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Variational methods for discontinuous potentials II. Global trial functions

J A Hendry† and M A Hennell‡

† Computer Centre, University of Birmingham, Birmingham B15 2TT, UK
‡ Department of Computational and Statistical Science, University of Liverpool, Liverpool L69 3BX, UK

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Abstract. When conventional variational trial functions are used to solve systems such as Schrödinger's equation with discontinuous potentials, it is found that the convergence rate is very slow when compared with that for continuous potentials. In a previous paper, the authors demonstrated how this convergence rate could be improved using local variational methods (i.e. finite elements). In this paper we demonstrate the construction of trial functions for global variational methods which results in a very substantial improvement in the obtained convergence rate. The technique, which is numerically stable, is based on orthogonal polynomials with suitable core functions incorporated.

1. Introduction

In a previous paper (Hendry and Hennell 1976, to be referred to as HH), the construction of a suitable variational trial function for use with square-well like potentials was discussed, it being demonstrated that a significant improvement in the convergence rate could be achieved by the inclusion of a suitable discontinuous core term to match the discontinuity in the second derivative of the solution. The variational approach outlined in HH was local in nature (i.e. the finite-element method was used), but an alternative global variational approach exists in which the trial functions used have influence over the whole region of interest. For the reasons outlined in HH, it is of interest to examine whether a similar improved convergence rate can be obtained within the global approach. Any such method should require only small modifications to existing computer codes for complicated problems. In § 2, the variational method and the choice of trial functions is outlined, while § 3 describes the results obtained for the potential of Bressel *et al* (1969) which was used previously in HH. Finally, §§ 4 and 5 contain a discussion of the results and some conclusions.

2. Calculational details

To illustrate the technique involved we restrict ourselves to the problem of finding the binding energy of a two-body s-wave system described by

$$-\frac{d^2u(r)}{dr^2}+V(r)u(r)=Eu(r) \qquad r\in[0,\infty] \tag{2.1}$$

where $V(r)$ is a given (discontinuous) potential. For the bound state, the boundary conditions associated with equation (2.1) are:

$$\begin{aligned} u(r) &\sim r \qquad r \to 0 \\ u(r) &\to 0 \qquad r \to \infty. \end{aligned} \tag{2.2}$$

Furthermore, for a discontinuous potential, $d^2u(r)/dr^2$ is discontinuous at the point r_c at which $V(r)$ has the discontinuity.

To solve the above problem numerically the variational Rayleigh–Ritz procedure was used. As in HH, the variational trial function was expanded as the sum of two types of term, consisting of core terms (to reproduce some particular feature of the solution—in this case the second derivative discontinuity) together with the customary systematic (or background) expansion set. The trial function has the form,

$$\psi_N^{(M)}(r) = \sum_{i=1}^{M} \alpha_{c,i} h_{c,i}(r) + \sum_{i=1}^{N} \alpha_{b,i} h_{b,i}(r) \tag{2.3}$$

where there are M core terms $h_{c,i}$ and N background terms $h_{b,i}$. Thus there are a total of $(M+N)$ variational parameters $\alpha_{l,i}$ ($l = b, c$) in (2.3) to be found by the Rayleigh–Ritz procedure. In this case, the trial functions incorporated the boundary conditions (2.2), so that $h_{c,i}$ and $h_{b,i}$ were taken to have the forms:

$$\begin{aligned} h_{c,i} &= \begin{cases} 0 & r \geqslant r_c \\ (r-r_c)^2 P_{c,i}(r) & r \leqslant r_c \end{cases} \\ h_{b,i} &= P_{b,i}(r)\, e^{-\beta r} \end{aligned} \tag{2.4}$$

where $P_{c,i}$ and $P_{b,i}$ are polynomials in r which are $O(r)$ at the origin and β is an adjustable non-linear parameter.

Note that (2.4) ensures that $h_{b,i}$ and all its derivatives are everywhere continuous, but that the second (and higher) derivatives of $h_{c,i}$ are discontinuous at $r = r_c$. For example, the second-order discontinuity of $h_{c,i}$ is

$$\left[\frac{d^2 h_{c,i}}{dr^2}\right]_{r=r_c+} - \left[\frac{d^2 h_{c,i}}{dr^2}\right]_{r=r_c-} = -2P_{c,i}(r_c).$$

Initially, for simplicity, the monomials were chosen for $P_{c,i}$ and $P_{b,i}$, but this proved to be a bad choice in practice due to the resulting numerical instability. When using a global variational method, it is desirable (for stability reasons) to use an orthogonal set of trial functions (see Mikhlin 1971). Rather than attempt to construct an orthogonal set of trial functions, a somewhat less involved procedure was used which proved to be completely satisfactory in overcoming the numerical instabilities. In this procedure the polynomials were taken to be

$$\begin{aligned} P_{c,i}(r) &= rP_{i-1}^{(4,2)}(2r/r_c - 1), \qquad i = 1, 2, \ldots \\ P_{b,i}(r) &= rL_{i-1}^{(2)}(2\beta r), \qquad i = 1, 2, \ldots \end{aligned}$$

where $P_n^{(l,m)}$ is the Jacobi polynomial of type (l, m) and degree n and $L_n^{(m)}$ is the associated Laguerre polynomial of type m and degree n. (Further details of these functions can be found in Abramowitz and Stegun (1964).) With this choice of

functions, the core terms and the background terms are separately orthogonal (to within a constant), i.e.

$$\int_0^{r_c} h_{c,i}h_{c,j}\,\mathrm{d}r = \delta_{ij} = \int_0^{\infty} h_{b,i}h_{b,j}\,\mathrm{d}r$$

but the core is not orthogonal to the background.

The Rayleigh–Ritz procedure then reduces equation (2.1) to the matrix eigenvalue problem

$$\mathscr{L}\boldsymbol{a} = E\mathscr{N}\boldsymbol{a}$$

where $\mathscr{L}$ and $\mathscr{N}$ are symmetric $(M+N)\times(M+N)$ matrices and $\boldsymbol{a}$ is an $(M+N)$ vector with elements

$$a_k = \begin{cases} \alpha_{c,k} & k \leqslant M \\ \alpha_{b,(k-M)} & M < k \leqslant N+M. \end{cases}$$

Note that the choice of trial functions ensures that the normalization matrix $\mathscr{N}$ has a simple block structure, the two diagonal blocks being themselves diagonal matrices, but the two off-diagonal blocks are full (i.e. non-zero) matrices.

3. Results

The discontinuous potential used to illustrate the technique was the $^1S_0$ realistic nucleon–nucleon potential of Bressel *et al* (1969), modified by a factor of 1·4 to produce a bound state. The detailed form of this potential is given in HH, together with an estimate of the exact value of the binding energy it produces, namely,

$$E = -0{\cdot}0377155.$$

The magnitude of the second-order discontinuity is (from HH)

$$\Delta u'' = \frac{[\mathrm{d}^2u/\mathrm{d}r^2]_{r=r_c+} - [\mathrm{d}^2u/\mathrm{d}r^2]_{r=r_c-}}{u(r_c)} = 36{\cdot}38. \tag{3.1}$$

Figure 1 shows the results obtained for the binding energy from the global variational method outlined in § 2. The required matrix elements were evaluated by numerical quadrature, a scaled Gauss–Legendre rule being used in $[0, r_c]$ with a scaled Gauss–Laguerre rule in $[r_c, \infty]$. The results were stable against these integration rules when sufficiently-high-order Gaussian rules were used. The results quoted here correspond to a thirty-point rule being used in each range, these being indistinguishable from the results obtained with smaller numbers of points. The results in figure 1 are presented for $\beta = 1{\cdot}5$ (see equation (2.4)), this being chosen as the optimal value from runs with a small number of trial functions. The differences $E_N - E$, where E_N is the estimate of the binding energy using N background terms, have been plotted on a logarithmic scale for various numbers of core terms M. Also shown are straight lines which are the best fits (by eye) to the various sets of results. The gradients G of these lines are also given on

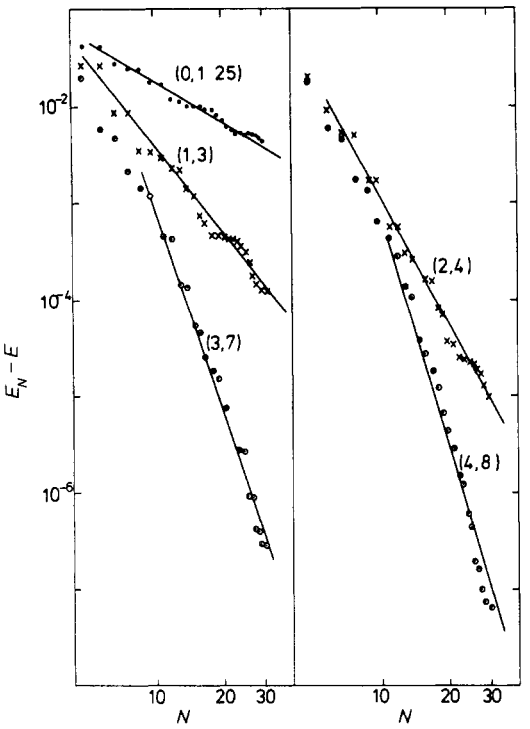

Figure 1. $E_N - E$ against N for various numbers of core terms M. The figures in brackets are (M, G) where G is the asymptotic convergence rate of § 3.

figure 1. Note that this gradient gives the asymptotic convergence rate, i.e. for large N

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

$$\ln (E_N - E) = \text{constant} - G \ln N.$$

It is immediately apparent that for all values of M, the difference $E_N - E$ steadily decreases with increasing N in accordance with the separation theorem for symmetric matrices (Delves 1973). This contrasts with the behaviour in HH where monotonic convergence was only obtained for a sufficiently large number of trial functions.

The results for $M = 0$ (no core terms) confirm the expected slow convergence rate, but with the inclusion of a single core term ($M = 1$) there is an appreciable improvement both in the asymptotic convergence rate and in the absolute errror for the same number of background trial functions. The systematic inclusion of more core terms results in a steady improvement until $M = 4$ is reached where the convegence rate is approximately $O(N^{-8})$. For $M > 4$, satisfactory results are still obtained. However, these have not been included here since it becomes difficult to detect any significant improvement in the convergence rate obtained over the convergence rate for $M = 4$.

Figure 2 shows the results for the discontinuity $\Delta\psi_N^{(M)}$ defined as in (3.1) with u replaced by the trial function $\psi_N^{(M)}$. Again it is apparent that for each value of M, convergence to the exact value is taking place as N increases, the larger-M values producing better approximations than do the smaller-M values. These results confirm the expectation that the core terms can indeed be used to systematically build up better approximations to the discontinuity.

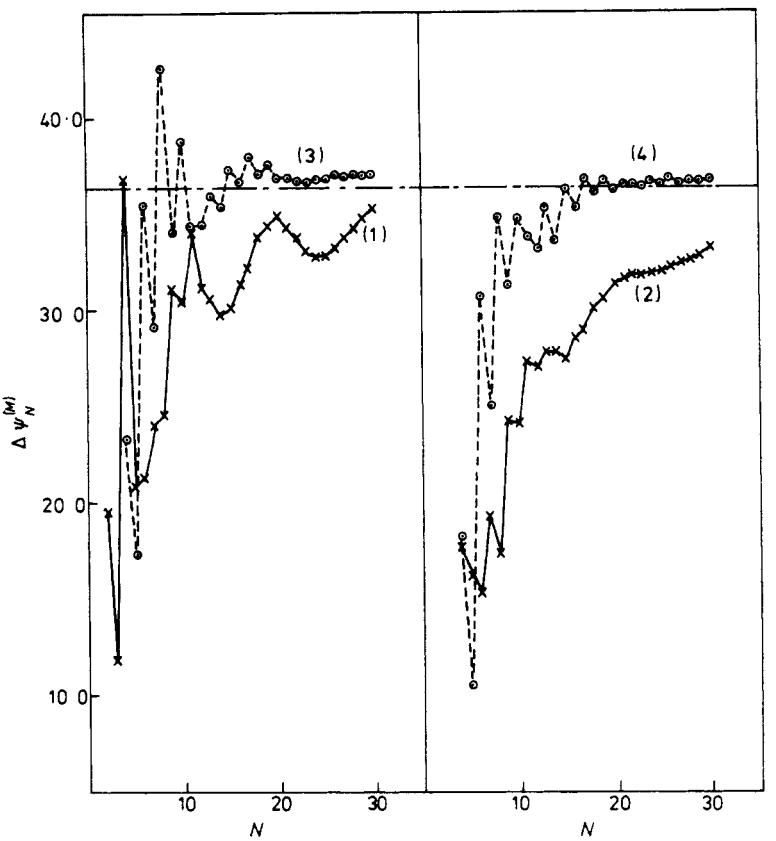

Figure 2. $\Delta\psi_N^{(M)}$ against N for various numbers of core terms M. The figure in brackets is (M); — · — · — exact value.

4. Discussion

The global variational method described here uses a trial function which has second (and higher) derivative discontinuities only at the point r_c. Thus the core terms can permit not only an accurate approximation of the second derivative discontinuity but will also allow the third and higher derivative discontinuities at r_c to be represented.

Yates (1975) has shown that the asymptotic convergence rate to be expected from a variational method depends on the choice of functions in the expansion set and on the lowest derivative discontinuity present in the exact solution. For $M \leqslant 4$, the results obtained here indicate that as the number of core terms M increases, so does the asymptotic convergence rate. Since for each value of M, the background part of the trial function has the same form, it is reasonable to conclude that these improved convergence rates are a reflection of better approximations to the lowest derivative discontinuities.

This behaviour should be contrasted with that found earlier in HH. There the cubic spline approach uses a trial function which has third derivative discontinities not only at r_c but also at the knots defining the spline positions. Hence in this latter approach, the third derivatives of the exact solution can never be approximated everywhere, and the convergence rate achieved is essentially governed by the degree of spline used.

5. Conclusions

In this paper we have demonstrated that the inclusion of a small number of core terms in a global trial function can significantly improve the convergence rate of the method when applied to a discontinuous potential. Moreover, the approach outlined here is easily generalized to a potential consisting of any number of square wells (or indeed more general discontinuous shape) by adding extra core terms based on the appropriate points of discontinuity.

Finally we are not claiming that either the global or piecewise approximation is better. We merely emphasize that existing computer codes (for both types of approximation) should be modified by including a suitable number of core terms to represent the appropriate discontinuities in the solution, in order to achieve adequate convergence rates.

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