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Variational methods with trial functions not satisfying prescribed boundary conditions

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Abstract. Some variational methods are considered in which the trial functions used are not required to satisfy prescribed boundary conditions. Applications of these methods are made to a two-body system interacting via a hard-core potential.

1. Introduction

It is a widely held belief that the trial functions used in a variational calculation should exactly satisfy (by construction) the boundary conditions of the particular problem. In fact this is not so, and there exist in the literature methods for handling a particular type of derivative boundary condition (Mikhlin 1964, Morse and Feshbach 1953) and various boundary conditions have been considered using complementary variational methods (Arthurs 1970, 1973, Anderson and Arthurs 1972 and references therein).

It frequently happens that the most attractive coordinate system for describing a problem is not the most convenient for implementing the given boundary conditions. For example, in the nuclear three-body problem, a hyperspherical coordinate system is attractive for expressing the problem but this system does not lend itself conveniently to the construction of variational trial functions which incorporate the boundary conditions when a hard-core potential (eg the potential of Hamada and Johnston 1962) or a boundary condition model (BCM, Lomon and Feshbach 1968) is used to describe the underlying two-body interactions.

In this paper we examine two possible methods for dealing with multiparticle problems when hard-core interactions are used. These methods are variational in nature, but the trial functions used are not required to explicitly satisfy the boundary conditions.

The first method (I) is a simple generalization of the existing method which enables us to compare with a recently developed variational method (Yates 1974). In this case the hard-core interaction is considered in two ways, firstly as the limit of a BCM and then directly.

The second method (II) is derived from first principles and, as far as the authors are aware, has not previously been applied to an eigenvalue problem.

These methods are derived in §§ 2 and 3. In § 4, method I is applied to the BCM for a two-boson system, while in §§ 5, 6 and 7, methods I and II are respectively applied to the Hamada–Johnston hard-core potential (HJ potential) for the same system. Finally some comparisons are given in § 8.

Throughout the paper, the HJ potential used is the $^1S_0$ potential of Hamada and Johnston (1962) with the strength parameter adjusted by a factor of 1·4 to produce a single bound state.

2. Method I

Consider a linear equation

$$L\Psi = f. \tag{2.1}$$

As has been stated elsewhere (Delves 1973, Stakgold 1968), the functional

$$F(\eta, \phi) = (\eta, L\phi) - (\eta, f) - (f, \phi)$$

is stationary about the true solutions of equation (2.1) and of

$$L^+\eta = f.$$

Here (η, ϕ) is some suitable inner product, the usual definition being

$$(\eta, \phi) = \int \eta\phi \, \mathrm{d}t,$$

the integration being performed over the region of interest. L^+ is the Hermitian conjugate operator of L and is explicitly defined in terms of the inner product by

$$(\eta, L\phi) = (L^+\eta, \phi).$$

Likewise for the eigenvalue problem

$$L\Psi = E\Psi \tag{2.2}$$

the functional

$$F(\eta, \phi) = (\eta, L\phi) - E(\eta, \phi)$$

is stationary about the true solution of equation (2.2).

Now consider the eigenvalue problem

$$L\Psi = E\Psi \tag{2.3a}$$

subject to the boundary condition

$$M\Psi = 0. \tag{2.3b}$$

Using the ideas outlined above, the functional

$$F(\eta, \phi) = (\eta, L\phi) - E(\eta, \phi) + \beta(\eta, M\phi)_B \tag{2.4}$$

is stationary (in the sense of Stakgold 1968, p 357) about the true solution of equations (2.3) and their corresponding adjoints. Here β is an arbitrary parameter and (η, ϕ) and $(\eta, \phi)_B$ represent inner products over and on the boundary of the region of interest respectively.

Introducing, as usual, a complete set h_i (which does not satisfy the given boundary conditions) gives suitable expansions for the trial functions

$$\eta_t = \sum_{i=1}^{N} b_i h_i$$

$$\Psi_t = \sum_{i=1}^{N} a_i h_i.$$

Substituting these expansions into functional (2.4) gives

$$F(\eta_t, \Psi_t) = b^+ La - Eb^+ Na + \beta b^+ Ma$$

where a, b, N, L, M are matrices with elements $a_i, b_i, (h_i, h_j), (h_i, Lh_j)$ and $(h_i, Mh_j)_B$ respectively. The stationary value of this functional gives the matrix eigenvalue problem.

$$(L + \beta M)a = E_T Na \tag{2.5}$$

where E_T is a variational estimate of the eigenvalue. We note at this point that intuitively the parameter β is some measure of how strongly the variational method feels the boundary condition. For instance, for small β the effect of the boundary condition will be small whilst for large β, the boundary condition will dominate. For inhomogeneous equations (2.1) it has been found that the method is relatively insensitive to the value of β over a wide range. (This is a private communication with D Yates, the results shortly to be produced in thesis form in Yates (1974).)

3. Method II

Here we consider the eigenvalue problem

$$L\Psi = E\Psi \tag{3.1}$$

where L is a second-order linear differential operator, subject to the boundary condition

$$\Psi = 0 \tag{3.2}$$

over the same prescribed boundary B. Then, as is well known, the functional

$$F(\phi) = (\phi, L\phi) - E(\phi, \phi) \tag{3.3}$$

is stationary about the true solution of (3.1) provided that the inner product in (3.3) has been chosen to make the operator L formally Hermitian. This can be achieved by using the usual inner product and ensuring that the trial function ϕ satisfies the prescribed boundary conditions.

However, suppose we now relax the condition that ϕ should satisfy the boundary condition. Then by adding a term to (3.3) we can produce a function which is stationary about the true solution of (3.1) without requiring that the trial functions satisfy (3.2). This functional is

$$F(\phi) = (\phi, L\phi) - E(\phi, \phi) - \left(\frac{\partial \phi}{\partial n}, \phi\right)_B \tag{3.4}$$

where $(\phi, \phi)_B$ is some appropriate inner product defined over the boundary B and $\partial\phi/\partial n$ is the normal derivative, n being the outward normal to the boundary. With the

usual definition of the inner product, this of course means that the operator L is no longer Hermitian since we have (by Green's theorem) that

$$(\phi, L\psi) = (L\phi, \psi) + \left(\frac{\partial \phi}{\partial n}, \psi\right)_B - \left(\phi, \frac{\partial \psi}{\partial n}\right)_B.$$

The idea of adding boundary terms to a functional of the form of (3.3) has previously been considered within the framework of complementary variational principles (Arthurs 1970, 1973, Anderson and Arthurs 1972).

With the usual choice of expansion functions, the functional (3.4) now becomes stationary if

$$(L+M)a = E_T N a$$

where the notation is the same as in (2.5) except that now M is the matrix with elements $(\partial h_i/\partial n, h_j)_B$. Note that this method is not derivable from method I, since there the analogous operator M would be unity and thus M would have elements $(h_i, h_j)_B$.

4. Method I and the BCM

We now demonstrate how the BCM fits into the framework developed in § 2. We consider the binding energy of a two-boson system, the equations which describe this system being

$$\begin{aligned} &-\frac{d^2}{dr^2}u(r) + V(r)u(r) = Eu(r), && r > c \\ &\frac{d}{dr}u(r) = \lambda u(r), && r = c. \end{aligned} \tag{4.1}$$

If we use the notation of § 2 then

$$L = -\frac{d^2}{dr^2} + V(r)$$

$$M = \frac{d}{dr} - \lambda.$$

Suitable definitions for the required inner products are (Delves 1973)

$$(h_i, Lh_j) = \int_c^\infty h_i \left(-\frac{d^2}{dr^2} + V(r)\right) h_j \, dr$$

$$(h_i, h_j) = \int_c^\infty h_i h_j \, dr$$

$$(h_i, Mh_j)_B = \left(h_i \frac{dh_j}{dr} - \lambda h_i h_j\right)_{r=c}.$$

The resulting matrix equation which we solve is

$$(L + \beta M)a = E_T N a.$$

Having obtained the solution to this eigenvalue problem we premultiply by a^+ to get

$$E_T = (a^T L a + \beta a^T M a)/a^T N a. \tag{4.2}$$

We note that this expression is very similar to the normal Rayleigh–Ritz principle. If we define

$$u_t = u + \epsilon$$

where ϵ is the amount by which the variational estimate $u_t = \Sigma_{i=1}^{N} a_i h_i$ varies from the true solution u, then we can show that (see appendix, equation (A.2)):

$$E_T = E + (1+\beta)O(\epsilon) + O(\epsilon^2).$$

Thus for general β the variational principle gives an estimate E_T which differs from the true value E by an amount which is first order in ϵ. However, the special choice $\beta = -1$ gives

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

ie a second-order estimate. We also note (see appendix, equation (A.3)) that the matrix

$$H(\beta) = L + \beta M$$

is not in general symmetric, but again the choice $\beta = -1$ results in a symmetric H. For the special case $\beta = -1$, the resultant principle is identical to the existing method for handling a set of equations like (4.1) (Mikhlin 1964, Morse and Feshbach 1953). As a test of the variational principle we may restrict ourselves to the pure BCM (ie we do not consider an external potential in this section). Then we have

$$-\frac{d^2}{dr^2}u(r) = Eu(r), \qquad r > c$$

$$\frac{d}{dr}u(r) = \lambda u(r), \qquad r = c.$$

It is easily seen that for negative values of λ this system has a bound state with energy $E = -\lambda^2$. For trial functions we used

$$u_t = \sum_{i=1}^{N} a_i r^i e^{-\alpha r} \tag{4.3}$$

where α is a nonlinear parameter. Figure 1 shows the results for E_T for the values of the parameters c and λ considered. The value of α used was obtained by finding a range over which the rate of convergence was not markedly affected and choosing a suitable value of α from this range. It is immediately apparent that for all β the energy estimates obtained from the variational method are converging to some value consistent with the true solution $E = -0{\cdot}25$. However, it is also clear that the results for $\beta = -1$ converge much more rapidly than the results for other β values. This is merely a direct demonstration of the result obtained earlier which predicted second-order convergence for $\beta = -1$ and first-order otherwise. Figure 2 shows results for the ratio λ_T obtained from the variational solution u_t by

$$\lambda_T = \left(\frac{du_t/dr}{u_t}\right)_{r=c}.$$

These results behave much as one would expect, the larger values of $|\beta|$ reproducing the prescribed boundary conditions with a small number of terms. However, we note that the special value $\beta = -1$ has no effect in this case since from the appendix we know that λ_T converges to λ to first order in ϵ irrespective of the value of β. To emphasize these

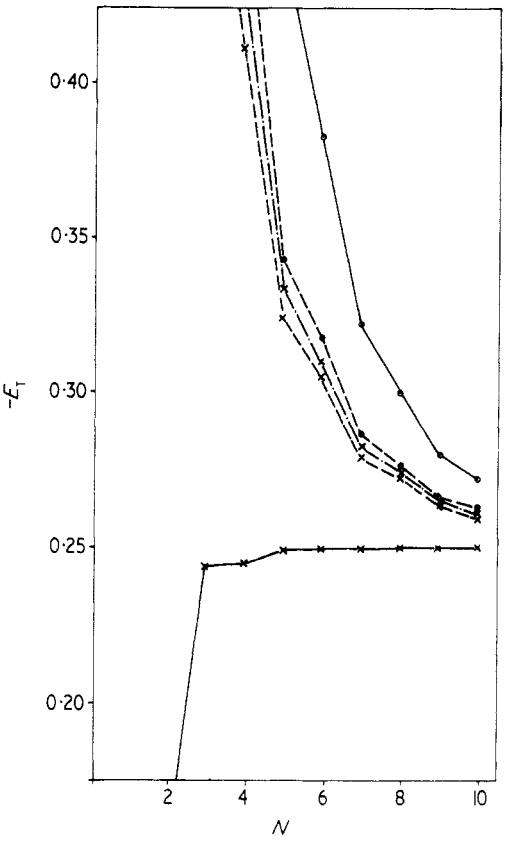

Figure 1. Binding energy E_T against number of variational terms N. Parameters are $\alpha = 1{\cdot}5$, $\lambda = -0{\cdot}5$, $c = 0{\cdot}7$. Full curves: $\beta = -1$ (with crosses), 1 (with open circles); broken curves: $\beta = -10$ (with crosses), 10 (with open circles); chain curve: $\beta = -100$ (with crosses).

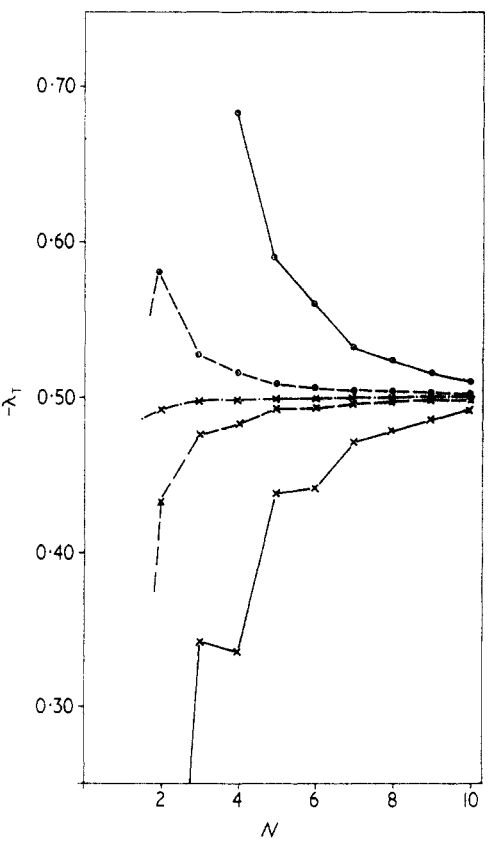

Figure 2. $\lambda_T = ((du_t/dr)/u_t)_c$ against N. Parameters as in figure 1.

points further, figure 3 shows the results obtained for the differences $|E_T - E|$ and $|\lambda_T - \lambda|$ as a function of N on a logarithmic scale. From an analysis of the convergence of simple problems one would expect there to be a linear relationship between these quantities and N (or at least asymptotically this should hold). Figure 3 clearly demonstrates that such a linear relationship holds. (The straight lines are merely a guide to the eye.) However, more important are the relative rates of convergence of the two quantities. For $\beta = +1$, both are converging at approximately the same rate (since the lines are parallel) whereas for $\beta = -1$, the rate for E_T is approximately twice that for λ_T. These results merely reinforce our simple analysis of the error given in the appendix.

5. A limiting case of method I and the BCM

In § 4, method I was applied to the pure BCM (ie no external potential). In this section we consider a hard-core potential as the limit of an external potential and the BCM acting

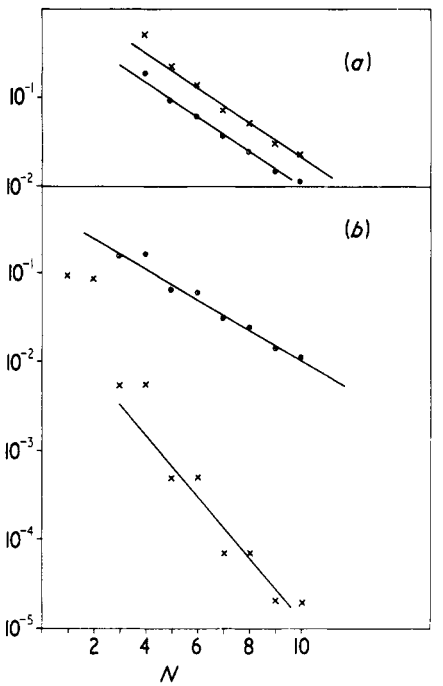

Figure 3. $|E_T - E|$ (full curve with crosses) and $|\lambda_T - \lambda|$ (full curve with open circles) against N for: (*a*) $\beta = 1$; and (*b*) $\beta = -1$. Other parameters as in figure 1.

at the core. Consider the boundary condition

$$\frac{du}{dr} - \lambda u = 0, \qquad r = c.$$

Then in limit $|\lambda| \to \infty$, this reduces to the condition that

$$u = 0, \qquad r = c.$$

Thus a hard-core potential can be considered as the limiting case of the BCM. The detailed problem we consider here is that of a two-boson system interacting via the HJ potential. We first solved this problem in the traditional way (the trial functions satisfying the boundary condition at $r = c$ explicitly) to enable us to quote the exact solution to four significant figures. We then relaxed the condition that the trial functions should satisfy the boundary condition and used the expansion (4.3) in method I for various values of λ, fixing $\beta = -1$ in order to obtain second-order convergence.

The results are shown in figure 4. Here we have plotted the converged value of E_T (as a function of N) for the various values of λ considered. The results clearly show that the predicted binding energy is converging to the exact solution of the HJ potential. It is interesting to note that whilst the energy of the pure BCM is tending to infinity ($E = -\lambda^2$) the combined system in fact feels the effect of the BCM less and less as λ increases. Since large values of λ are required, from the computational point of view, the method is possibly unstable, since the term $\lambda\,(\Psi, \Psi)_B$ may tend to swamp any other term due to the finite precision arithmetic in the computer.

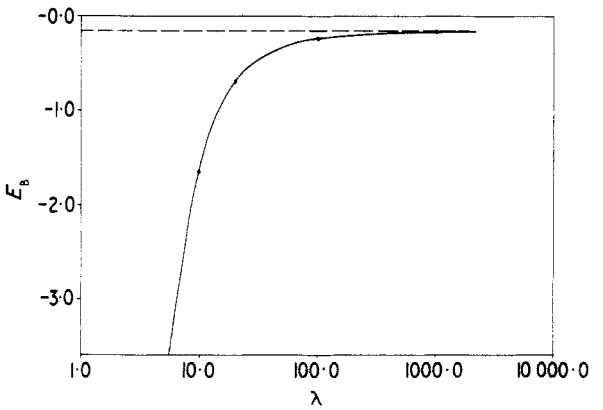

Figure 4. Converged value of E_T against λ for the HJ potential considered as the limit of a BCM (α = 1·50). The broken line is the exact solution.

6. Method II and the HJ potential

In this section the method of § 3 is applied to the HJ potential. For two bosons, the eigenvalue equation is

$$-\frac{d^2u}{dr^2}+V(r)u = Eu, \qquad r > c \tag{6.1}$$

subject to the boundary conditions at the hard core

$$u = 0, \qquad r = c. \tag{6.2}$$

Thus in the notation of § 3, we have

$$L \equiv -\frac{d^2}{dr^2}+V(r)$$

$$\frac{\partial}{\partial n} \equiv \frac{d}{dr}.$$

If we introduce a complete set h_i, which does not satisfy (6.2), substitute into functional (3.4) and find the stationary value as usual, the matrix equation

$$(L+M)a = E_T N a$$

arises, where M is the matrix given by

$$M_{ij} = \left(\frac{dh_i}{dr}h_j\right)_{r=c}.$$

In appendix 2, it is explicitly shown that for a system defined by equations (6.1) and (6.2) the energy estimate which will result from this method is second-order in the error.

In figure 5, we have plotted the results obtained from using this method with the trial function given by (4.3). Also shown on this graph are the results from the traditional

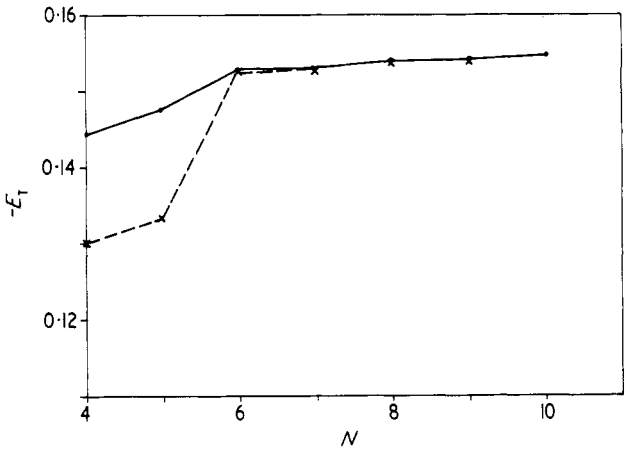

Figure 5. E_T against N for the HJ potential ($\alpha = 1{\cdot}75$). Full curve: traditional method; broken curve: method II.

method (ie the boundary condition explicitly included in the trial function). It can be seen from the graphs that both sets of results are converging at approximately the same rate, the results for method II lagging slightly behind those of the traditional method for each value of N. That this is so is not surprising since method II is having to work much harder than the traditional method as it is required to estimate the eigenvalue and at the same time reproduce the boundary condition. Figure 6 shows the results for the value of the modulus of the normalized wavefunction at $r = c$ obtained from method II. As N increases, the value of the quantity is becoming smaller showing that the method is reproducing the boundary condition (6.2) at the hard-core radius. (The slightly anomalous kink around $N = 7$ can be explained by the value of the trial function changing sign around $N = 6$.)

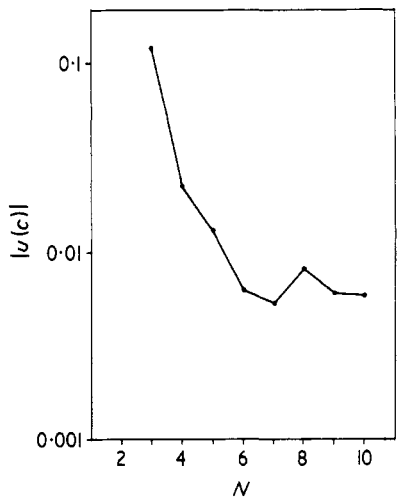

Figure 6. $|u(c)|$ against N for the HJ potential using method II ($\alpha = 1{\cdot}75$).

7. Method I and the HJ potential

In this section the method of § 2 is applied directly to the HJ potential. As in § 6 we require to solve (6.1) subject to the boundary condition (6.2). Thus in the notation of § 2 we have

$$L = -\frac{d^2}{dr^2} + V(r)$$

$$M = I \text{ (the identity operator).}$$

Introducing a complete set h_i, which do not satisfy (6.2) into functional (2.4) results in the matrix equation

$$(L+\beta M)a = E_T N a$$

where M is given by

$$M_{ij} = (h_i h_j)_{r=c}.$$

Figure 7 shows the results obtained from this method using a trial function of the form (4.3). Here we have plotted E_T against β for various values of N. It should be immediately apparent that for small fixed β (~ 10) there is no convergence of the estimates E_T as N increases. However, for large β (~ 1000), convergence clearly takes place as N increases. A possible explanation of this fact is as follows. The functional of this section (ie method I) differs only from that used in § 6 (ie method II) in the boundary terms, which are respectively $\beta(\Psi_t, \Psi_t)_B$ and $(d\Psi_t/dr, \Psi_t)_B$. Thus if β is chosen so that

$$\beta\Psi_t = \frac{d\Psi_t}{dr}, \qquad r = c, \tag{7.1}$$

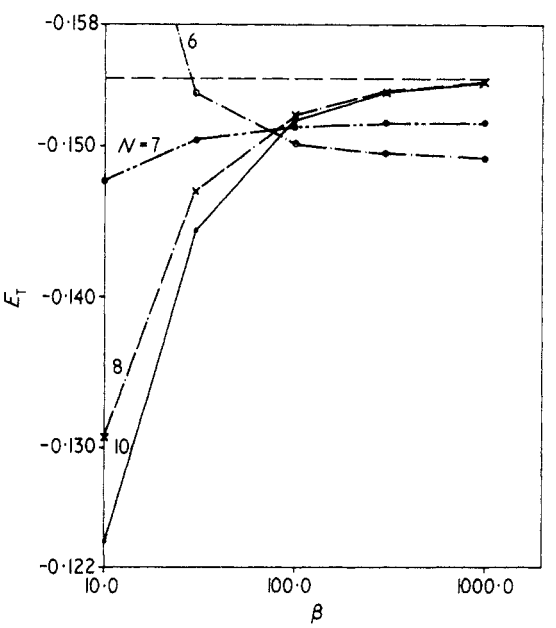

Figure 7. E_T against β for various N for the HJ potential using method I ($\alpha = 1{\cdot}75$). The broken line is the exact solution.

the two methods will coincide. Now if the method is converging, we would expect Ψ_t to become small (to reproduce the boundary condition) whereas $d\Psi_t/dr$ will tend to a fixed nonzero limit at $r = c$. Thus the value of β from (7.1) will become large. Hence, if convergence is to be obtained at all, we would only expect it for large values of β, as the results bear out. In figure 8, the value of the normalized wavefunction at $r = c$ is shown as a function of β and N. Again it is apparent that for large β the boundary condition is being well reproduced.

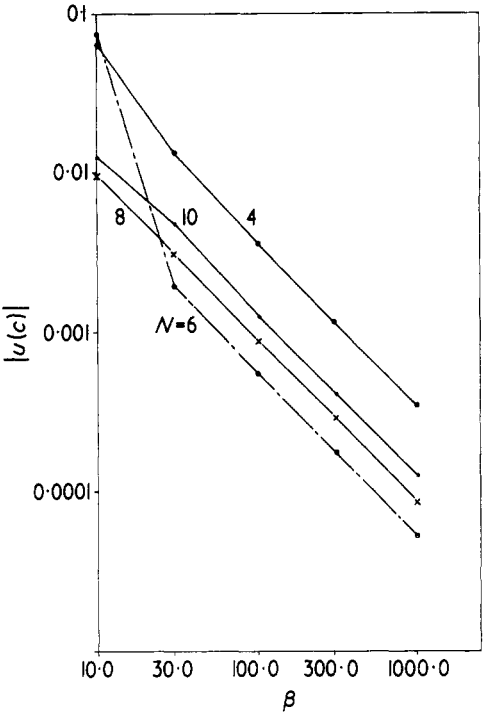

Figure 8. $|u(c)|$ against β for various N for the HJ potential using method I ($\alpha = 1{\cdot}75$).

8. Conclusions

In this paper we have demonstrated three variational techniques which can be used to solve a system with a hard-core potential, without requiring the trial functions to explicitly satisfy the given boundary conditions. These techniques have been applied to a simple two-boson system to demonstrate some of the characteristics.

Two distinct methods were presented. The second of these involves no limiting process whatsoever and gives an eigenvalue estimate which is second-order in the error. However, it does require the normal derivative of the trial function at the hard-core radius and this could be a significant disadvantage of the method in a complex system.

The first method was applied in two different ways to solve the hard-core system, both of which required some limiting procedure. The first application was to consider the hard core as the limit of a BCM ($\lambda \to \infty$). To implement this required first derivatives and again this may be a disadvantage in complex systems. Once again the method can be made to give a second-order estimate of the eigenvalue.

In the second application the method was applied directly to the hard-core interaction. It was shown that when the coupling between the volume and surface terms was made large, the method converged to the correct result.

Acknowledgments

We would like to thank one of the referees for several useful suggestions and for bringing to our notice the references to complementary variational principles.

Appendix 1

We have from equation (4.2)

$$E_T = (a^+ La + \beta a^+ Ma)/a^+ Na$$

which can be rewritten in the alternative form

$$E_T = [(u_t, Lu_t) + \beta(u_t, Mu_t)_B]/(u_t, u_t)$$

where $u_t = \Sigma_{i=1}^{N} a_i h_i = u + \epsilon$, u being the true solution of

$$Lu = Eu$$

$$Mu = 0.$$

Thus

$$E_T = [(u+\epsilon, L(u+\epsilon)) + \beta(u+\epsilon, M(u+\epsilon))_B]/(u_t, u_t).$$

Now

$$(u+\epsilon, L(u+\epsilon)) = (u, Lu) + (\epsilon, Lu) + (u, L\epsilon) + (\epsilon, L\epsilon) = E(u,u) + E(\epsilon, u) + (u, L\epsilon) + (\epsilon, L\epsilon)$$

but

$$\begin{aligned}(u, L\epsilon) &= \int_c^\infty u\left(-\frac{d^2}{dr^2} + V(r)\right)\epsilon \, dr \\ &= -\left[u\frac{d\epsilon}{dr}\right]_c^\infty + \left[\frac{du}{dr}\epsilon\right]_c^\infty + \int_c^\infty \epsilon\left(-\frac{d^2}{dr^2} + V(r)\right)u \, dr \\ &= \left(u\frac{d\epsilon}{dr}\right)_c - \left(\frac{du}{dr}\epsilon\right)_c + (\epsilon, Lu) \\ &= (u, M\epsilon)_B + \lambda(u, \epsilon)_B - \lambda(u, \epsilon)_B + (\epsilon, Lu) \\ &= (u, M\epsilon)_B + E(u, \epsilon).\end{aligned}$$

Thus

$$\begin{aligned}&(u+\epsilon, L(u+\epsilon)) \\ &\quad = E(u,u) + E(\epsilon, u) + E(u, \epsilon) + (\epsilon, L\epsilon) + (u, M\epsilon)_B \\ &\quad = E(u_t, u_t) + (\epsilon, (L-E)\epsilon) + (u, M\epsilon)_B. \qquad \text{(A.1)}\end{aligned}$$

Similarly

$$(u+\epsilon, M(u+\epsilon))_B = (u, M\epsilon)_B + (\epsilon, M\epsilon)_B$$

and so

$$\begin{aligned} E_T &= [E(u_t, u_t) + (\epsilon, (L-E)\epsilon) + (u, M\epsilon)_B + \beta(u, M\epsilon)_B + \beta(\epsilon, M\epsilon)_B]/(u_t, u_t) \\ &= [E + (1+\beta)(u, M\epsilon)_B/(u_t, u_t)] + [(\epsilon, (L-E)\epsilon) + \beta(\epsilon, M\epsilon)_B]/(u_t, u_t) \\ &= E + (1+\beta)O(\epsilon) + O(\epsilon^2). \end{aligned} \tag{A.2}$$

We also have

$$H(\beta) = L + \beta M$$

where the (i,j)th element of H is given by

$$\begin{aligned} H_{ij}(\beta) &= (h_i, Lh_j) + \beta(h_i, Mh_j)_B \\ &= \int_c^\infty h_i \left(-\frac{d^2}{dr^2} + V(r) \right) h_j \, dr + \beta \left(h_i \frac{dh_j}{dr} - \lambda h_i h_j \right)_c \\ &= (1+\beta)\left(h_i \frac{dh_j}{dr} \right)_c + \int_c^\infty \left(\frac{dh_i}{dr} \frac{dh_j}{dr} + h_i V h_j \right) dr - \beta\lambda(h_i h_j)_c \\ &\neq H_{ji}(\beta). \end{aligned} \tag{A.3}$$

H is only symmetric for $\beta = -1$. Finally the ratio λ_T is given by

$$\begin{aligned} \lambda_T &= \left(\frac{du_t/dr}{u_t} \right)_c \\ &= \lambda + \left[u_t \left(\frac{du_t/dr - \lambda u_t}{(u_t u_t)} \right) \right]_c \\ &= \lambda + (u_t, Mu_t)_B/(u_t, u_t)_B \\ &= \lambda + (u_t, Mu)_B/(u_t, u_t)_B + (u_t, M\epsilon)_B/(u_t, u_t)_B \\ &= \lambda + O(\epsilon). \end{aligned} \tag{A.4}$$

Appendix 2

As in appendix 1, the energy estimate E_T of method II is given by

$$E_T = [(u_t, Lu_t) + (du_t/dr, u_t)_B]/(u_t, u_t).$$

Now let $u_t = u + \epsilon$, where u is the exact solution of equations (6.1) and (6.2). Then, as in appendix 1, we get

$$\begin{aligned} E_T &= [E(u,u) + E(\epsilon,u) + (u, L\epsilon) + (\epsilon, L\epsilon) + (du_t/dr, u_t)_B]/(u_t, u_t) \\ &= [E(u,u) + E(\epsilon,u) + (u, d\epsilon/dr)_B - (du/dr, \epsilon)_B + E(\epsilon, Lu) + (\epsilon, L\epsilon) \\ &\quad + (du/dr, u)_B + (du/dr, \epsilon)_B + (d\epsilon/dr, u)_B + (d\epsilon/dr, \epsilon)_B]/(u_t, u_t) \\ &= [E(u,u) + E(\epsilon,u) + E(\epsilon,u) + (\epsilon, L\epsilon) + (d\epsilon/dr, \epsilon)_B]/(u_t, u_t) \\ &= E + [(\epsilon, (L-E)\epsilon) + (d\epsilon/dr, \epsilon)_B]/(u_t, u_t) \\ &= E + O(\epsilon^2). \end{aligned}$$

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