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Variational methods for scattering problems with trial functions not satisfying prescribed boundary conditions

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Abstract. Two variational methods are presented for scattering problems which do not require the trial functions used to satisfy prescribed boundary conditions. The methods are applied to a two-body system interacting via a hard-core potential.

1. Introduction

In a previous paper (Hennell and Hendry 1975, to be referred to as HH), two variational methods were derived which did not require the trial functions to explicitly satisfy prescribed boundary conditions. These methods were applied to find the binding energy of a two-body nuclear system interacting via a hard-core potential.

Alternatively, interest may lie in determining the scattering quantities associated with such a system. Variational methods (based on a differential equation approach) exist for scattering problems. The Kohn variational principle (see Schwartz 1961) is a widely used method, but requires the trial functions to explicitly satisfy the prescribed boundary conditions. However, for the reasons given in HH, it may be convenient to relax this condition on the trial function.

Within the framework of complementary variational principles (Arthurs 1970), Anderson *et al* (1970a) have developed variational methods, for upper and lower bounds on the scattering length, which do not necessarily require the trial functions to satisfy the boundary conditions.

It should be noted that if the scattering problem is approached by way of an integral equation, then any variational method derived does not require boundary conditions on the trial functions (Anderson *et al* 1970a, b).

In this paper, possible extensions of the ideas of HH are used to derive variational methods for scattering problems. The methods presented here are similar to the conventional Kohn variational principle (referred to as CKVP throughout), in that they reduce to it if the trial functions do satisfy the boundary conditions.

In §§ 2 and 3, the methods are briefly outlined, whilst in §§ 4 and 5 they are applied to the nuclear system considered in HH. Some comments on the methods and results are contained in § 6.

Throughout this paper, the hard-core potential used is the $^1S_0$ potential of Hamada and Johnston (1962, to be referred to as HJ) with the strength adjusted by a factor of 1·4 for consistency with HH.

2. Method I

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

$$\mathscr{L}u = 0, \qquad \mathscr{L} = -\frac{d^2}{dr^2} + V(r) - k^2 \tag{2.1}$$

where $V(r)$ is the potential describing the force between the particles and k^2 is the energy.

Asymptotically $(r \to \infty)$

$$u \to [(\sin kr)/k] + q \cos kr \tag{2.2a}$$

and

$$q = (\tan \delta)/k$$

with δ being the scattering phase shift. Associated with (2.1) will be a boundary condition

$$\mathscr{M}u = 0, \qquad r = c \tag{2.2b}$$

where $\mathscr{M}$ is some suitable operator. The solution of (2.1), subject to (2.2a) can be written as

$$u = F + qG + w$$

where as $r \to \infty$,

$$F \to (\sin kr)/k \qquad G \to \cos kr \qquad w \to 0.$$

Nuttall (1969) has shown that (2.1) may then be written as the inhomogeneous matrix operator equation,

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

where

$$L = \begin{bmatrix} \mathscr{L} & \mathscr{L}G \\ (G, \mathscr{L}\cdot) & (G, \mathscr{L}G) \end{bmatrix}$$

and

$$\Psi = \begin{bmatrix} w \\ q \end{bmatrix} \qquad P = -\begin{bmatrix} \mathscr{L}F \\ (G, \mathscr{L}F) \end{bmatrix}.$$

Here $(,)$ is the usual inner product defined over the region of interest and $(G, \mathscr{L}\cdot)$ means that something has still to be included in the inner product when the matrix multiplication takes place. Similarly, boundary condition (2.2b) can be written

$$M\Psi = Q \tag{2.3b}$$

with

$$M = \begin{bmatrix} \mathscr{M} & \mathscr{M}G \\ (G, \mathscr{M}\cdot)_B & (G, \mathscr{M}G)_B \end{bmatrix} \qquad Q = -\begin{bmatrix} \mathscr{M}F \\ (G, \mathscr{M}F)_B \end{bmatrix}.$$

In (2.3b), $(,)_B$ is the inner product defined on the boundary. Further details of the inner products can be found in HH.

The variational method described in § 2 of HH can now be used to determine the solution of the inhomogeneous equations (2.3). We first define generalized inner products $\{\,,\}$ for vectors $\Psi_i = \begin{bmatrix} w_i \\ q_i \end{bmatrix}$ by

$$\{\Psi_1, \Psi_2\} = (w_1, w_2) + q_1 q_2$$

$$\{\Psi_1, \Psi_2\}_B = (w_1, w_2)_B + q_1 q_2.$$

As in HH, introduce the functional

$$I(\eta, \psi) = (\{\eta, L\psi\} - \{\eta, P\} - \{P, \psi\}) + \beta(\{\eta, M\psi\}_B - \{\eta, Q\}_B - \{Q, \psi\}_B) \tag{2.4}$$

and the equations adjoint to (2.3)

$$L^+\eta = P, \qquad M^+\eta = Q.$$

Then the functional I is stationary about the true solution Ψ of the direct problem (ie (2.3)) for variations $\delta\eta$ in the adjoint vector η and *vice versa*. For further details, see Stakgold (1968). As usual we expand η, Ψ in terms of a complete set h_i (which does not satisfy the prescribed boundary conditions)

$$\Psi_N = \begin{bmatrix} \sum_{i=1}^{N} a_i h_i \\ q_t \end{bmatrix} \qquad \eta_N = \begin{bmatrix} \sum_{i=1}^{N} b_i h_i \\ \lambda_t \end{bmatrix}$$

and insert into functional (2.4). The stationary value of the functional then gives the set of $(N+1)$ linear equations

$$\begin{bmatrix} \boldsymbol{H}_{NN} & \boldsymbol{H}_{NG} \\ \boldsymbol{H}_{GN} & H_{GG} \end{bmatrix} \begin{bmatrix} \boldsymbol{a}_t \\ q_t \end{bmatrix} = \begin{bmatrix} \boldsymbol{R}_{NF} \\ R_{GF} \end{bmatrix}. \tag{2.5}$$

In equation (2.5) the quantities which arise are,

$\boldsymbol{H}_{NN}$	$(N \times N)$ matrix,	elements	$H_{ij} = (h_i, \mathscr{L}h_j) + \beta(h_i, \mathscr{M}h_j)_B$
$\boldsymbol{H}_{NG}$	N-row vector,	elements	$H_{iG} = (h_i, \mathscr{L}G) + \beta(h_i, \mathscr{M}G)_B$
$\boldsymbol{H}_{GN}$	N-column vector,	elements	$H_{Gi} = (G, \mathscr{L}h_i) + \beta(G, \mathscr{M}h_i)_B$
H_{GG}	scalar,	element	$H_{GG} = (G, \mathscr{L}G) + \beta(G, \mathscr{M}G)_B$
$\boldsymbol{R}_{NF}$	N-row vector,	elements	$-R_{iF} = (h_i, \mathscr{L}F) + \beta(h_i, \mathscr{M}F)_B$
R_{GF}	scalar,	element	$-R_{GF} = (G, \mathscr{L}F) + \beta(G, \mathscr{M}F)_B$
$\boldsymbol{a}_t$	N-row vector,	elements	a_i.

The structure of equation (2.5) is very similar to that of the first-order estimate of the CKVP. The essential difference is that the H_{ij}, etc, now include a term associated with the boundary condition. The solution of equation (2.5) can be found in the usual way by solving a set of $N \times N$ linear equations (see Delves 1973, § 5.1.3 for details).

3. Method II

In HH (§ 3), a variational method for an eigenvalue problem was derived from the conventional Rayleigh–Ritz principle by relaxing the boundary conditions on the trial

functions and adding a compensating term to the variational functional. Here we do the same thing for the CKVP.

As in §2, we require to solve (2.1) subject to the asymptotic condition (2.2*b*) with the boundary condition

$$u = 0, \qquad r = c. \tag{3.1}$$

Delves (1973, § 5.1.2) gives a very simple derivation of the CKVP. If we use the ideas of this derivation but take account of the trial function u_t not satisfying condition (3.1), then the functional

$$[q_t^{(2)}] = q_t^{(1)} - \int_c^\infty u_t \mathcal{L} u_t \, dr - \left(\frac{du_t}{dr} u_t\right)_{r=c} \tag{3.2}$$

is stationary about the solution of (2.1) subject to condition (3.1). Here, stationary is used in the sense that the difference between $q_t^{(2)}$ and the exact value q is second-order in the error ϵ in the trial function, ie,

$$q_t^{(2)} = q + O(\epsilon^2) + O(\epsilon d\epsilon/dr).$$

Appendix 2 of HH gives the details for the analogous case of the bound state problem.

As in § 2, we take as trial function

$$u_t = F + q_t^{(1)} G + \sum_{i=1}^{N} a_i h_i$$

where F, G and h_i do not satisfy (3.1). Inserting this expansion into functional (3.2) then gives the set of equations (2.5) with the $\beta(X, Y)_B$ term replaced by $[(dX/dr)Y]_{r=c}$ for all possible combinations of X and Y.

Having solved for the first-order estimate $q_t^{(1)}$ and $\boldsymbol{a}_t$, substitution into the functional then gives a second-order estimate $q_t^{(2)}$ of q. Note that this formalism is very similar to the CKVP, differing only in the matrix elements having the derivative terms at the core added. Finally, here we have considered a hard-core potential (ie, boundary condition (3.1)), but the same technique could handle an interaction described by a boundary condition model (Lomon and Feshbach 1968).

4. Method I and the HJ potential

The theory of § 2 has been applied to the HJ hard-core potential,

$$V(r) = -1{\cdot}4 \times 139{\cdot}4 \times 0{\cdot}08E(1 + 8{\cdot}7E + 10{\cdot}6E^2)/41{\cdot}5,$$
$$E = \exp(-\mu r)/\mu r, \qquad \mu = 1/1{\cdot}415$$

with the hard-core radius $c = 0{\cdot}486$ fm. (The factor 41·5 is the usual factor when working in MeV and fm, and the factor 1·4 is for consistency with HH.) For this hard-core potential, the operator $\mathcal{M}$ of § 2 is the identity operator. For functions, we have chosen

$$F = (\sin kr)/k, \qquad G = \cos kr, \qquad h_i = r^{i-1} e^{-\alpha r}. \tag{4.1}$$

Note that F, G and h_i have the correct asymptotic form ($r \to \infty$) while at $r = c$ they do not satisfy the prescribed boundary condition. The results obtained for method I are shown

in figure 1 for two typical values of k, corresponding to zero-energy scattering ($k = 0$) and a fairly high-energy scattering ($k = 0{\cdot}7$), which is equivalent to about 20 MeV). For each value of k, results are shown for two choices of the parameter β in equation (2.5). Also shown are the results from a CKVP calculation for the same system (see next section). From figure 1(a), it is apparent that for both values of β, the estimates q_t are converging to the exact value as N increases. It is also clear that the results for the larger β approach the exact solution much more rapidly than do those for the smaller β. Figure 1(b) shows $|u_t(c)|$ as a function of N. For N sufficiently large (≥ 4), this quantity is tending to decrease with N, showing that the exact boundary condition at the core is being reproduced. Again, the larger value of β gives the better results.

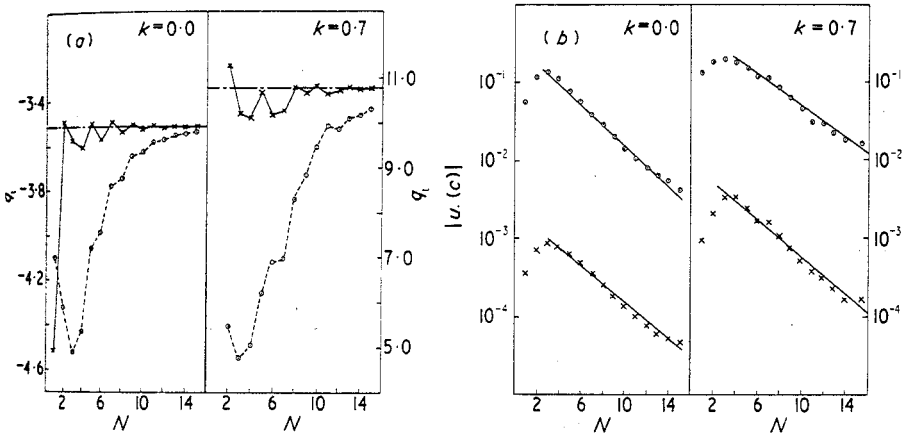

Figure 1. Method I for $k = 0{\cdot}0$, $0{\cdot}7$ ($\alpha = 2{\cdot}0$). (a) q_t against N; (b) $|u_t(c)|$ against N. —×—×—, $\beta = 1000$; —○—○—, $\beta = 10$; — — — —, exact value from CKVP.

The behaviour obtained here differs markedly from that of HH for method I. There, a large value of β was required in order to obtain any convergence, but here a small value of β can be used (provided that there is a compensating increase in the number of trial functions).

The behaviour found here is similar to that found by Yates (1975) in an investigation of method I applied to a variety of inhomogeneous partial differential equations (with associated boundary conditions) over various regions. He found that the method was relatively insensitive to the actual value of β provided it was neither too large (which means that the boundary conditions dominate at the expense of the equation) nor too small (trying to solve an equation ignoring boundary conditions). Finally, it should be noted that the results for $k = 0{\cdot}7$ are not quite as good as for $k = 0$. This is not surprising since for non-zero k, F and G are oscillatory whereas for $k = 0$ they are polynomial and have a much smoother behaviour.

5. Method II and the HJ potential

The theory described in § 3 has been applied to the system considered in § 4 using trial functions (4.1). The results obtained are shown in figure 2. Figure 2(a) shows the

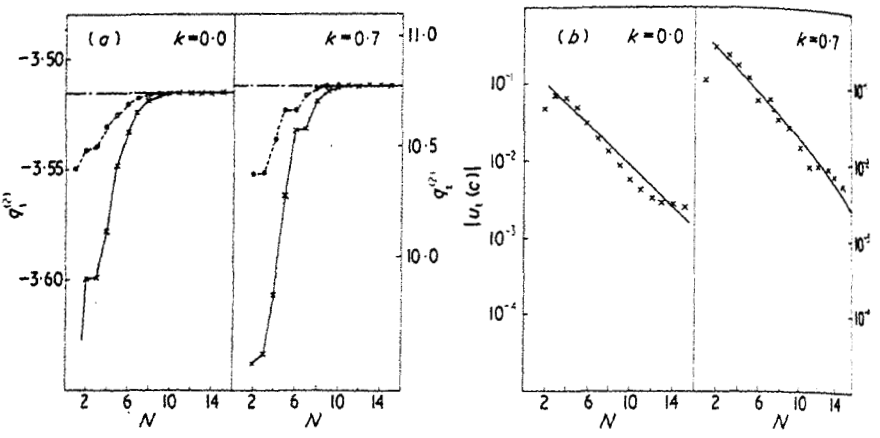

Figure 2. Method II for $k=0{\cdot}0$, $0{\cdot}7$ ($\alpha=2{\cdot}0$). (*a*) $q_t^{(2)}$ against N; (*b*) $|u_t(c)|$ against N. —×—×—, method II; —○—○—, CKVP; — — — —, exact value from CKVP.

second-order estimate $q_t^{(2)}$ for two values of k from method II. Also shown are the results from a CKVP calculation for this system (ie, the boundary conditions at $r=c$ are satisfied by including a suitable factor in the F and G terms and $h_i=(r-c)^i\,\mathrm{e}^{-\alpha r}$). It can be seen that as N increases the results for method II are converging to the same value as those of the CKVP but tend to lag slightly behind. This is typical of the results of HH, and as observed there, is not surprising since method II must work harder to reproduce the value of q and the boundary condition at $r=c$. Figure 2(*b*) shows $|u_t(c)|$ for both energies and as N increases this is tending to get smaller showing that the boundary condition is indeed being reproduced.

As in § 4, the results for $k=0$ are slightly better than those for $k=0{\cdot}7$.

6. Conclusions

In this paper, two variational methods have been demonstrated for scattering problems which do not require the trial functions to satisfy the boundary conditions. These methods have been explicitly set up for a two-body system, but analogous methods could be derived for more complex situations.

The first method requires no knowledge of derivatives, but would need the optimal choice of the coupling parameter β (which was found to be large for the system considered).

The second method requires derivatives at the core, but apart from this the formalism is very similar to the CKVP. Furthermore the results obtained are (almost) as good. It is also apparent from the figures that method I gives results which converge much less rapidly than do the corresponding results for method II. This can be easily understood. In method I, q_t is obtained from the solution of a set of linear equations (2.5) and is a first-order estimate of q. However, in method II, the first-order estimate $q_t^{(1)}$ is fed into functional (3.2) to give a second-order estimate $q_t^{(2)}$ of q. Hence we expect method II to give a better convergence rate than method I.

Thus the results obtained here, taken together with those of HH, show that it is possible to determine the quantities of interest in a nuclear system using variational methods with trial functions which do not satisfy the prescribed boundary conditions.

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