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Variational methods for discontinuous potentials

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Abstract. The problem of constructing variational trial functions for potentials such as the Bressel–Kerman–Rouben nucleon–nucleon potential is discussed. It is demonstrated that failure to provide suitable trial functions can result in a serious reduction in the convergence rate. The discontinuity in the trial functions is introduced by means of functions analogous to the *B*-splines. The technique advocated is to construct a core trial function using these functions which may then be used in conjunction with a systematic expansion set.

1. Introduction

There have been a large number of instances of the use of square well-like potentials in nuclear physics calculations (for example within the nuclear three-body problem there are the early calculations of Clapp 1949, Feshbach and Rarita 1949 and, more recently, Fuda 1971 and Kim and Tubis 1971). In few, if any, of these calculations is any cognizance taken of the second derivative of the wavefunction having a discontinuity (this fact follows from the Schrödinger equation since the potential is discontinuous and the wavefunction is continuous). In general this fact is of little interest and can safely be ignored. However, in a variational calculation of any system in which such a potential occurs, it is obviously desirable that the choice of trial function should reflect this property of the exact solution. No variational calculation (known to the authors) using such a potential has incorporated a trial function with a discontinuous second derivative, the reason for this being that the calculations with continuous trial functions converge to the exact solution to arbitrary accuracy. The only disadvantage computationally is that the convergence is somewhat slow, but for the simple systems usually considered this is not a severe disadvantage.

Nevertheless, there is one area in which the slow convergence rate does cause a severe problem. This is within the nuclear three-body problem with realistic potentials where the complexity of the problem makes it desirable to achieve the fastest possible convergence. Hennell and Delves (1972, 1973) and Delves and Hennell (1971) have carried out a series of variational calculations for the three-nucleon system (using typical nuclear potentials) in which the convergence of the calculations has been demonstrated. However, when they tried to use the same techniques on the potential of Bressel *et al* (1969, to be referred to as BKR), the calculations failed, the convergence rate being reduced to such an extent that the calculation was no longer feasible.

The BKR potential consists of a finite square barrier core and an attractive part at interparticle distances greater than the core radius. Thus a two-body system interacting via this potential would have a sizeable discontinuity in the second derivative of the wavefunction at the core radius. The trial functions used by Hennell and Delves did not contain this information about the two-body subsystems and they attributed their failure to this fact.

The variational approach of Hennell and Delves is global in the sense that each term of the trial function has influence everywhere in the region of interest. An alternative local variational approach exists in which each term of the trial function is only non-zero over a well defined portion of the region and hence is referred to as a finite element method. (For an introduction to this method and some recent applications, see Strang and Fix 1973 and Whiteman 1973.) In this paper the finite element method is used with piecewise cubic polynomials to examine the effects of the inclusion of the above mentioned discontinuity in the trial function. (We note that a somewhat similar idea has previously been used in different context by Fix *et al* 1973.)

In §§ 2 and 3 the trial functions are introduced, while in § 4, the method is applied to the realistic discontinuous BKR nuclear potential. Finally, in § 5, some conclusions are given and some comments on the use of such a technique within more complex problems are made.

2. Trial functions

The cubic splines which we shall use are the B-splines of Schoenberg (1946). They are defined in terms of an equidistant mesh on the real line, the mesh points (or knots) being at the integers. We define

$$B_0(x) = \tfrac{1}{4}\begin{cases} 0 & |x| \geqslant 2 \\ (2-|x|)^3 & 2 > |x| \geqslant 1 \\ (2-|x|)^3 - 4(1-|x|)^3 & 1 > |x|. \end{cases}$$

(The definition of the B-spline given in Shore (1973) contains a misprint and should be as quoted above.) Then, as is easily checked, B_0, B_0' and B_0'' vanish outside the range $x \in [-2, 2]$ while within this range they are continuous. Note that B_0''' is discontinuous. If we define B_i by

$$B_i(x) = B_0(x-i)$$

then we see that B_i is the spline centred on the point $x = i$ and so the linear combination

$$\psi(x) = \sum_{i=0}^{N} a_i B_i(x)$$

is (in general) non-zero for $x \in [-2, N+2]$ and ψ, ψ' and ψ'' are continuous at the knots ($x = -2, -1, \ldots, N+2$). However, as stated in the introduction, we wish to allow for the possibility of there being a discontinuous second derivative at a certain point.

Suppose we define

$$Q_0(x) = \tfrac{1}{4}\operatorname{sgn}(x)\begin{cases} 0 & |x| \geqslant 2 \\ (2-|x|)^3 & 2 > |x| \geqslant 1 \\ (2-|x|)^3 - 8(1-|x|)^3 & 1 > |x| \end{cases}$$

where

$$\mathrm{sgn}(x) = x/|x| = \begin{cases} +1 & x > 0 \\ -1 & x < 0. \end{cases}$$

Then, Q_0 and its derivatives vanish outside $x \in [-2, 2]$ but within this range Q_0 and Q_0' are continuous whilst Q_0'' has a discontinuity at $x = 0$, the magnitude of this discontinuity being

$$Q_0''(0-) - (Q_0''(0+) = 18.$$

As before, we define Q_i by

$$Q_i(x) = Q_0(x - i)$$

and we can show that

$$\phi(x) = \sum_{i=0}^{N} a_i B_i(x) + b_k Q_k(x) \qquad 0 \leqslant k \leqslant N$$

is non-zero for $x \in [-2, N+2]$ with ϕ and ϕ' continuous everywhere but ϕ'' has a discontinuity at $x = k$ with magnitude

$$\phi''(k-) - \phi''(k+) = 18 b_k.$$

3. Calculation details

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

$$-\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} + Vu = Eu, \qquad r \in [0, \infty] \tag{3.1}$$

where V is a given potential. For the bound state, the boundary conditions associated with (3.1) are

$$u(r) \sim r, \qquad r \to 0 \tag{3.2}$$

and

$$u(r) \to 0, \qquad r \to \infty. \tag{3.3}$$

Rather than work with the infinite interval $r \in [0, \infty]$, we map this region to a finite interval $x \in [0, M]$, M being a positive integer, by

$$r = f(x) \tag{3.4}$$

where we have explicitly chosen

$$f(x) = \alpha x/(M - x). \tag{3.5}$$

In (3.5), α is a parameter that can be used to position the important part of the r region in the centre of the x region. On applying this transformation to equation (3.1), we have

$$H(x)\psi(x) \equiv \left[-\frac{1}{f'^2}\left(\frac{d^2}{dx^2} - \frac{f''}{f'}\frac{d}{dx}\right) + U(x) \right]\psi(x) = E\psi(x) \tag{3.1a}$$

where

$$\psi(x) = u(f(x))$$

$$U(x) = V(f(x))$$

and the boundary conditions are replaced by

$$\psi(x) \sim x, \qquad x \to 0 \tag{3.2a}$$

$$\psi(x) \to 0, \qquad x \to M. \tag{3.3a}$$

For trial functions we shall use the B-splines defined in § 2. However, before we can use them in a conventional variational method, we must ensure that the prescribed boundary conditions are automatically satisfied. If we define

$$\begin{aligned} S_0(x) &= B_0(x) - \tfrac{1}{4}B_{-1}(x) && 0 \leqslant x \leqslant 2 \\ S_1(x) &= B_1(x) - B_{-1}(x) && 0 \leqslant x \leqslant 3 \\ S_i(x) &= B_i(x) && 2 \leqslant i \leqslant M-2,\ 0 \leqslant x \leqslant M \end{aligned} \tag{3.6}$$

then it is a simple matter to check that the $S_i(x)$ satisfy boundary conditions (3.2a) and (3.3a).

The linear combination

$$\phi(x) = \sum_{i=0}^{M-2} c_i S_i(x) + b_k Q_k(x), \qquad M-2 \geqslant k \geqslant 2 \tag{3.7}$$

has the property that ϕ, ϕ' and ϕ'' are everywhere continuous for $x \in [0, M]$, except at $x = k$ where ϕ'' is discontinuous, and satisfies the boundary conditions (3.2a) and (3.3a). Thus (3.7) is a suitable trial function for use with a discontinuous potential (eg BKR) provided that the transformation (3.4) maps the core radius r_c onto $x = k$.

Shore (1973) has previously considered B-splines in variational calculations but has approached the problem somewhat differently. Rather than work with the infinite interval, he cuts off equation (3.1) at a suitably chosen r_{max} and then maps $r \in [0, r_{max}]$ onto $x \in [0, M]$ by

$$r = S[\exp(S_2 x) - 1], \qquad S_2 = M^{-1} \ln[1 + (r_{max}/S)]$$

S being a free parameter. Thus, there are two parameters r_{max} and S which have to be optimized in some sense. For the (continuous) Coulomb potential, it was found that transformation (3.5), with α suitably chosen, and trial function (3.7) (omitting the Q_k term) gave results as accurate as those of Shore for the same number of trial parameters. Thus we feel that (3.5) is a more attractive choice for the transformation (since it has only one parameter to be adjusted). Furthermore, the same techniques used on a realistic continuous nuclear potential (Reid soft core (Reid 1968), to be referred to as RSC) gave good results, the energy converging to its correct value at a rate $O(N^{-6})$, where N is the number of variational parameters.

This section has been formulated for the case of an s-wave bound state, but the extension to higher angular momentum is straightforward. Equation (3.1) then includes the angular momentum barrier term $l(l+1)/r^2$ and (3.2) is replaced by

$$u(r) \sim r^{l+1}, \qquad r \to 0.$$

For $l = 1, 2$ it is possible to construct combinations of the B-splines (as was done in (3.6)) to satisfy the boundary condition near $x = 0$, but for $l \geqslant 3$ this cannot be done

(since we are only using cubic functions). Instead, one would have to replace the boundary condition at $r = 0$ by $u(0) = 0$, or the conventional variational method would have to be replaced by one which does not explicitly require the trial function to satisfy the boundary conditions (see Hennell and Hendry 1975 and references therein). Shore (1973) has effectively used the former procedure for all partial waves for $l \geqslant 1$.

4. Discontinuous potential

For a realistic discontinuous potential we have taken

$$V(r) = \begin{cases} 670 \times 1{\cdot}4/41{\cdot}5 & r < r_c \\ -1{\cdot}4 \times 139{\cdot}4 \times 0{\cdot}08E(1+8{\cdot}7E+10{\cdot}6E^2)/41{\cdot}5 & r > r_c \\ r_c = 0{\cdot}688 \text{ fm}, E = \exp(-\mu r)/\mu r, & \mu = 1/1{\cdot}415, \end{cases}$$

this being the $^1S_0$ potential of Bressel *et al* (1969) adjusted by a factor 1·4 to produce a bound state. (The factor 41·5 is the usual conversion when working in Mev and fm.) For this potential, we know that the discontinuity of the wavefunction's second derivative is

$$\Delta u'' = 36{\cdot}38$$

where

$$\Delta u'' = \left(\left[\frac{d^2u}{dr^2} \right]_{r_c+} - \left[\frac{d^2u}{dr^2} \right]_{r_c-} \right) (u(r_c))^{-1}.$$

For the trial function we have taken

$$\phi_N(x) = \sum_{i=0}^{N} c_i S_i(x) + b_k Q_k(x) \qquad 2 \leqslant k \leqslant N. \tag{4.1}$$

We use the transformation

$$r = \alpha x/(N+2-x)$$

but α cannot take any value since we must ensure that the core radius r_c maps onto the point $x = k$ in (4.1). To achieve this, we have introduced a parameter R which describes the position of the core ($x = k$) relative to the final point of interest in the x region (ie $x = N+2$). Having chosen a suitable value of R, k is then found by

$$k = \text{nearest integer to } ((N+2)/R), \qquad k \geqslant 2.$$

Thus as N increases, the position of k moves outwards. Once k has been found, α is given by

$$\alpha = r_c(N+2-k)/k.$$

With the above trial function (4.1), the Rayleigh–Ritz procedure then replaces equation (3.1) by the matrix eigenvalue problem

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

where $\mathscr{L}$, $\mathscr{N}$ are symmetric $(N+2)\times(N+2)$ matrices and $\boldsymbol{a}$ is an $(N+2)$ vector. The elements of $\mathscr{L}$ and $\mathscr{N}$ are evaluated in the usual way, each element having contributions

from at most four adjacent subintervals in x. Numerically, it was found that a low-order Gauss–Legendre rule over each subinterval gave sufficient accuracy for the evaluation of these integrals.

For $\boldsymbol{a}$ we have

$$a_i = c_i \qquad 1 \leqslant i \leqslant N+1$$

$$a_{N+2} = b_k.$$

Figure 1 shows the results that were obtained using trial function (4.1). Also shown are the results omitting the Q_k term from the trial function. Both sets of results have been

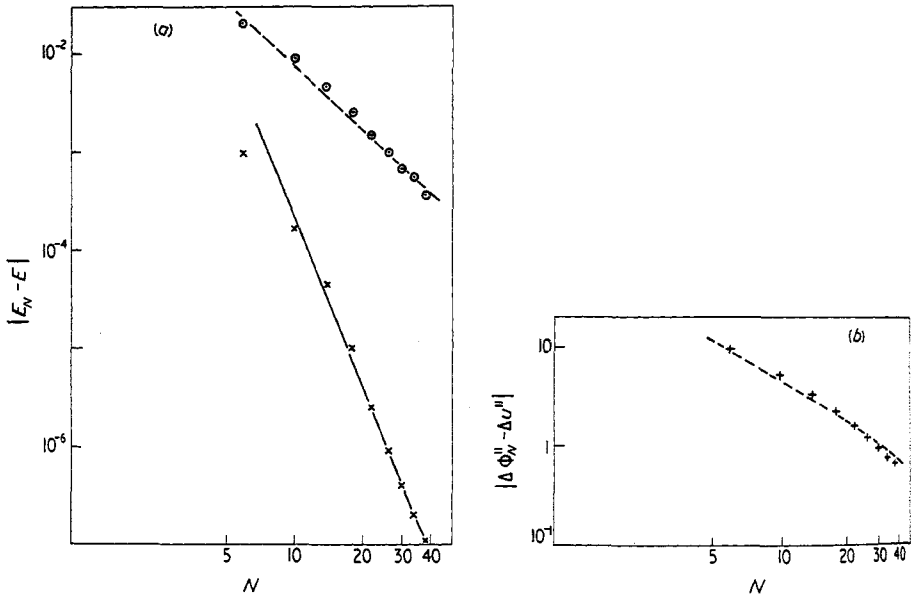

Figure 1. (*a*) $|E_N - E|$ against N for BKR potential × including Q_k; ⊙ no Q_k; —— line of gradient (-6); – – – line of gradient (-2). (*b*) $|\Delta\phi_N'' - \Delta u''|$ against N for BKR potential $+|\Delta\phi_N'' - \Delta u''|$; – – – line of gradient (-1).

calculated using $R = 4{\cdot}0$ and $N = 6(4)38$. Figure 1(*a*) shows $|E_N - E|$ against N on a logarithmic scale, where for the exact value E we have taken E_{42} (including Q_k term) which is

$$E \equiv E_{42} = -0{\cdot}0377155.$$

It is immediately apparent that the inclusion of the single Q_k term has made a significant difference both to the convergence rate and the number of trial functions required for a given accuracy. From the lines drawn we see that the convergence rate has increased from approximately $O(N^{-2})$ to $O(N^{-6})$, this last rate being similar to that mentioned in § 3 for the continuous RSC potential. For accuracy we note that for $N = 10$ the results with (without) Q_k are respectively accurate to 0·4% (25%) while for $N = 22$ the corresponding figures are 0·007% (4%). The results for no Q_k confirm the statement made in the introduction that a slow convergence rate would be obtained, but provided we use sufficient terms the energy can be accurately estimated.

Figure 1(*b*) shows the results for the magnitude of the discontinuity at r_c. From (4.1) we can calculate this magnitude to be

$$\Delta\phi''_N = 18b_k/[f'(k)^2(0{\cdot}25c_{k-1}+c_k+0{\cdot}25c_{k+1})].$$

We have plotted $|\Delta\phi''_N-\Delta u''|$ against N and as the graph indicates this converges at a rate proportional to $O(N^{-1})$, the results for $N = 38$ being accurate to about 2·0%. Finally the results quoted here are typical of those obtained for a range of values of R.

5. Conclusion

The results of the previous sections have shown that the inclusion of a single term Q_k in the trial function has enabled us to recover a convergence rate of $O(N^{-6})$ for a discontinuous potential (BKR), this being the rate we achieved for the continuous potential (RSC). We also note that the convergence rate for $\Delta u''$ is $O(N^{-1})$. From the graphs presented, it is apparent that the convergence for E_N is monotonic for sufficiently large N (both with and without the inclusion of the Q_k term). This is not necessarily so for small $N(\lesssim 3)$, an observation which has previously been noted by Shore (1973). This behaviour should be contrasted with that of a global variational method (GVM), where monotonic convergence in N is assured by the separation theorem for symmetric real matrices (Wilkinson 1965, Delves 1973).

Unpublished results (Hennell) for the BKR of § 4 using the GVM with Hylleras trial functions (ie $r^n e^{-\alpha r}$) show a similar behaviour to that obtained here with the cubic splines (without Q_k). Likewise for RSC, results similar to those of the cubic splines are obtained.

The results shown here strongly suggest that the convergence rate of the GVM will also improve substantially if discontinuous terms are incorporated in the trial function. In view of the fact that constructing an expansion set with the second derivative discontinuity explicit is non-trivial, the simplest strategy is to use the usual expansion sets together with a single function incorporating the discontinuity (ie a core function). Core terms in variational calculations are usually *ad hoc* functions which in some way incorporate the gross features (or some particular feature) of the exact solution.

Although in this paper, we have used a piecewise approximation everywhere, we are not on the evidence of this paper advocating the use of this method in multiparticle problems. It appears to us that where computer codes already exist for these problems there is nothing to be gained from duplication. For the case of square well-like potentials a simple modification to incorporate a term analogous to those used here in existing codes should be adequate.

References

Bressel C N, Kerman A K and Rouben B 1969 *Nucl. Phys.* A **124** 624–36
Clapp R E 1949 *Phys. Rev.* **76** 873–4
Delves L M 1973 *Advances in Nuclear Physics* vol 5, eds M Baranger and E Voigt (New York: Plenum)
Delves L M and Hennell M A 1971 *Nucl. Phys.* A **168** 347–83
Feshbach H and Rarita W 1949 *Phys. Rev.* **75** 1384–8
Fix G J, Gulati S and Wakoff G I 1973 *J. Comput. Phys.* **13** 209–28
Fuda M G 1971 *Phys. Rev.* C **3** 485–93

Hennell M A and Delves L M 1972 *Phys. Lett.* **40B** 20–2
—— 1973 *Nucl. Phys.* A **204** 552–60
Hennell M A and Hendry J A 1975 *J. Phys.* A: *Math. Gen.* **8** 299–312
Kim Y E and Tubis A 1971 *Phys. Rev.* C **4** 693–9
Reid R V 1968 *Ann. Phys., NY* **50** 411–48
Schoenberg I J 1946 *Q. Appl. Math.* **4** 45–9
Shore B W 1973 *J. Phys.* B: *Atom. Molec. Phys.* **6** 1923–32
Strang G and Fix G J 1973 *An Analysis of the Finite Element Method* (New Jersey: Prentice-Hall)
Wilkinson J H 1965 *The Algebraic Eigenvalue Problem* (Oxford: Clarendon)
Whiteman J R (ed) 1973 *The Mathematics of Finite Elements and Applications* (New York: Academic)