An effective Hamiltonian method for the solution of the Schrodinger equation. I. The one-dimensional problem

An effective Hamiltonian method for the solution of the Schrödinger equation I. The one-dimensional problem

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Abstract. A method is presented for solving the one-dimensional Schrödinger equation in which the potential is approximated by a step function. This effective Hamiltonian is then solved exactly by a continued fraction technique which enables the convergence properties to be studied. The method is particularly suitable for the solution of scattering problems for which upper and lower bounds can be obtained for the phase shifts.

1. Introduction

The approximation discussed here is the simple one of replacing a smooth potential by a step function potential. This technique has been used before in a number of fields such as obtaining Green functions (Hennell 1968) but also by Canosa and Gomes de Oliveira (1970) for solving bound-state problems in the one-dimensional Schrödinger equation. The method presented here is devised principally for solving the scattering problem for which upper and lower bounds can be obtained for tan δ.

2. The method

The one-dimensional Schrödinger equation for the scattering of two particles (bound-states will be discussed later) is

$$\frac{d^2}{dr^2}\psi(r) + k^2\psi(r) - U(r)\psi(r) = 0 \tag{1}$$

where k is the relative momentum of the two particles. For simplicity, only the $l = 0$ case will be discussed although the method can cope quite easily with $l \neq 0$. The boundary conditions are then

$$\psi(0) = 0, \qquad \lim_{r \to \infty} \psi(r) = A(\sin kr + \tan \delta \cos kr)$$

δ being the phase shift.

The approximation is to replace the potential $U(r)$ by the step potentials

$$U(r) \approx V(r) = V_n, \qquad r/h \in [n-1, n] \qquad (n = 1, 2, \ldots, N) \tag{2}$$

where h is the step length and for the moment take $V_n = U[(n-\frac{1}{2})h]$ ie the value of $U(r)$

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at the midpoint of the nth region. Then in the nth region with the approximation (2) the equation (1) becomes

$$\frac{d^2}{dr^2}\psi_n(r) + k_n^2\psi_n(r) - V_n\psi_n(r) = 0 \tag{3}$$

for which the exact solution is

$$\psi_n(r) = A_n \sin p_n r + B_n \cos p_n r \tag{4}$$

with $p_n^2 = k^2 - V_n > 0$ (for $p_n^2 < 0$ the sinh and cosh solutions may be taken). The constants A_n and B_n may be obtained from the constants A_{n-1} and B_{n-1} of the $(n-1)$th region by requiring continuity of the solutions and their first derivatives at the region interfaces. The result of this is

$$D_n = \frac{a_n + D_{n-1}b_n}{c_n + D_{n-1}d_n} \qquad D_n = \frac{B_n}{A_n} \tag{5}$$

with

$$a_n = \cot p_{n-1}R - K \cot p_n R$$

$$b_n = -(1 + K \cot p_n R \cot p_{n-1}R)$$

$$c_n = -(K + \cot p_n R \cot p_{n-1}R)$$

$$d_n = (-K \cot p_{n-1}R + \cot p_n R)$$

$$K = p_n/p_{n-1}$$

$$R = nh.$$

In the first region the boundary condition at the origin is $\psi_1(0) = 0$ from which $D_1 = 0$. Thus the continued fraction (5) can be summed outwards to any region quite simply. If the sequence (2) is now terminated at the Nth region, ie the potential being zero for $r \geqslant Nh$, then

$$D_{N+1} = \tan \delta_{R,h}$$

where $\delta_{R,h}$ is the exact scattering phase shift for the effective Hamiltonian.

The method then is to choose a step length h and, starting from the origin, step outwards until convergence with respect to N of $\tan \delta_{R,h}$ is obtained to a given accuracy. The technique is then repeated for a smaller h, out to the same point R as before and this process of reducing h is repeated until $\tan \delta_{R,h}$ has converged with respect to changes in h.

In figure 1 the central curve shows results for the potential $U(r) = e^{-r^2}$. This shows that as $h \to 0$ and with $R = 5.0$ (for four significant figures), $\tan \delta$ converges towards the 'exact' solution (which in this case was obtained both by variational and finite difference routines).

In appendix 1 it is shown that if $V_n = U[(n-\frac{1}{2})h]$ then the method is of order h^2 ie the error term decreases as the square of the step length. This result is confirmed in figure 4 where a graph is drawn of $\lg(\tan \delta_{R,h} - \tan \delta_\infty)$ against $\lg h$ (δ_∞ is the exact phase shift for the given potential $U(r)$ ie $\delta_\infty = \delta_{R,0}$). It may be seen that the result is a straight line of slope 2.0 approximately.

Since (5) is a continued fraction, the problems of convergence may be studied from this viewpoint, particularly since a considerable amount of work has been expended on the convergence problem (Wall 1948). A formal analysis of convergence on this basis
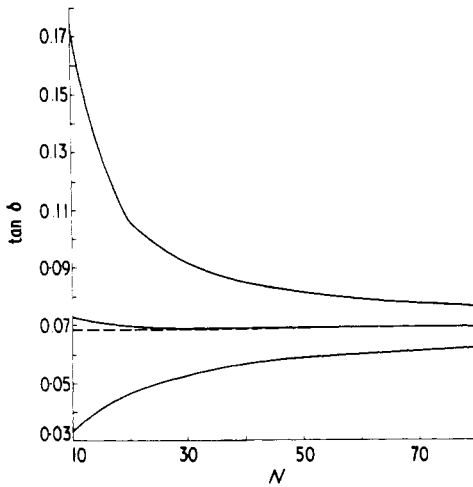
Figure 1. $V(r) = e^{-r^2}$; the central curve gives the results for $\tan \delta$ against h for the midpoint method whilst the outer two curves are the upper and lower bounds. The broken line gives the exact solution. $k^2 = 0.01$, $R = 5.0$.

will be presented elsewhere. The class of potentials for which convergence can be proved is, as yet, rather restrictive; however in practice the method converges to the correct solutions for a number of realistic nucleon–nucleon potentials.

3. Bounds for δ

In any region, the point at which $U(r)$ is evaluated is arbitrary. Intuitively, it would seem that evaluating $U(r)$ at the midpoint is likely to prove the best approximation. In the case of a wholly attractive potential, if V_n is evaluated so that

$$V_n = \max|U(r)|, \qquad (n-1)h \leqslant r \leqslant nh$$

an effective Hamiltonian can be constructed which is everywhere more attractive than $U(r)$ and the $\tan \delta_{R,h}$ for this effective Hamiltonian will be an upper bound on $|\tan \delta|$ for $U(r)$ (see appendix 2). In general it would be necessary only to evaluate $U(r)$ at the step length to obtain $V_n^{\max}$ with the exception of turning points, for which it is necessary to obtain the turning point itself and in the region encompassing the turning point, $U(r)$ should be evaluated there.

Similarly lower bounds can be obtained by taking $V_n = \min|U(r)|, (n-1)h \leqslant r \leqslant nh$. In this case there is no problem with the turning points and V_n will be given by $V_n = \min$ of $\{U[(n-1)h], U(nh)\}$.

In figure 2 upper and lower bounds are shown for $U(r) = e^{-\mu r}/\mu r, \mu = 1/1.58$, whilst in figure 1 the bounds are given for $U(r) = e^{-r^2}$. Although the Yukawa potential has a singularity at the origin, this does not affect either the midpoint approximation or the lower bounds. For the upper bounds, however, V_1 is infinite which forces $\psi_1 = 0$ so that the iteration technique starts from region 2 with $D_2 = 0$. In appendix 1 it is shown that with the effective potential evaluated at the region boundaries the method is of order h, hence the bounds are significantly slower to converge than the midpoint method, a point which is clearly seen in figures 1 and 2.

For the case of potentials which oscillate in sign, it is possible to obtain upper bounds (say) by taking the effective step potentials greater than $U(r)$ for the attractive
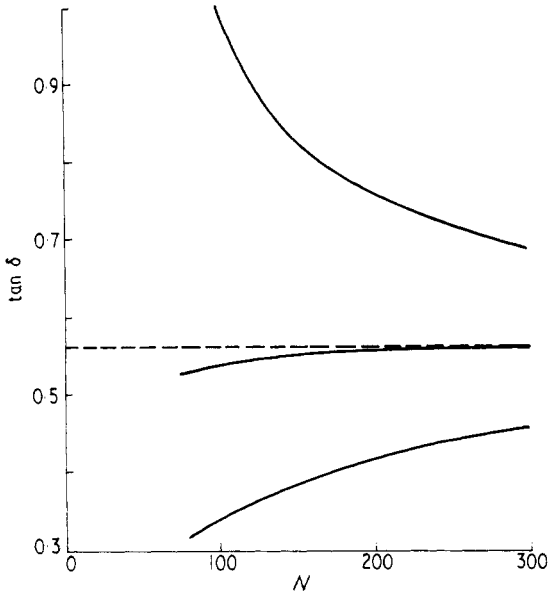
Figure 2. $V(r) = e^{-\mu r}/\mu r$, $\mu = 1/1\cdot58$; the central curve gives the results for tan δ against h for the midpoint method whilst the outer two curves are the upper and lower bounds. The broken line gives the exact solution. $k^2 = 12\cdot0$, $R = 16\cdot0$.

components and less than $U(r)$ for the negative components, and vice versa for the lower bounds. This is illustrated by figure 3 where bounds are presented for the potential

$$U(r) = -10\cdot463\frac{e^{-x}}{x} - 1650\cdot6\frac{e^{-4x}}{x} + 6484\cdot2\frac{e^{-7x}}{x}$$

(this is the $^1S_0$ nucleon–nucleon potential of Reid). Clearly the bounds are converging to the exact result.

So far in this discussion the choice of step length has not been considered. Since it is not necessary to use a constant step length it is possible to use a number of schemes for estimating an optimum value. For instance, initially a large h may be chosen and
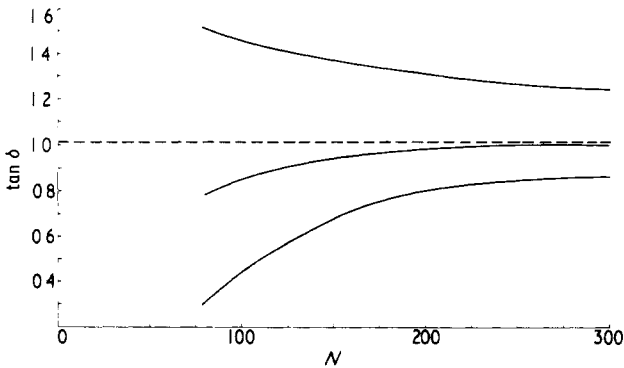

Figure 3. $V(r)$ is the Reid $^1S_0$ nucleon–nucleon potential; the central curve gives the results for tan δ against h for the midpoint rule whilst the outer curves are the upper and lower bounds. The broken line gives the exact solution. $k^2 = 12\cdot0$, $R = 16\cdot0$.

$D_2(h)$ evaluated, then the step is reduced to $h/2$ and the $D_3(h/2)$ obtained with this step length should agree with $D_2(h)$ to some specified accuracy. If this is not true then the step should be reduced to $h/4$ and the process repeated until a suitable step length is obtained. This step length can then be used for the next 10 (say) steps and then another search for h (preferably larger) can be made and so on. The effect of this is to obtain the required accuracy with just one run on a computer. In the calculations presented here the step length has been kept fixed.

4. Bound-states

The case of bound-states has been treated by Canosa and Gomes de Oliveira (hereafter referred to as CG) who have used the technique of approximating $U(r)$ by a step function. Their method is to solve the system of equations obtained by matching at the boundaries and obtain the A_n and B_n explicitly. At the same time they obtain the eigenvalues. For the case of bound-states it would appear that the method of CG has more to offer than the method presented here. It is clear that the approximations to $V(r)$ presented in § 3 will also give upper and lower bounds for the eigenvalues when used in the method of CG, a point not discussed by them. Also, the proof that the bound-state method is of order h^2 follows by carrying over the proof given in appendix 1 to the Rayleigh–Ritz formula. (CG were unable to produce such a proof.)

A further point is the question of round-off error. In their paper CG emphasize that their method (without resorting to some clever tricks) suffers from severe round-off errors for rapidly varying or deep potentials (terms such as $\cosh 100 - \sinh 100$ occurring). It is worth noting that the method outlined in this paper does not appear to have
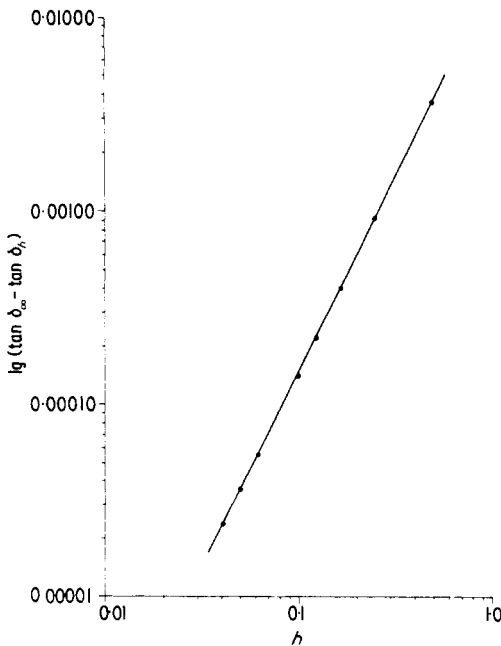

Figure 4. $\lg(\tan \delta_\infty - \tan \delta_h)$ against h. The slope is 2·0, showing that the midpoint method is $\theta(h^2)$.

this disadvantage, successive runs with the Reid potential have shown agreement to at least eight significant figures between computer runs in single (11 significant figures) and double (23 significant figures) precision.

5. Conclusion

The method presented here arose from attempts to solve integral equations by step potential approximations and a further paper will be presented demonstrating this technique. The method has also been demonstrated for the case of coupled ODE's in particular for the case of the coupled triplet states in neutron–proton scattering.

It is also intuitively obvious that although the method outlined above is only an h^2 method, an improvement can be obtained $[\theta(h^3)]$ if instead of approximating with square wells a trapezium approximation is used. Higher-order methods also appear possible. The important point here is that rigorous bounds can still be obtained, these cannot be obtained by finite difference methods.

The method is extremely simple to implement and if only phase shifts are required, the storage requirements are negligible, making the method attractive to users of small computers. Since the step length is optional it is possible to construct algorithms which reduce the number of steps considerably.

Acknowledgments

Appendix 1

The variational estimate for the phase shift is

$$\tan \delta = \tan \delta_t + \int_0^\infty \psi_t (H - E)\psi_t \, dr + \theta(\delta\psi_t^2) \tag{A1.1}$$

where ψ_t is a trial function, δ_t is the corresponding trial phase shift and $H = T + V(r)$, T being the kinetic energy. For ψ_t, take the exact solution ψ_n for the effective Hamiltonian. This satisfies the equation

$$(T + V_n - E)\psi_n = 0, \qquad (n-1)h \leqslant r \leqslant nh.$$

Then

$$(T + U - E)\psi_n = [T + V_n - E + (U - V_n)]\psi_n$$
$$= (U - V_n)\psi_n$$

from which (A1.1) becomes:

$$\tan \delta = \tan \delta_t + \sum_{n=1}^N \int_{(n-1)h}^{nh} \psi_n(r) [U(r) - V_n]\psi_n(r) \, dr.$$

Transforming to $y = r - (n-1)h$ gives

$$\tan \delta = \tan \delta_t + \sum_{n=1}^{N} \int_0^h \psi_n(y)[U(y) - V_n]\psi_n(y)\,\mathrm{d}y.$$

Consider an arbitrary point $y = \alpha h$, then $\psi_n(y)$ and $U(y)$ may be expanded about this point so that

$$\psi_n(y) = \psi_n(\alpha h) + z\psi_n'(\alpha h) + \frac{z^2}{2}\psi_n''(\alpha h) + \dots$$

$$U(y) = U(\alpha h) + zU'(\alpha h) + \frac{z^2}{2}U''(\alpha h) + \dots$$

where

$$z = y - \alpha h \qquad \text{and} \qquad -2\alpha h \leqslant z \leqslant h(1-\alpha).$$

Transforming the integral and inserting the expansion for $\psi_n(y)$ and $U(y)$ gives, after integration and collecting up the terms in powers of h:

$$\int_0^h \psi_n(y)[U(y) - V_n]\psi_n(y)\,\mathrm{d}y$$

$$= h\psi_n(\alpha h)^2[U(\alpha h) - V_n] + h^2(1 - 2\alpha)[\psi_n(\alpha h)U(\alpha h)\psi_n'(\alpha h) + \psi_n(\alpha h)\psi_n'(\alpha h)U(\alpha h)]$$

$$+ h^3(\dots) + \dots.$$

From this expression it can be seen that if V_n is chosen to be the value of $U(r)$ at any arbitrary point ie $V_n = U[(n-1+\alpha)h]$, then the first term of this expression vanishes. The second term vanishes only when $\alpha = \frac{1}{2}$ ie if $V_n = U[(n-\frac{1}{2})h]$. Thus the local truncation error for $\tan \delta$ is $\theta(h^2)$ for V_n evaluated at an arbitrary point and $\theta(h^3)$ for the special case of the midpoint rule.

Since there are N such regions, the global error estimate will be $\theta(h)$ and $\theta(h^2)$ for the two cases ($N = R_{\max}/h$). This analysis shows that the midpoint method has the smallest error estimate $\theta(h^2)$ whilst both the upper and lower bound methods will be $\theta(h)$.

Appendix 2

Consider the variational estimate and error term for the phase shift ie

$$\tan \delta_1 = \tan \delta_t + \int_0^\infty \psi_t(H_1 - E)\psi_t\,\mathrm{d}r + \int_0^\infty \epsilon(H_1 - E)\epsilon\,\mathrm{d}r$$

where, $H_1 = T + V_1$, $\psi = \psi_t + \epsilon$ is the exact solution and ψ_t is a trial function. Now let $V_2 = V_1 + v$, then

$$\tan \delta_2 = \tan \delta_t + \int_0^\infty \psi_t(H_2 - E)\psi_t\,\mathrm{d}r + \int_0^\infty \epsilon(H_2 - E)\epsilon\,\mathrm{d}r$$

$$= \tan \delta_1 + \left(\int_0^\infty \psi_t v(r)\psi_t\,\mathrm{d}r + \int_0^\infty \epsilon v(r)\epsilon\,\mathrm{d}r \right).$$

Hence, for $v(r) > 0$ for all r, $\tan \delta_2$ will be an upper bound on $\tan \delta_1$. Similarly, if $v(r) < 0$ for all r, then $\tan \delta_2$ will be a lower bound on $\tan \delta_1$.

References

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