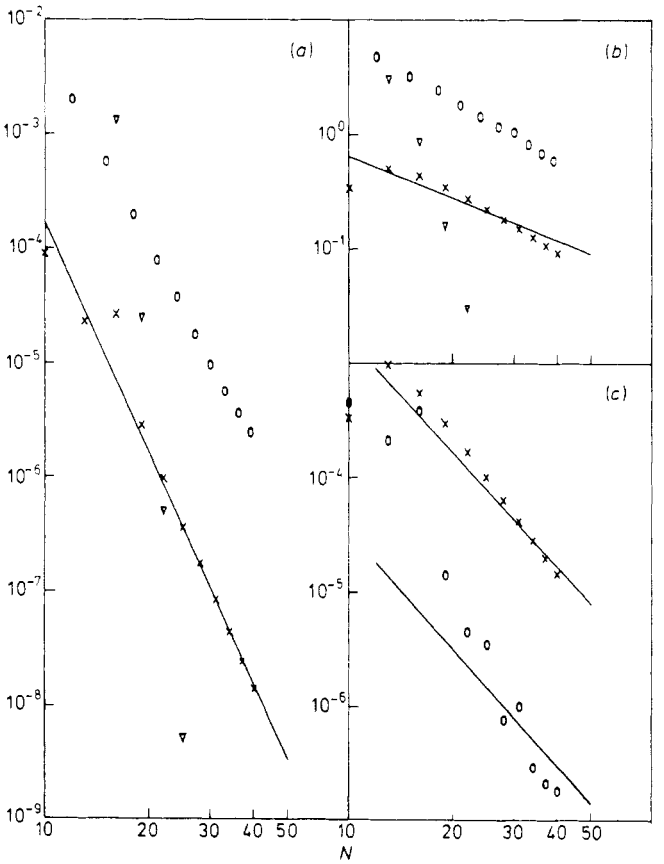

Figure 1. (*a*) Convergence of the computed value $q_r^{(2)}$ to exact value q against total number of variational parameters N. ×, present results; ○, using method of HH1; ▽, using method of HH2. The straight line has gradient −6. (*b*) Convergence of computed value of second-derivative discontinuity D at r_c to the exact value against total number of variational parameters N. The notation is the same as in (*a*) and the straight line has gradient −1. (*c*) Function interface conditions against N. ×, r_c; ○, r_b. The straight lines have gradient −3.

thus being a total of $N = 4 + 3N_b$ variational parameters. The nonlinear parameter β in equation (2.7) had the value 1·5 and $k = 0{\cdot}7$, these being the values used earlier in HH2. Figure 1(*a*) shows the convergence of the second-order estimate $q_t^{(2)}$ to the exact value q (taken from HH2) as a function of N. As N increases, satisfactory convergence is obtained, the convergence rate, as indicated by the gradient of the straight line, being approximately $O(N^{-6})$, i.e. for large N

$$|q_t^{(2)} - q| = CN^{-6} \qquad C = \text{constant}.$$

Figure 1(*b*) shows results for the convergence of the computed second-order derivative discontinuity D at r_c to the exact value (see HH2 for the definition of these quantities). Again, satisfactory convergence is obtained, the rate being approximately $O(N^{-1})$.

These results should be contrasted with those which would be obtained from a CKVP calculation using a continuous trial function. For such calculations for a smooth potential, a convergence rate $O(N^{-6})$ for $q_t^{(2)}$ would be expected, while for a discontinuous potential a significantly lower rate would be obtained. (The results in HH1 would indicate $O(N^{-2})$.) Thus the method outlined in the present paper has enabled the recovery of the $O(N^{-6})$ convergence rate for a discontinuous potential while at the same time reproducing the second-derivative discontinuity present in the solution.

An important feature of the GEM is the implicit imposition of the interface conditions (2.2*c*). Figure 1(*c*) shows the results for the function interface conditions at r_c, r_b. Here the quantities

$$|w_c(r_c-) - w_m(r_c+)| \qquad |w_m(r_b-) - w_b(r_b+)|$$

have been plotted against N. As N increases, both quantities decrease. Furthermore, on either side of the interfaces, the solutions stabilise indicating that the interface conditions are being reproduced. As indicated, the results at r_c are well fitted by a line of gradient -3 but those at r_b would appear to converge somewhat faster (perhaps due to the influence of the global trial functions).

Similar results are obtained for the derivative interface conditions.

3.2. Comparison with previous methods

In HH1 a scheme for including a suitable discontinuous term in a cubic spline basis was described and applied to the binding energy of the BKR potential (via the Rayleigh–Ritz principle). Figure 1 also contains the results from this approach modified to fit into the CKVP. The trial function is then

$$w = \bar{F} + q_t\bar{G} + \sum_{i=0}^{M-2} c_i S_i(x) + b_k Q_k(x)$$

where $\bar{F}$ and $\bar{G}$ satisfy the boundary conditions at $r = 0$ and have the correct asymptotic form F, G. The $S_i(x)$ are combinations of the B-splines satisfying the boundary conditions at $r = 0$ while Q_k is a specially constructed spline having a second-derivative discontinuity at $x = k$. The infinite region $r \in [0, \infty]$ was mapped to $x \in [0, M]$ by

$$r = \alpha x/(M - x),$$

α being chosen so that $x = k$ corresponded to $r = r_c$ and was at a fixed ratio R to the end point $x = M$ (see HH1 for fuller details). The results presented correspond to $R = 3{\cdot}0$, this appearing from experiment to be the optimal value. Again for $q_t^{(2)}$ and D

convergence rates of approximately $O(N^{-6})$ and $O(N^{-1})$ are obtained. However, judged by the criteria of the total number of variational parameters N, these results are inferior to those of § 3.1, being about 100 times less accurate for $q_i^{(2)}$ and about 10 times worse for D.

Figure 1 also shows the results from HH2 for a GEM calculation using global functions everywhere (i.e. Legendre polynomials were used in subregion m). As indicated, very fast (exponential) convergence is obtained. For small N, these are the worst results presented, but for $N \geq 20$ they are significantly better (especially for D). Presumably in both regional methods there are overheads due to the implicit satisfaction of the interface conditions. It is interesting to note that these appear to be less significant for small N when using the spline basis.

3.3. Solution of the linear equations

As indicated in § 2.4, an efficient solution technique (avoiding the direct solution of the full matrix equation (2.8)) is possible. Figure 2 shows the solution times plotted against N_b using

(i) a direct solver (Gauss) on equation (2.8);

(ii) the rank modification scheme of equations (2.11) and (2.12) using a banded solver for $\mathbf{L}_{mm}$ (and a direct solver for $\mathbf{L}_{bb}$).

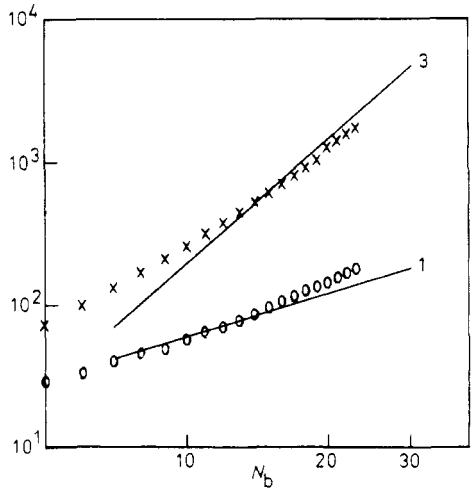

Figure 2. Timings (arbitrary units) for equation solution against N_b. ×, direct method; ○, rank modification method. The straight lines have gradient 3 and 1 as indicated.

As can be seen, the times in (i) grow rapidly and for large N_b approach the $O(N_b^3)$ cost, indicated by the straight line, that would be expected.

The corresponding times for (ii) are much smaller and, over the range of N_b shown, depend linearly on N_b (due to banded solver). Ultimately these times would also rise like N_b^3 since a direct solver was used for $\mathbf{L}_{bb}$. Nevertheless, these timings indicate that there are savings to be obtained by using the rank modification solution scheme. Indeed, further savings could be obtained by using the iterative solver described by Delves and Phillips (1976) for $\mathbf{L}_{bb}$ (with associated cost $O(N_b^2)$).

4. Conclusions

In this paper, it has been demonstrated that a regional variational method (with implicit matching across interfaces) can successfully reproduce the discontinuity present in the solution of the Schrödinger equation with a discontinuous potential. It would also appear that the results are better than those from a conventional approach using cubic splines augmented by a single discontinuous term.

Moreover, a possible method of including known solution features in a FEM calculation (without having two types of trial function in any part of the region) has been indicated. The equations which result from such an approach can be solved by techniques reflecting the structure of the trial function in various subregions. This latter point is important since it permits the extension of existing FEM programs in a relatively straightforward manner.

References

Bressel C N, Kerman A K and Rouben B 1969 *Nucl. Phys.* A **124** 624–36
Delves L M 1973 *Advances in Nuclear Physics* vol 5 eds M Baranger and E Voigt (New York: Plenum)
Delves L M and Hall C A 1976 *J. Inst. Math. Applic.* to appear
Delves L M and Phillips C 1976 *J. Inst. Math. Applic.* to appear
Fix G J, Gulati S and Wakoff G I 1973 *J. Comput. Phys.* **13** 209–28
Hendry J A and Hennell M A 1976 *J. Phys. A: Math. Gen.* **9** 11–8
—— 1977 *J. Phys. A: Math. Gen.* **10** 343–8
—— 1978 *J. Comput. Phys.* **28** 376–94
Mikhlin S G 1971 *The Numerical Performance of Variational Methods* (Amsterdam: Noordhoff)
Strang G and Fix G J 1973 *An Analysis of the Finite Element Method* (New Jersey: Prentice-Hall)