JOURNAL OF COMPUTATIONAL PHYSICS 28, 376–394 (1978)

The Global Element Method Applied to a Discontinuous Nuclear Potential

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Received August 23, 1977

A new variational technique, the Global Element Method (GEM), is applied to a well-known nuclear physics problem. The GEM enables the solution region to be divided into physically meaningful subregions and appropriate expansion functions to be used in each of these subregions. The continuity of the trial functions (and their derivatives) at the subregion interfaces, together with the prescribed boundary conditions is enforced by the variational principle. It is demonstrated that for the bound-state and scattering problems for a typical discontinuous nuclear potential, the GEM obtains significantly faster convergence rates than previous variational methods. Moreover this new approach will enable the major components of existing computer programs, using conventional global variational methods, to be reused after suitable modification. The GEM, with the possibility of high convergence rates, should hopefully prove to be a useful computational tool in many areas of computational physics.

1. INTRODUCTION

Variational methods (or the closely related, but more widely applicable, Galerkin methods) are at present popular numerical techniques for the solution of differential equations. Two practical implementations of these methods have developed. In the finite element approach (FEM), the trial functions are chosen to be nonzero only over a small part (element) of the region under consideration, continuity being imposed explicitly across the interface of each region and convergence being obtained by increasing the number of elements (see, for example, Strang and Fix [1]). Typically, a low-order polynomial, e.g., cubic spline is used as the trial function in a FEM. Alternatively, in the global variational approach (GVM), the trial functions are chosen to exist everywhere in the region of interest and typically, orthogonal polynomials are used, convergence being obtained by increasing the degree of the polynomial (see, for example, Mikhlin [2]).

0021-9991/78/0283-0376$02.00/0

Conventionally in both a GVM and FEM, the trial functions are chosen to explicitly satisfy the essential boundary conditions associated with the differential equation. However, in many circumstances, this constraint can prove inconvenient and it is preferable to work within a variational formalism which does not require this condition on the trial functions. Some attempts along these lines within a FEM can be found in Zienkiewicz [3]. Likewise, within a GVM, attempts to relax the boundary conditions have been made by Arthurs [4], Yates [5], Hennell and Hendry [6] and Davies and Hendry [7]. It should be noted that there are some possible advantages to be obtained from using a GVM in preference to a FEM. There are three main points. Firstly, Delves and Mead [8] have shown that high rates of (asymptotic) convergence can be expected when the GVM is applied to a particular class of problem; in practice the convergence rates obtained are usually much higher than from a FEM using low-order elements. Secondly, the matrices produced in a GVM, though nonsparse are typically much smaller than those from a FEM and efficient iterative techniques (Delves [9]) exploiting the structure of the matrices have been developed to improve on the $O(N^3)$ cost associated with the direct solution of an $N \times N$ matrix. Finally, although difficult to characterize completely, there should be a class of problems for which the GVM is more efficient than a FEM. The GVM is best adapted to relatively simple regions (e.g., squares, circles) for which a natural choice of trial functions can be made, whereas the FEM is best for irregular shaped regions.

Both methods however give poor convergence rates for problems having a solution containing nonpolynomial behavior (e.g., singular derivatives at a reentrant corner, Fix, *et al.* [10], or a discontinuous second derivative at a point, Hendry and Hennell [12, 13]). In these cases it is possible to improve the convergence rate by including in the trial functions core terms (which reproduce the appropriate behavior) in addition to the normal polynomial terms. However a certain amount of caution must be exercised, since the systematic inclusion of core terms (to represent more precisely the nonpolynomial behavior) tends to lead to progressively more ill-conditioned matrices due to the presence of the two types of terms (Fix, *et al.* [10]).

Recently, there has been proposed by Delves and Hall [11] a new variational method, the global element method (GEM). This method attempts to retain the flexibility of the FEM for irregular shaped regions while at the same time retaining the high convergence rate associated with the GVM. In the GEM, the region under consideration is subdivided into a small number of subregions, the choice of these subregions being dictated by the geometry of the region or by the anticipated different solution behavior within the various parts of the region. Within each subregion, a suitable expansion set is chosen, continuity across the interfaces of the subregions being imposed implicitly in the variational functional (using an approach similar to that used in Davies and Hendry [7] to relax the boundary conditions). Note that by this approach it is hoped that terms describing nonpolynomial behavior can be systematically and straightforwardly included without leading to ill-conditioned matrices, since there will only be one type of trial function associated with each subregion.

A somewhat similar regional approach (and variational functional allowing the

implicit imposition of the interface conditions) has previously been proposed in the nuclear engineering field [19, 20]. However the present approach differs significantly in the treatment within each subregion and the present variational functional permits the relaxation (if so desired for convenience) of the essential boundary conditions associated with the differential equation.

In nuclear physics, square well potentials (or more general discontinuous potentials) are often used to describe nuclear forces [12]. As indicated before, if a conventional variational method (either GVM or FEM) is used to solve the Schrödinger equation for such a discontinuous potential, it is found that the obtained convergence rate is very slow due to the second derivative of the true solution containing a discontinuity (see Hendry and Hennell [12, 13]). In [12, 13], this convergence rate was significantly improved by including suitable core terms having an explicit second-order discontinuity at the appropriate point. However, this process of systematically including more core terms to better represent the discontinuity (and hence improve the convergence rate) could not be continued indefinitely since it was found that after a few core terms had been included no significant improvement was obtained [13].

Since the continuity conditions across an interface imposed in the GEM are exactly the physical conditions associated with the solution of the Schrödinger equation for such a discontinuous potential, it is of interest to examine the performance of the GEM to see whether it can reproduce the second-order discontinuity in the wavefunction and at the same time achieve a high convergence rate.

In this paper the GEM is applied to the two-body s-wave system interacting via the potential of Bressel, *et al.* [14], which was previously used in [12, 13]. In Section 2, the GEM is outlined for the bound-state problem and the results from the method presented. Similarly, Section 3 describes the GEM and the results for the scattering problem with the elements being chosen to reflect the regions which arise naturally in this case.

Finally Section 4 contains some conclusions.

2. The Global Element Method Applied to the Bound-State Problem

2.1. *Problem*

We will be concerned with finding the binding energy of the two-body s-wave system

$$\mathscr{H}u(r) = Eu(r) \qquad r \in [0, \infty[, \tag{2.1a}$$

where

$$\mathscr{H} \equiv -\frac{d^2}{dr^2} + V(r) \tag{2.1b}$$

and $V(r)$ is a given (discontinuous) potential.

Associated with Eq. (2.1) are the boundary conditions,

$$\begin{aligned} u(r) &\sim r, \qquad r \to 0, \\ u(r) &\to 0, \qquad r \to \infty. \end{aligned} \tag{2.1c}$$

For future reference, Fig. 1a shows a typical nuclear potential with a discontinuity at $r = r_c$.

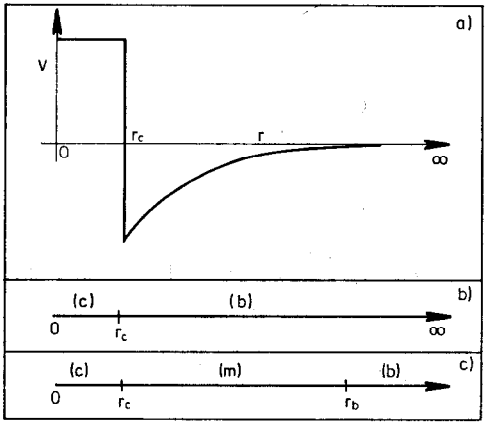

FIG. 1. A typical discontinuous nuclear potential V, showing the elements used in Sections 2 and 3.

2.2. *Global Elements*

The GEM applied to an inhomogeneous second-order elliptic differential equation has previously been described in detail in [11]. For completeness, the modifications required to handle a homogeneous problem and a brief outline of the method are given here.

Referring to Fig. 1a, it is natural to identify two distinct regions for the potential V,

$$\begin{aligned} &\text{(i)} \quad \text{a core region } (c), && 0 \leqslant r \leqslant r_c, \\ &\text{(ii)} \quad \text{a background region } (b), && r_c \leqslant r \leqslant \infty. \end{aligned} \tag{2.2}$$

Accordingly, as indicated in Fig. 1b, we choose to implement the GEM with two elements, these being the regions (b) and (c) in (2.2). Following [11], we then recast Eq. (2.1) as the pair of equations

$$\begin{aligned} \mathscr{H} u_c(r) &= E u_c(r), \qquad 0 \leqslant r \leqslant r_c, \\ \mathscr{H} u_b(r) &= E u_b(r), \qquad r_c \leqslant r \leqslant \infty, \end{aligned} \tag{2.3a}$$

subject to the boundary conditions

$$u_c(r) \sim r, \qquad r \to 0,$$
$$u_b(r) \to 0, \qquad r \to \infty, \tag{2.3b}$$

and the interface conditions,

$$u_c(r_c-) = u_b(r_c+),$$
$$u_c'(r_c-) = u_b'(r_c+), \tag{2.3c}$$

where

$$u' \equiv \frac{du}{dr}.$$

Then, as shown in Appendix I, the functional

$$E_T(w_c, w_b) = \frac{\int_0^{r_c} w_c \mathscr{H} w_c \, dr + \int_{r_c}^{\infty} w_b \mathscr{H} w_b \, dr + (w_c w_c')_{r=0} + (w_b w_c' - w_b' w_c)_{r=r_c}}{\int_0^{r_c} w_c w_c \, dr + \int_{r_c}^{\infty} w_b w_b \, dr} \tag{2.4}$$

is stationary for arbitrary variations in the trial functions w_c, w_b about the true solutions of Eq. (2.3). Note that these trial functions do not exactly satisfy the boundary conditions at $r = 0$ (although they do satisfy these at $r = \infty$) or the interface conditions at $r = r_c$. The variational method will then reproduce the conditions, at $r = 0$, r_c and at the same time approximate the solution in the interior of regions (b) and (c).

We introduce appropriate expansion sets in the two regions

$$w_c = \sum_{i=1}^{N_c} \alpha_{c,i} h_{c,i}(r),$$
$$w_b = \sum_{i=1}^{N_b} \alpha_{b,i} h_{b,i}(r). \tag{2.5}$$

Inserting these expansions into (2.4) and finding the stationary value of the functional leads to the symmetric matrix eigenvalue problem ($\mathscr{H}$ is Hermitian).

$$\begin{pmatrix} \underline{\underline{\mathbf{H}}}_{cc} & \underline{\underline{\mathbf{B}}}_{cb} \\ \underline{\underline{\mathbf{B}}}_{cb}^T & \underline{\underline{\mathbf{H}}}_{bb} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}_c \\ \boldsymbol{\alpha}_b \end{pmatrix} = E_T \begin{pmatrix} \underline{\underline{\mathbf{M}}}_{cc} & \underline{\underline{\mathbf{O}}} \\ \underline{\underline{\mathbf{O}}} & \underline{\underline{\mathbf{M}}}_{bb} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}_c \\ \boldsymbol{\alpha}_b \end{pmatrix} \tag{2.6}$$

Equation (2.6) is a (2 × 2) block-matrix eigenvalue problem and the definitions of the various matrix quanties $\underline{\underline{\mathbf{H}}}_{cc}$, $\underline{\underline{\mathbf{B}}}_{cb}$, etc. are given in Appendix I. As the notation implies, the matrix $\underline{\underline{\mathbf{H}}}_{cc}$ is the matrix of the operator $\mathscr{H}$ in region (c), while the matrix $\underline{\underline{\mathbf{B}}}_{cb}$ is the matrix describing the interface term in functional (2.4). In Eq. (2.5) N_c and N_b can take any suitable values, and thus the matrix $\underline{\underline{\mathbf{B}}}_{cb}$ is not necessarily square.

It should also be noted that the trial functions $h_{c,i}$ and $h_{b,i}$ need not have the same form—rather, they should be chosen to reflect the anticipated solution behavior in the appropriate region.

Finally, as should be apparent from the functional (2.4) and Eq. (2.6), the GEM is very similar in concept to the conventional Rayleigh-Ritz approach—indeed this latter approach can be interpreted (if so desired) as a single element GEM (with no interface conditions).

2.3. *Results*

For a realistic nuclear discontinuous potential we have taken

$$V(r)\begin{cases} = 670 \times 1.4/41.5 & r \leqslant r_c\,, \\ = -1.4 \times 139.4 \times 0.08Z(1 + 8.7Z + 10.6Z^2)/41.5 & r \geqslant r_c\,, \\ r_c = 0.688\,fm \qquad Z = \exp(\mu r)/\mu r & \mu = 1/1.415, \end{cases} \tag{2.7}$$

this being the $^1S_0$ potential of Bressel, *et al.* [14], adjusted by a factor of 1.4 to produce a bound state. From previous work using this potential [12, 13], the value of the binding energy is

$$E = -0.0377155$$

and the exact value of the wavefunction discontinuity at the core $\Delta u'$ is

$$\Delta u' = 36.3816,$$

where

$$\Delta u' = \left(\left[\frac{d^2u}{dr^2}\right]_{r_c+} - \left[\frac{d^2u}{dr^2}\right]_{r_c-}\right)\Big/u(r_c). \tag{2.8}$$

When using global trial functions, it is desirable for stability reasons to use orthogonal polynomials (see Mikhlin [15]). Accordingly, in Eq. (2.5)

$$\begin{aligned} h_{c,i}(r) &\equiv P_{i-1}(2r/r_c - 1) & i &= 1,\ldots, N_c\,, \\ h_{b,i}(r) &\equiv L_{i-1}(2\beta(r - r_c))\, e^{-\beta r} & i &= 1,\ldots, N_b\,, \end{aligned} \tag{2.9}$$

where in (2.9), P_i and L_i are, respectively, Legendre and Laguerre polynomials (see Abramowitz and Stegun [16]). With this choice of trial functions, the boundary condition at $r = 0$ is not satisfied exactly (but that at $r \to \infty$ is) and the normalization matrices $\underline{\underline{\mathbf{M}}}_{cc}$ and $\underline{\underline{\mathbf{M}}}_{bb}$ in Eq. (2.6) are diagonal as desired.

The required matrix elements in (2.6) were evaluated by numerical quadrature, a scaled Gauss–Legendre rule being used in $[0, r_c]$ and a scaled Gauss–Laguerre rule in $[r_c, \infty]$. The results presented here used a 30-point rule in each region, it being found that stable results were produced for sufficiently high-order quadrature rules. The nonlinear parameter β in Eq. (2.9) was set to 1.5 this being the value previously used

in [13]. Figure 2(a) shows the results (plotted on a logarithmic scale) obtained for $|E_N - E|$ where E_N is the estimate of the binding energy for $N = N_c + N_b$ trial functions. Two distinct sets of results are shown for the choices

$$\begin{aligned} &\text{(i)} \quad N_b = N_c, \qquad N = 2N_c, \\ &\text{(ii)} \quad N_b = 2N_c, \qquad N = 3N_c. \end{aligned} \tag{2.10}$$

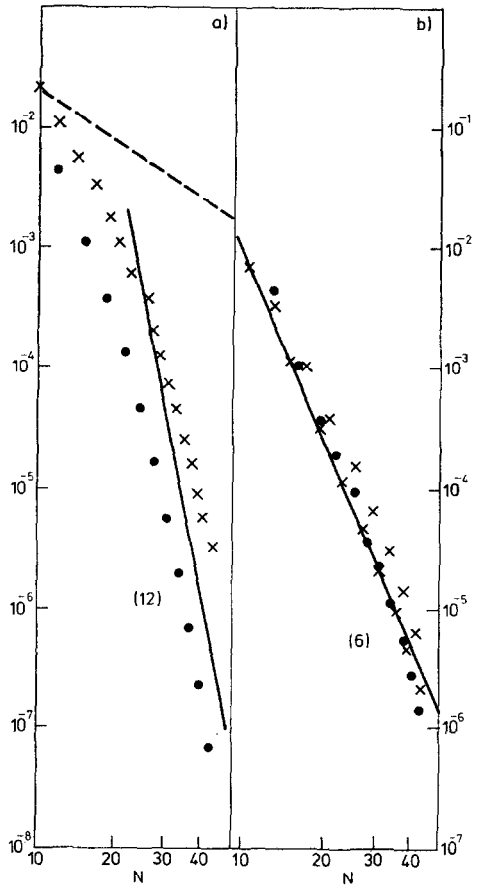

FIG. 2. Results for the bound-state problem of Section 2, in which X indicates $N_b = N_c$ and indicates $N_b = 2N_c$. The gradient of the straight line is indicated thus (G), where G is the asymptotic convergence rate of Section 2.3: (a) $|E_N - E|$ -- results from Ref. [13]; and (b) $|w_c(r_c-) - w_b(r_c+)|$.

As is clear from the graph, both sets of results converge as N increases. However it is also apparent that the results for choice (ii) in (2.10) are much better in the sense that for a total number of trial functions N, more accurate results are obtained. This is not surprising, since the form of the potential (2.7) would lead one to expect the true solution to have a more complicated form in region (b) than in region (c), and

hence require more trial functions to give a good description. Figure 2(a) also shows a straight line which is the best fit (by eye) to both sets of results. The gradient G of this line is a measure of the asymptotic convergence rate, i.e.. for large N.

$$| E_N - E | = (\text{constant})\, N^{-G}.$$

As indicated on the graph, $G \simeq 12$ confirming the hope mentioned in the introduction of achieving high convergence rates in the GEM. For comparison, we have also included on Fig. 2(a) the results obtained in [13] from the conventional R–R approach (with continuous t.f.s.). Clearly there has been a significant improvement. It should also be noted that the GEM here has achieved a convergence rate better than that in [13] even with the inclusion of core terms.

Fig. 2(b) shows the discontinuity in the solution across the interface at r_c

$$\Delta u = | w_c(r_c-) - w_b(r_c+)|$$

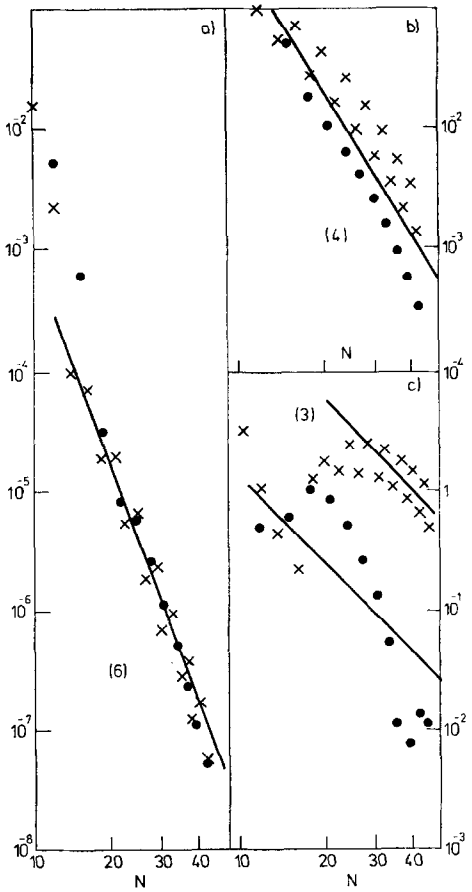

FIG. 3. As Fig. 2: (a) $| w_b(0)|$; (b) $| w_c'(r_c -) - w_b'(r_c +)|$; and (c) D (see Section 2.3).

for a total of N trial functions. Again it is apparent that as N increases, both sets of results are tending to zero, showing that the GEM is indeed reproducing the interface conditions (2.3c). The results for choice (i) in (2.10) display the "double convergence" effect very often seen in global varational methods, but those for (ii) appear to decrease smoothly. Also shown is the best fit line to the results, and from this we deduce an approximate convergence rate $O(N^{-6})$ as might be expected from the result of Fig. 2a. Figure 2b only demonstrates that the discontinuity in the solution decreases as N increases—it should be emphasized that both $w_c(r_c-)$ and $w_b(r_c+)$ separately converge.

Figure 3(a) shows the reproduction of the boundary condition at $r = 0$, i.e., $|\, w_c(0)|$. As N increases, this quantity is tending to decrease, the convergence rate being similar to that obtained for Δu.

The discontinuity in the first derivative at $r = r_c$,

$$\Delta u' = |\, w_c'(r_c-) - w_b'(r_c+)|$$

is shown in Fig. 3b. Comments similar to these for Δu apply in this case, with the exception that the convergence rate is now approximately $O(N^{-4})$.

The results obtained for Δu and $\Delta u'$ are not totally unexpected since the variational functional has been deliberately constructed in order to force these quantities to be continuous across the interface. However, there is no analogous term for the second derivative discontinuity. In order to represent this quantity, we must rely on obtaining a good numerical solution in both regions by systematic increase of the terms in the expansion sets.

Figure 3c shows the quantity

$$D = |\, \Delta w'' - \Delta u''\,|,$$

where $\Delta u''$ is given by (2.8) and $\Delta w''$ is the similar quantity constructed from the numerical solution,

$$\Delta w'' = \left[\left(\frac{d^2 w_b}{dr^2}\right)_{r_c+} - \left(\frac{d^2 w_c}{dr^2}\right)_{r_c-}\right] \Big/ [(w_c(r_c-) + w_b(r_c+))/2].$$

The sets of results in Fig. 3c display a different behavior, but after an erratic start, they tend to decrease for large N. For the results corresponding to choice (i) in (2.10), a reasonable estimate of the convergence rate is $O(N^{-3})$ as shown. However for the choice (ii) in (2.10) no sensible estimate can be obtained, but an $O(N^{-3})$ rate is not totally incompatible with these results.

In the results presented here we have chosen $h_{c,i}$ so that the boundary condition at $r = 0$ is not satisfied exactly. If $h_{c,i}$ is chosen to exactly satisfy this condition, results very similar to those presented here are obtained, the only difference being that they are slightly more accurate for small values of N ($\lesssim 10$).

3. The GEM Applied to a Scattering Problem

3.1. *Problem*

The s-wave scattering of a two-body s-wave system is described by

$$\mathscr{L}u(r) = 0, \qquad 0 \leqslant r \leqslant \infty, \tag{3.1a}$$

where

$$\mathscr{L} \equiv -\frac{d^2}{dr^2} + V(r) - k^2 \tag{3.1b}$$

and k^2 is the energy. As in Section 2, V is a (discontinuous) potential.

Asymptotically ($r \to \infty$),

$$u \to F + qG, \tag{3.1c}$$

where

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

and δ is the scattering phase shift. The boundary condition at $r = 0$ is

$$u(r) \sim r. \tag{3.1d}$$

3.2. *Global Elements*

In this section, we indicate the application of the GEM to a scattering problem. Two elements could be used, but since in the scattering problem it is possible to identify (and to handle simply) a third region, we use three elements by introducing a break point r_b (see Fig. 1c) chosen so that for $r \geqslant r_b$ the potential V is essentially zero.

Thus there are now three regions,

$$\begin{aligned} &\text{(i) a core region (c),} && 0 \leqslant r \leqslant r_c\,; \\ &\text{(ii) a middle region (m),} && r_c \leqslant r \leqslant r_b\,; \\ &\text{(iii) a background region (b),} && r_b \leqslant r \leqslant \infty. \end{aligned} \tag{3.2}$$

Following Section 2.2, we introduce the problems

$$\mathscr{L}u_l = 0 \qquad l = c, m, b, \tag{3.3a}$$

subject to the conditions

$$\begin{aligned} &u_c \sim r, && r \to 0, \\ &u_b \to F + qG, && r \to \infty, \end{aligned} \tag{3.3b}$$

and the interface conditions at r_c and r_b,

$$\begin{aligned} u_c(r_c-) &= u_m(r_c+), \qquad u_m(r_b-) = u_b(r_b+), \\ u_c'(r_c-) &= u_m'(r_c+), \qquad u_m'(r_b-) = u_b'(r_b+). \end{aligned} \tag{3.3c}$$

Then, as is shown in Appendix II, the functional

$$[q_T^{(2)}] = q_T - \int_0^{r_c} w_c \mathscr{L} w_c \, dr - \int_{r_c}^{r_b} w_m \mathscr{L} w_m \, dr - \int_{r_b}^{\infty} w_b \mathscr{L} w_b \, dr$$

$$- (w_c w_c')_{r=0} - (w_m w_c' - w_m' w_c)_{r=r_c} - (w_b w_m' - w_b' w_m)_{r=r_b}$$

is stationary for arbitrary variations in the trial functions about the true solutions of Eq. (3.3) provided that (as in the conventional Kohn Variational Principle, see [17])

$$w_b = F + q_T G + w$$

and $w \to 0$ as $r \to \infty$. Note also that the trial functions neither satisfy the boundary condition at $r = 0$, nor the interface conditions at r_c, r_b. As the notation implies, the functional gives a second-order estimate of the quantity q.

Introducing appropriate expansion sets in the three regions

$$\begin{aligned} w_l &= \sum_{i=1}^{N_l} \alpha_{l,i} h_{l,i}, \qquad l = c, m, \\ w_b &= F + q_T G + \sum_{i=1}^{N_b} \alpha_{b,i} h_{b,i} \end{aligned} \tag{3.4}$$

and finding the stationary value of the functional leads to the equations for the variational parameters $\boldsymbol{\alpha}_l$ ($l = c, m, b$) and q_T,

$$\begin{pmatrix} \underline{\underline{\mathbf{L}}}_{cc} & \underline{\underline{\mathbf{B}}}_{cm} & \underline{\underline{\mathbf{O}}} & \mathbf{O} \\ \underline{\underline{\mathbf{B}}}_{cm}^T & \underline{\underline{\mathbf{L}}}_{mm} & \underline{\underline{\mathbf{B}}}_{mb} & \mathbf{B}_{mG} \\ \underline{\underline{\mathbf{O}}} & \underline{\underline{\mathbf{B}}}_{mb}^T & \underline{\underline{\mathbf{L}}}_{bb} & \mathbf{L}_{bG} \\ \mathbf{O} & \mathbf{B}_{mG}^T & \mathbf{L}_{bG}^T & L_{GG} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}_c \\ \boldsymbol{\alpha}_m \\ \boldsymbol{\alpha}_b \\ q_T \end{pmatrix} = \begin{pmatrix} \mathbf{O} \\ -\mathbf{B}_{mF} \\ -\mathbf{L}_{bF} \\ \tfrac{1}{2}(1 - 2L_{GF}) \end{pmatrix}. \tag{3.5}$$

The definitions of the various quantities in this (4 × 4) block matrix equation are given in Appendix II.

The variational parameters are found by solving the matrix equation (3.5) as indicated in Appendix II. From these values, the second order estimate $q_T^{(2)}$ is found by substitution into the functional.

3.3. *Results*

We again consider the potential of Eq. (2.7). From the detailed form of the potential, it is possible (within a constant) to write down the exact solution in region (c). Accordingly the trial functions were chosen as

$$h_c = \begin{matrix}\sinh(|p|r),\ p^2 \geqslant 0\\ \sin(|p|r),\ p^2 \leqslant 0\end{matrix}\Big\} \quad p^2 = V(r_c/2) - k^2,$$

$$h_{m,i} = P_{i-1}((2r - r_b - r_c)/(r_b - r_c)), \qquad i = 1,\ldots, N_m,$$

$$h_{b,i} = L_{i-1}(2\beta(r - r_b))\, e^{-\beta r} \qquad i = 1,\ldots, N_b,$$

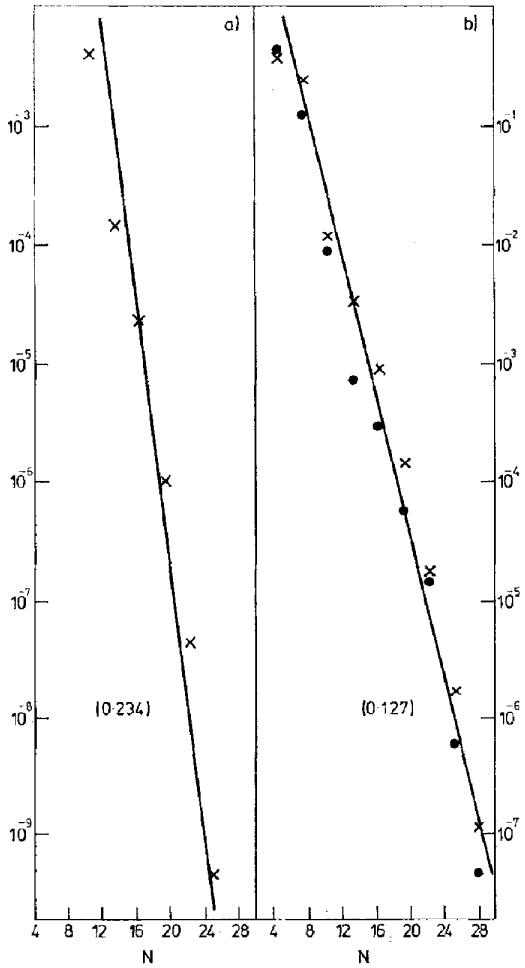

FIG. 4. Results for the scattering problem of Section 3. The gradient of the straight line is indicated (γ), where γ is the (exponential) convergence rate of Section 3.3: in (a) X indicates $|\, q_N^{(2)} - q\,|$; and in (b) X indicates $|\, w_c(r_c -) - w_m(r_c +)|$ and · indicates $|\, w_m(r_b -) - w_b(r_b +)|$.

where L_i, P_i are as in Section 2.3. Note that there is only one trial function in region (c) and that h_c explicitly satisfies the boundary condition at $r = 0$. The results presented below correspond to using the same type of integration rules as in Section 2.2, the parameter β being fixed at the same value as was previously used. The value of k was chosen to be 0.7 (corresponding to an energy of about 20 MeV) and for this value the exact value of the scattering quantity q was taken to be (to eight significant figures)

$$q = 2.9833377.$$

(This value of q was obtained from a previous spline calculation based on the tech-

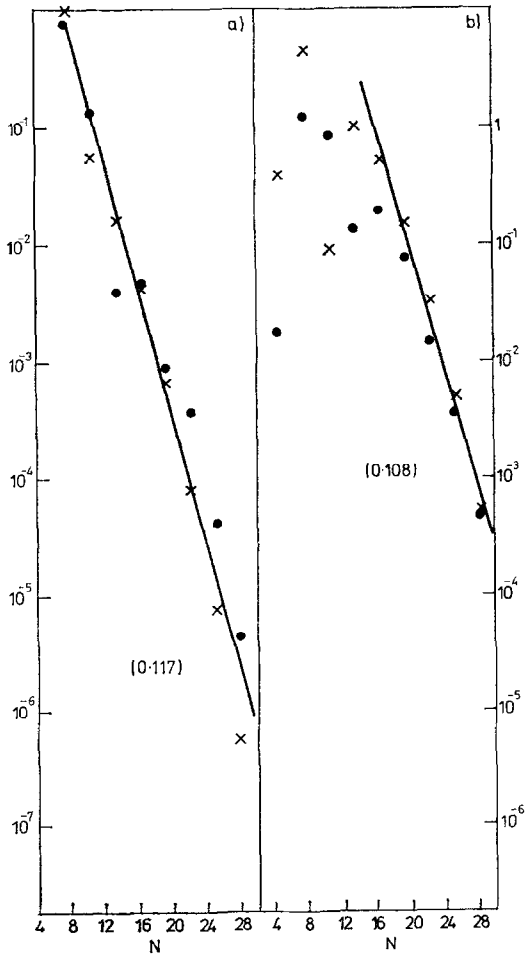

FIG. 5. As for Fig. 4: in (a) X indicates $|w_c'(r_c -) - w_m'(r_c +)|$ and · indicates $|w_m'(r_b -) - w_b'(r_b +)|$; and in (b) X indicates D and · indicates $|w_m''(r_b -) - w_b''(r_b +)|$.

niques used in [12] and confirmed by the results obtained here.) It was also found "best" in practice to set $N_m = 2N_b$ and thus the total number of trial functions is $N = 3N_b + 1$. A suitable value of r_b was taken to be $r_b = 4r_c$.

The results obtained are shown in Fig. 4 and 5. It should be noted that these results have been plotted on a log–linear scale. If the results presented in this section are plotted on a log–log plot (as in Section 2), then the trend of the results has a distinct downward curvature for large N (much more pronounced than in Section 2), indicating the possibility of exponential convergence.

Figure 4a shows the results for

$$| q_N^{(2)} - q |$$

against N, where $q_N^{(2)}$ is the second-order estimate of q produced by the GEM using a total of N trial functions. Clearly satisfactory convergence is obtained. Also shown is the best fit (by eye) line to these results, the gradient γ of this line being indicated on the graph. Note that γ is a measure of the asymptotic convergence rate,

$$| q_N^{(2)} - q | = (\text{Const}) \exp(-\gamma N)$$

Figure 4b shows the corresponding results for the discontinuities in the solution across the two interfaces at r_c and r_b. As N increases, both sets of results are tending to zero, at approximately the same rate (as indicated by the straight line).

Similar remarks apply for the derivative discontinuities shown in Fig. 5a.

Finally Fig. 5b shows the results for the known second derivative discontinuity at r_c (the quantity D defined in Section 2.3 with w_b replaced by w_m) and the discontinuity at r_b

$$| w_m''(r_b-) - w_b''(r_b+)|.$$

After an erratic start ($N \lesssim 12$), both of these sets of results settle down and converge smoothly at a rate as indicated on the graph.

Results, not presented here, for the scattering problem using two elements as in Section 2 were found to have a behavior similar to those obtained earlier in Section 2. There has been a significant improvement, both in the asymptotic convergence rate and in the attained accuracy by the introduction of a third region. This improvement is not due to using the exact solution in $0 \leqslant r \leqslant r_c$, since the results using Legendre polynomials as the expansion set in this region show a behavior very similar to those described in this section (differing only in the number of trial functions being $4N_b$). Hence the improvement must be a reflection of breaking the region into suitable subregions and using appropriate expansion sets within each subregion, in particular, the sinusoidal terms now only contribute in the asymptotic region ($r \geqslant r_b$) where the potential V is essentially zero.

4. Conclusions

In this paper, a recently proposed global variational method has been considered. The results, for the example used, indicate that the method has been successful in achieving, as hoped, a high convergence rate and at the same time reproducing the nonsmooth behavior in the solution. Moreover, the GEM used here has attained a convergence rate significantly higher than previous attempts [12, 13] using a conventional variational method with the inclusion of specially constructed core terms. The results also indicate that by choosing the elements of the GEM to reflect the physics of the problem, an exponential convergence rate can be achieved.

The method is very similar to the conventional GVM in overall concept, and existing computer programs require little adaptation to handle the GEM.

In this paper, we have not been primarily concerned with the efficiency of the GEM from the point of view of the operational cost (i.e., the numerical quadrature required to set up the matrices and the resulting linear equation solution). Rather by considering a one-dimensional problem, for which this cost is not very large, we have concentrated on the convergence rate and the reproduction of the second derivative discontinuity. For a two-dimensional problem, however, a naive implementation of the GEM could lead to a prohibitively large operational count, but recent theoretical developments [18] have indicated how these may be significantly reduced by careful choices of trial functions, elements, quadrature technique, and linear equation solution technique.

Appendix I

Consider the functional

$$E_T(w_c, w_b) = N(w_c, w_b)/D(w_c, w_b)$$

where

$$N(w_c, w_b) = \int_0^{r_c} w_c \mathscr{H} w_c \, dr + \int_{r_c}^{\infty} w_b \mathscr{H} w_b \, dr + (w_c w_c')_{r=0} + (w_b w_c' - w_b' w_c)_{r=r_c}$$

and

$$D(w_c, w_b) = \int_0^{r_c} w_c w_c \, dr + \int_{r_c}^{\infty} w_b w_b \, dr.$$

We expand the trial functions w_c, w_b about the true solutions of Eq. (2.3)

$$w_c = u_c + \epsilon v_c \quad w_b = u_b + \epsilon v_b$$

where ϵ is a scalar and v_c, v_b are arbitrary variations in the appropriate quantity.

Then

$$N(w_c, w_b) = \int_0^{r_c} u_c \mathscr{H} u_c \, dr + \int_{r_c}^{\infty} u_b \mathscr{H} u_b \, dr + (u_c u_c')_{r=0} + (u_b u_c' - u_b' u_c)_{r=r_c}$$
$$+ \epsilon \left\{ \int_0^{r_c} (v_c \mathscr{H} u_c + u_c \mathscr{H} v_c) \, dr + \int_{r_c}^{\infty} (v_b \mathscr{H} u_b + u_b \mathscr{H} v_b) \, dr \right.$$
$$\left. + (v_c u_c' + v_c' u_c)_{r=0} + (v_b u_c' + u_b v_c' - u_b' v_c - v_b' u_c)_{r=r_c} \right\}$$
$$+ \epsilon^2 N(v_c, v_b)$$

Using relations (2.3a) and (2.3b) and inverting the order of integration in the ϵ term lead to

$$N(w_c, w_b) = E \left\{ \int_0^{r_c} u_c u_c \, dr + \int_{r_c}^{\infty} u_b u_b \, dr \right\} + 2\epsilon E \left\{ \int_0^{r_c} u_c v_c \, dr + \int_{r_c}^{\infty} u_b v_b \, dr \right.$$
$$\left. + ((u_c' - u_b')(v_c + v_b) - (u_c - u_b)(v_c' + v_b'))_{r=r_c} \right\} + \epsilon^2 N(v_c, v_b)$$
$$= ED(u_c, u_b) + 2\epsilon E \left\{ \int_0^{r_c} u_c v_c \, dr + \int_{r_c}^{\infty} u_b v_b \, dr \right\} + \epsilon^2 N(v_c, v_b)$$
$$= ED(w_c, w_b) + \epsilon^2 \left\{ \int_0^{r_c} v_c (\mathscr{H} - E) v_c \, dr + \int_{r_c}^{\infty} v_b (\mathscr{H} - E) v_b \, dr \right.$$
$$\left. + (v_c v_c')_{r=0} + (v_b v_c' - v_b' v_c)_{r=r_c} \right\}.$$

Hence

$$E_T(w_c, w_b) = E + O(\epsilon^2).$$

Thus the functional $E_T(w_c, w_b)$ is stationary about the true solution of Eq. (2.3) without requiring that the trial functions w_c, w_b should satisfy the boundary condition at $r = 0$ nor the interface conditions at $r = r_c$.

Introducing suitable expansion sets $h_{c,i}$ and $h_{b,i}$ (see Eq. (2.5)) and finding the resultant stationary value of the functional lead to the block matrix equations.

$$\begin{pmatrix} \underline{\underline{\mathbf{H}}}_{cc} & \underline{\underline{\mathbf{B}}}_{cb} \\ \underline{\underline{\mathbf{B}}}_{cb}^T & \underline{\underline{\mathbf{H}}}_{bb} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}_c \\ \boldsymbol{\alpha}_b \end{pmatrix} = E_T \begin{pmatrix} \underline{\underline{\mathbf{M}}}_{cc} & \underline{\underline{\mathbf{O}}} \\ \underline{\underline{\mathbf{O}}} & \underline{\underline{\mathbf{M}}}_{bb} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}_c \\ \boldsymbol{\alpha}_b \end{pmatrix},$$

where the matrices are given by

$$\underline{\underline{\mathbf{H}}}_{cc} \equiv \frac{1}{2} \left\{ \int_0^{r_c} (h_{c,i} \mathscr{H} h_{c,j} + h_{c,j} \mathscr{H} h_{c,i}) \, dr + (h_{c,i} h_{c,j}' + h_{c,j} h_{c,i}')_{r=0} \right\}, \quad i, j = 1, \ldots, N_c,$$

$$\underline{\underline{\mathbf{H}}}_{bb} \equiv \frac{1}{2}\left\{\int_{r_c}^{\infty} (h_{b,i}\mathscr{H}h_{b,j} + h_{b,j}\mathscr{H}h_{b,i})\, dr\right\}, \qquad i,j = 1,\ldots, N_b\,,$$

$$\underline{\mathbf{B}}_{cb} \equiv \frac{1}{2}\{h'_{c,i}h_{b,j} - h_{c,i}h'_{b,j}\}_{r=r_c}, \qquad j = 1,\ldots, N_b\,,$$

$$\underline{\underline{\mathbf{M}}}_{cc} \equiv \int_0^{r_c} h_{c,i}h_{c,j}\, dr, \qquad i,j = 1,\ldots, N_c\,,$$

$$\underline{\underline{\mathbf{M}}}_{bb} \equiv \int_{r_c}^{\infty} h_{b,i}h_{b,j}\, dr, \qquad i,j = 1,\ldots, N_b\,,$$

$$\boldsymbol{\alpha}_c \equiv \alpha_{c,i}\,, \qquad i = 1,\ldots, N_c\,,$$

$$\boldsymbol{\alpha}_b \equiv \alpha_{b,i}\,, \qquad i = 1,\ldots, N_b\,,$$

$\underline{\underline{\mathbf{O}}} \equiv$ zero matrix of appropriate size.

Appendix II

Consider the functional

$$[q_T^{(2)}] = q_T - \int_0^{r_c} w_c\mathscr{L}w_c\, dr - \int_{r_c}^{r_b} w_m\mathscr{L}w_m\, dr - \int_{r_b}^{\infty} w_b\mathscr{L}w_b\, dr$$

$$- (w_cw'_c)_{r=0} - (w_mw'_c - w_cw'_m)_{r=r_c} - (w_bw'_m - w_mw'_b)_{r=r_b}$$

As in Appendix I, we introduce

$$w_l = u_l + \epsilon v_l \qquad l = c, m, b,$$

where u_l is the solution of Eq. (3.3).

Using the ideas of the rapid derivation of the Kohn Variational Principle given in Delves and the result

$$w_b - u_b = \epsilon v_b \to (q_T - q)G, \qquad r \to \infty,$$

together with the manipulations given in Appendix I, leads to the functional $[q_T^{(2)}]$ being stationary about the true solution of Eq. (3.2) without requiring the trial functions w_l to satisfy the interface conditions. Moreover, $[q_T^{(2)}]$ gives a second order estimate of q,

$$[q_T^{(2)}] = q + O(\epsilon^2)$$

Introducing the expansions for w_l given in Eq. (3.4) and finding the stationary value

of the functional leads to the (4×4) block matrix equation (3.5) for the variational parameters.

The definition of the various quantities in Eq. (3.5) are

$$\underline{\underline{\mathbf{L}}}_{cc} \equiv \frac{1}{2}\left\{\int_0^{r_c} (h_{c,i}\mathscr{L}h_{c,j} + h_{c,j}\mathscr{L}h_{c,i})\,dr + (h_{c,i}h'_{c,j} + h_{c,j}h'_{c,i})_{r=0}\right\}, \qquad i,j = 1,\ldots,N_c,$$

$$\underline{\underline{\mathbf{L}}}_{mm} \equiv \frac{1}{2}\left\{\int_{r_c}^{r_b} (h_{m,i}\mathscr{L}h_{m,j} + h_{m,j}\mathscr{L}h_{m,i})\,dr\right\}, \qquad i,j = 1,\ldots,N_m,$$

$$\underline{\underline{\mathbf{L}}}_{bb} \equiv \frac{1}{2}\left\{\int_{r_b}^{\infty} (h_{b,i}\mathscr{L}h_{b,j} + h_{b,j}\mathscr{L}h_{b,i})\,dr\right\}, \qquad i,j = 1,\ldots,N_b,$$

$$\underline{\underline{\mathbf{B}}}_{pq} \equiv \frac{1}{2}\{(h'_{p,i}h_{q,j} - h_{p,i}h'_{q,j})_{r=r_p}\}, \qquad i = 1,\ldots,N_p, \quad j = 1,\ldots,N_q, \quad pq = cm, mb,$$

$$\mathbf{L}_{bA} \equiv \frac{1}{2}\left\{\int_{r_b}^{\infty} (h_{b,i}\mathscr{L}A + A\mathscr{L}h_{b,i})\,dr\right\}, \qquad i = 1,\ldots,N_b, \quad A = F, G,$$

$$\mathbf{B}_{mA} \equiv \frac{1}{2}\{(Ah'_{m,i} - A'h_{m,i})_{r=r_b}\}, \qquad i = 1,\ldots,N_m, \quad A = F, G,$$

$$L_{AB} \equiv \frac{1}{2}\left\{\int_{r_b}^{\infty} (A\mathscr{L}B + B\mathscr{L}A)\,dr\right\}, \qquad AB = FF, GG, GF,$$

$$\alpha_l \equiv \alpha_{l,i}, \qquad l = c, m, b, \quad i = 1,\ldots,N_l,$$

$O \equiv$ zero matrix or vector of appropriate size.

To solve Eq. (3.5), we introduce the quantities β_l, γ_l, such that

$$\alpha_l = -(\beta_l + q_T\gamma_l) \qquad l = c, m, b$$

and solve the pair of equations

$$\begin{pmatrix} \underline{\underline{\mathbf{L}}}_{cc} & \underline{\underline{\mathbf{B}}}_{cm} & \underline{\underline{\mathbf{O}}} \\ \underline{\underline{\mathbf{B}}}^T_{cm} & \underline{\underline{\mathbf{L}}}_{mm} & \underline{\underline{\mathbf{B}}}_{mb} \\ \underline{\underline{\mathbf{O}}} & \underline{\underline{\mathbf{B}}}^T_{mb} & \underline{\underline{\mathbf{L}}}_{bb} \end{pmatrix} \begin{pmatrix} \beta_c & \gamma_c \\ \beta_m & \gamma_m \\ \beta_b & \gamma_b \end{pmatrix} = \begin{pmatrix} \mathbf{O} & \mathbf{O} \\ \mathbf{B}_{mF} & \mathbf{B}_{mG} \\ \mathbf{L}_{bF} & \mathbf{L}_{bG} \end{pmatrix}$$

from which

$$q_T = \tfrac{1}{2}(1 - 2L_{GF} + 2\mathbf{B}^T_{mG}\cdot\beta_m + 2\mathbf{L}^T_{bG}\cdot\beta_b)/(L_{GG} - \mathbf{B}^T_{mG}\cdot\gamma_m - \mathbf{L}^T_{bG}\cdot\gamma_b).$$

Substitution of q_T and α_l, $l = c, m, b$, into the functional then leads to the second-order estimate $[q_T^{(2)}]$.

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