

Pseudo-bound wavefunctions in the generator-coordinate method

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1982 J. Phys. A: Math. Gen. 15 2383

(<http://iopscience.iop.org/0305-4470/15/8/018>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 30/05/2010 at 16:04

Please note that [terms and conditions apply](#).

Pseudo-bound wavefunctions in the generator-coordinate method

R G Lovas^{†‡} and M A Nagarajan[†]

[†] Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England

[‡] Institute of Nuclear Research, Debrecen, PO Box 51, H-4001, Hungary[§]

Received 14 January 1982

Abstract. The method of using square-integrable trial functions for representing resonant and scattering states is adapted to the generator-coordinate description of two-cluster systems. Numerical tests in an exactly soluble two-particle model indicate that the method is suitable for locating a resonance and is surprisingly accurate in predicting scattering phase shifts. The method is shown to be closely related to the Kohn variational scattering formalism used in the framework of the generator-coordinate method.

1. Introduction

The possibility of describing a scattering state as a sum of bound states was first investigated by Temkin (1966) who applied it to the study of the excited states of the H^- system. This approach was studied in great detail by Hazi and Taylor (1970), and since then the representation of unbound states by square-integrable functions has been widely used in atomic physics (Reinhardt 1979). In nuclear physics this idea was introduced in the description of stripping reactions to resonant states (Fortune *et al* 1969, Cole *et al* 1970, Coester and Schlessinger 1973). The use of square-integrable functions has proved to be a reasonable approximation for not-too-broad resonances (Schlessinger and Payne 1972, Barz *et al* 1973). Its merit lies in its simplicity and applicability in other approaches and fields as well. For instance, in the framework of the coupled reaction channels method the use of the square-integrable representation seems to be the only way of including unbound residual states (Lovas 1977). Square-integrable functions have also been used in structure calculations in order to discretise the single-particle continuum (Hird and Huang 1973, Csernai *et al* 1978). Recently Filippov and Okhrimenko (1980) used a square-integrable basis in the resonating group method for a scattering calculation. The description of cluster states in the framework of the generator-coordinate method (GCM) (see e.g. Mihailović and Rosina 1973) also lends itself to treating unbound states as if they were bound, and it is common to apply it to resonances (see e.g. Mihailović and Poljšak 1978).

But it is by no means self-evident that square-integrable functions can be used to represent positive-energy states if the model Hamiltonian allows particle emission. It is in this case that we call the square-integrable model wavefunctions pseudo-bound (PB) and their application to describing unbound states the pseudo-bound state method (PBSM). For them the familiar variational foundation of the ordinary bound-state

[§] Present address.

approximation methods does not give sufficient backing. For a potential model, however, Hazi and Taylor (1970) have shown that the PB states obtained by diagonalising the Hamiltonian on a harmonic oscillator basis are closely associated with the exact scattering states of the system.

Our aim is to explore the possibilities of the legitimate use of PB wavefunctions to describe unbound states in the framework of the GCM. We adapt Hazi and Taylor's PB diagonalisation method to the GCM and test various recipes for computing the measurable quantities (resonance parameters and phase shifts). To this end we have made calculations in an exactly soluble model with GCM-like trial functions. The GCM-like basis is found to behave largely similarly to the harmonic oscillator basis, thus the conclusions are probably more general. On the other hand, the GCM basis turns out to have some very favourable special properties, and that indicates its usefulness in atomic physics as well.

First of all, we shall briefly relate the PBSM to the bound-state variational methods and summarise the correspondence between the exact wavefunction of an unbound system and its PB approximant (§ 2). Then, in § 3, we shall show the model calculations for resonant and scattering states. In § 4 we shall discuss the working mechanism of the PBSM and clarify its relation to its closest relatives, the Kohn-type variational formalism of the GCM and the Hulthén variational method. In § 5 we shall outline how the PBSM can be implemented in actual GCM calculations. In § 6 we summarise the results and give an appraisal of the method.

2. Properties of the pseudo-bound states

The PBSM involves the solution of the time-independent Schrödinger equation above the particle emission threshold (zero energy) in a square-integrable function space. Since in such a space this equation is only fulfilled at discrete energy eigenvalues, the PBSM consists in solving energy eigenvalue problems. These can be viewed as true bound-state problems for the Hamiltonian projected onto the subspace spanned by the PB basis. Consequently, the PB solution can be found using the bound-state variational principle (see e.g. Moisewitsch 1966, pp 163–8).

According to this, the solution is provided by the stationary points of the energy functional

$$E[\chi] = \langle \chi | H | \chi \rangle / \langle \chi | \chi \rangle.$$

It follows from the properties of $E[\chi]$ that the approximate energy will be above the exact energy of the lowest lying state to which χ is not orthogonal (Temkin 1966). This implies that, when there is no bound state of some particular strict quantum numbers, the approximate energy of a state of these quantum numbers cannot be negative. An approximate energy is guaranteed to be greater than (or equal to) the exact one if the lower lying eigenstates are projected out from the trial function. Such a projection may be possible by the introduction of states that approximate the eigenstates but is likely to be complicated in the general case. If χ contains only linear variational parameters, the stationary points are obtained by diagonalising the Hamiltonian on the square-integrable basis that spans χ : $\chi = \sum_i c_i \chi_i$. Addition of any new element to the basis, while producing a new eigenvalue higher than the original ones, lowers all the others provided H is Hermitian, whether the energy is negative or positive. But this monotonicity does not guarantee that the increase of the basis

will improve the description of any particular positive-energy state since the lower lying states are not projected out from χ . Thus it is not obvious what a particular PB state represents.

Hazi and Taylor (1970) have observed that in the harmonic oscillator basis a PB wavefunction closely follows the scattering solution belonging to the same energy up to some distance Λ , which can be arbitrarily chosen by choosing the basis size, and then tends to zero sharply. If Λ is in the asymptotic region, the PB wavefunction carries information on the scattering phase shift. In this sense a PB state represents the scattering state of the same energy. A change of the basis size shifts the spectrum of eigenenergies, and hence the new set of PB states corresponds to continuum states of shifted energies. The diagonalisation usually positions a PB state at each resonance of the system, and the energy of this state is extremely stable against changes in the basis. This state carries information not only on the phase shift but also on the resonance parameters. Therefore, it can be considered to be a state that approximates a particular continuum state as well as being a discrete state representing the resonance.

The GCM is a linear variational method, thus all the general considerations put forward so far apply to it. But since its basis is very different from a harmonic oscillator one, it is important to see whether the above interpretation of the individual PB states is still valid. That is why we introduce the exactly solvable model and solve it approximately with a basis which bears all the essential features of the GCM.

3. Model calculations

3.1. Model for the generator-coordinate method

In the GCM description of two interactive clusters A and B the trial wavefunction is of the form

$$\Psi^{JM\pi} = P^{JM\pi} \int d\mathbf{S} f(\mathbf{S}) \mathcal{A} \left[\exp\left(-\frac{(\mathbf{r}-\mathbf{S})^2}{2b^2}\right) \Phi_A \Phi_B \right],$$

where Φ_A and Φ_B are the internal wavefunctions, r is the relative coordinate of A and B , b is an oscillator parameter, \mathcal{A} is the intercluster antisymmetriser, $f(\mathbf{S})$ is a variational function and $P^{JM\pi}$ is an angular momentum and parity projector. In practice the integral is discretised so that the wavefunction of the relative motion becomes a linear combination of shifted Gaussians centred around the discrete points \mathbf{S}_i :

$$\Psi^{JM\pi} = \sum_i c_i^{JM\pi} \Phi^{JM\pi}(\mathbf{S}_i) \quad (1)$$

with

$$\Phi^{JM\pi}(\mathbf{S}_i) = P^{JM\pi} \mathcal{A} \left[\exp\left(-\frac{(\mathbf{r}-\mathbf{S}_i)^2}{2b^2}\right) \Phi_A \Phi_B \right]. \quad (2)$$

When $\Psi^{JM\pi}$ is not a bound state, it has an oscillating tail in r , which requires the sum in (1) to be infinite with $\mathbf{S}_i \rightarrow \infty$ as $i \rightarrow \infty$. Therefore, when applied to unbound states, (1) is truncated, and the asymptotic region is usually taken care of by some other means. A PB approximation is obtained by just truncating this sum without any further provision for the asymptotic region.

Since Φ_A and Φ_B are frozen even in realistic calculations, the PB representation of the relative motion can be studied equally well by considering a two-body model. Furthermore, since this approximation concerns the asymptotic region, where the antisymmetrisation and the exact form of the interaction have little effect, it is justifiable to neglect the antisymmetrisation and to use a schematic interaction. We consider two spinless particles of the nucleon mass interacting in the relative s state via a potential consisting of a square well and a square barrier. In the examples to be shown the potential has been chosen to be

$$V(r) = \begin{cases} -40 \text{ MeV}, & 0 \leq r < 2 \text{ fm}, \\ 20 \text{ MeV}, & 2 \text{ fm} \leq r < d, \\ 0, & d \leq r, \end{cases} \quad d = 5 \text{ fm}.$$

Our basis is non-orthonormal and looks like

$$\begin{aligned} \phi_i(r) &= P^{00+} \exp\left(-\frac{(r-S_i)^2}{2b^2}\right) = \frac{u_i(r)}{r} Y_{00}(\hat{r}), \\ u_i(r) &\equiv u(S_i, r) = \pi^{1/2} \frac{b^2}{S_i} \left[\exp\left(-\frac{(r-S_i)^2}{2b^2}\right) - \exp\left(-\frac{(r+S_i)^2}{2b^2}\right) \right]. \end{aligned} \quad (3)$$

To get the PB eigenfunctions

$$u_n^{\text{PB}}(r) = \sum_{i=1}^N c_i u_i(r), \quad (4)$$

we solve the equation

$$\langle \delta u_n^{\text{PB}} | H - E_n | u_n^{\text{PB}} \rangle = 0,$$

which amounts to diagonalising H in the basis defined in (3). To be able to reach far away from the centre with a relatively convenient basis size, we have chosen the values of b and the steps $\Delta S = S_i - S_{i-1}$ as large as possible while still reasonably covering the region of the potential:

$$b = 0.65 \text{ fm}, \quad S_i = (i - 0.5) \text{ fm} \quad (i = 1, 2, \dots, N; N = 3, 4, \dots, 48).$$

The lowest pole of the S -matrix is at $(4.941 - 0.480i)$ MeV. The PB eigenvalues $E_n(S_N)$ belonging to node numbers $n = 0, 1, 2, 3$ and 4 as a function of N (or S_N) are plotted in figure 1. As is expected from the considerations of § 2, all the eigenvalues decrease monotonically as the basis is extended and apparently tend to zero energy as N is increased. (Note the logarithmic energy scale.)

3.2. Resonances

The resonance appears in the energy-versus-dimension 'curves' of figure 1 as inflexion points. The shoulders of the neighbouring curves could be joined together to form the 'stable' eigenvalue of Hazi and Taylor (1970). Our basis also bears out Hazi and Taylor's other finding, namely, that the narrower the resonance the flatter the shoulder.

We compare the exact Gamow wavefunction of the resonance with its PB representations belonging to different node numbers in figure 2. The two PB functions in each section of the figure correspond to energies that are more or less equally close to the exact energy. Of course, the approximate method cannot imitate the imaginary part and the exponentially increasing amplitude of the Gamow function, but it does

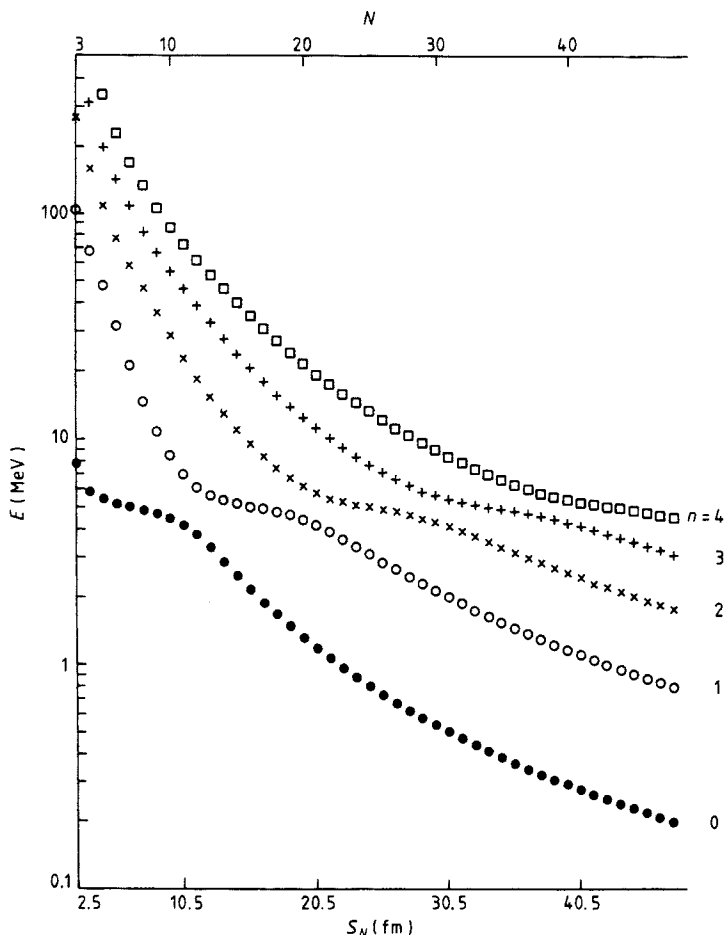


Figure 1. The eigenenergies belonging to node numbers $n = 0, 1, 2, 3, 4$ of the problem, defined in the text, in the PB bases of dimension N or last discretisation point S_N .

reproduce the 'nuclear' interior as well as the extrema and nodes of the tail of its real part up to the $(n + 1)$ th node. The basis sizes N that generate the resonance function of n nodes are distinguished by the fact that $S_N + b \leq r_{n+1}$, where r_{n+1} is the position of the $(n + 1)$ th node of the real part of the exact function.

In this manner there are an infinite number of PB wavefunctions belonging to the same resonance, but they are not quite equivalent. The first one is the PB state of Huby (1970) and Cole *et al* (1970), and it is only this one that follows very closely the Gamow function if both are properly normalised to unity (Lovas 1974). As we shall see, the PB functions that have at least one extremum in the asymptotic region rather closely follow the exact scattering wavefunction as well. This suggests that they should rather be normalised asymptotically like the continuum wavefunctions and interpreted as approximate scattering functions.

The 'stabilisation method' of Hazi and Taylor (1970) for finding a resonance consists in determining the $E_n(S_N)$ sets for several n and selecting out the stable value to be identified with the resonance energy ε . The resonance width can then be

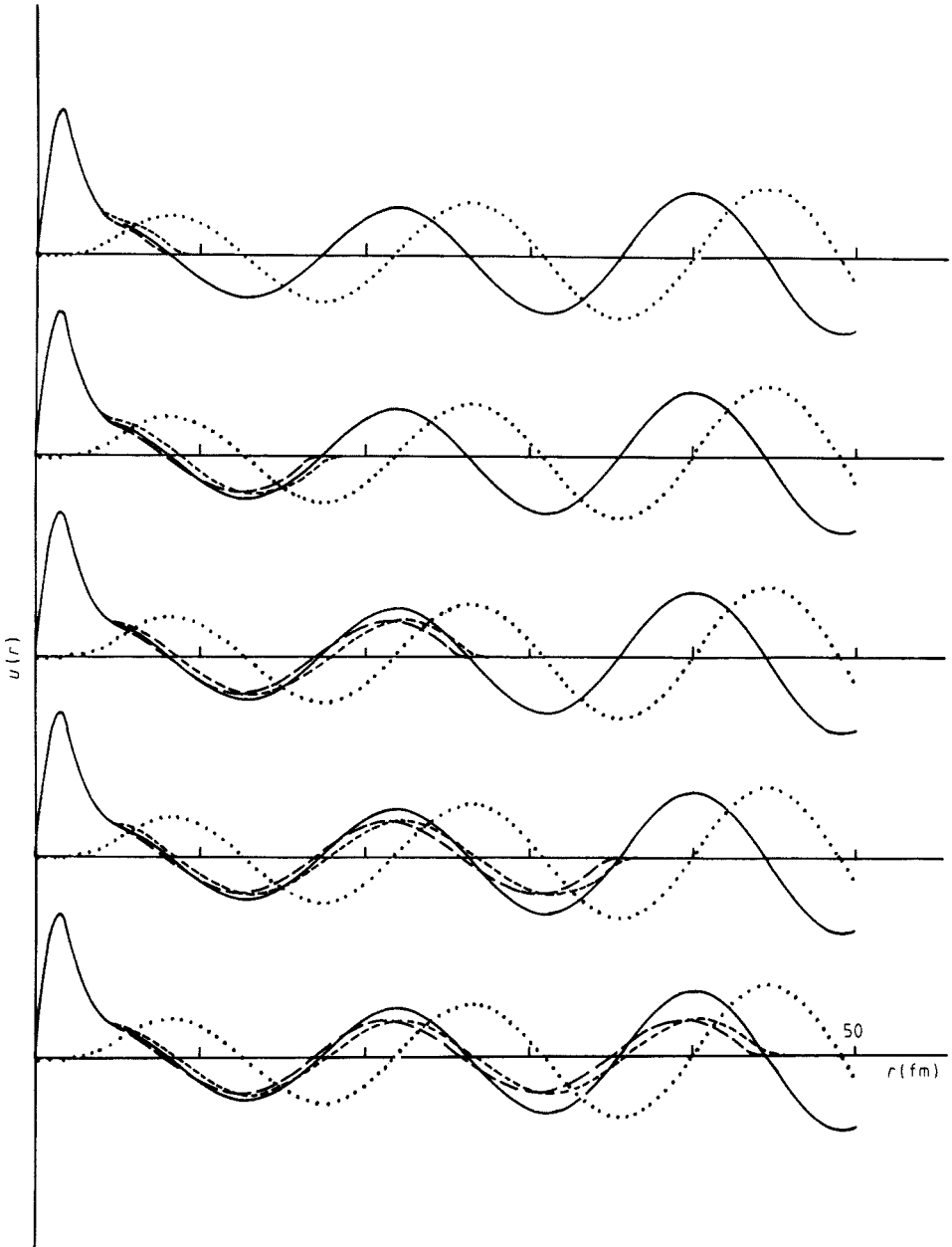


Figure 2. The exact resonance wavefunction (real part: full curve; imaginary part: dotted curve) and its two approximants belonging to slightly higher (long broken curve) and lower (short broken curve) energies, respectively, repeated for different node numbers n . The approximate wavefunctions belong to the following basis sizes: $N = 7, 8$ for $n = 0$; $N = 16, 17$ for $n = 1$; $N = 25, 26$ for $n = 2$; $N = 34, 35$ for $n = 3$; $N = 43, 44$ for $n = 4$. The phase of the exact function is chosen to make the function real at the first maximum of its modulus. The approximate functions are normalised so that they are equal to the exact function at this point.

calculated from any of the $E_n(S_N)$ curves by evaluating the slope of the curve at a point S_N close to the inflexion point. Rewriting equation (21) of Hazi and Taylor (1970), we obtain

$$\Gamma = -\frac{4}{\kappa} \left(\frac{2}{dE_n/dS_N} + \frac{S_N}{\varepsilon} \right),$$

where κ is the wavenumber corresponding to the resonance energy according to $\varepsilon = \frac{1}{2}\kappa^2$. The resonance energies and widths corresponding to the wavefunctions of figure 2 are given in table 1. The agreement with the exact values ($\varepsilon = 4.941$ MeV, $\Gamma = 0.960$ MeV) is not too bad though the width is systematically overestimated, and should we not know the exact energy and wavefunction, it would be difficult to tell which of the energies is the best. Indeed, in nuclear physics we need to analyse broader resonances as well, and for these the shoulders of $E_n(S_N)$ are even less well defined. For the resonance produced by the model potential with $d = 3.5$ fm at $E = \varepsilon - i\Gamma/2 = (2.040 - 2.171i)$ MeV, there are no shoulders at all. In general, the resonance energy cannot be determined much more accurately than within its width, and the search for a stable point is rather indirect.

Table 1. Approximate resonance energies $\varepsilon = E_n(S_N)$ and widths Γ .

n	N	ε (MeV)	Γ (MeV)
0	7	5.037	1.017
	8	4.878	1.056
1	16	5.037	0.987
	17	4.901	1.026
2	25	5.039	0.984
	26	4.918	1.024
3	34	5.040	0.981
	35	4.931	1.022
4	43	5.042	0.991
	44	4.942	1.035

It is therefore worth-while to compare the PBSM with an approximate method that takes into account the decaying nature of the resonance explicitly. The simplest way to improve on the PBSM in this respect is to include in the basis an outgoing wave that is regularised at the origin and belongs to the resonance wavenumber k to be determined. For example, in our case the inclusion of

$$\mathcal{O}(r) = (1 - e^{-\gamma r^2}) e^{ikr}$$

with $\gamma = 0.2 \text{ fm}^{-2}$ and $N = 5$ produces the resonance energy $E = (4.978 - 0.481i)$ MeV, and the agreement with the exact wavefunction (both in the real and imaginary parts) is excellent. The method of calculating the complex eigenvalues and the corresponding wavefunction has been demonstrated by Giraud *et al* (1981). The inclusion of the non-normalisable wavefunction $\mathcal{O}(r)$ does not cause any problems because it is always used in conjunction with the operator $(H - E_r)$, where E_r is the eigenvalue which defines the wavenumber k . The improvement gained by augmenting the basis with elements of larger S_i is very small and rapidly decreases with growing N . The difference

between the approximate and exact values is thus almost entirely due to the incompleteness of the Gaussian basis inside the potential.

This method is obviously more straightforward and accurate for describing a resonance than the PBSM. We remark, however, that the price we pay for the improvement is non-negligible. In the realistic case the computation of the matrix elements of \mathcal{O} is a delicate and time consuming matter. This method is discussed in detail elsewhere (Giraud *et al* 1981).

3.3. Scattering

Since one is used to regarding resonances as the analogues of bound states at positive energies, it is somewhat surprising that off-resonance scattering states appear to be equally well represented by a PB expansion. We test the idea for a quadruplet of PB states in the vicinity of 8.4 MeV. The PB wavefunctions u_n^{PB} of these states are compared with the exact scattering solutions at the same energies in figure 3. The agreement is excellent. In figure 4 a resonant PB wavefunction is compared with the scattering solution at the same energy. The agreement is actually less perfect here but still quite reasonable.

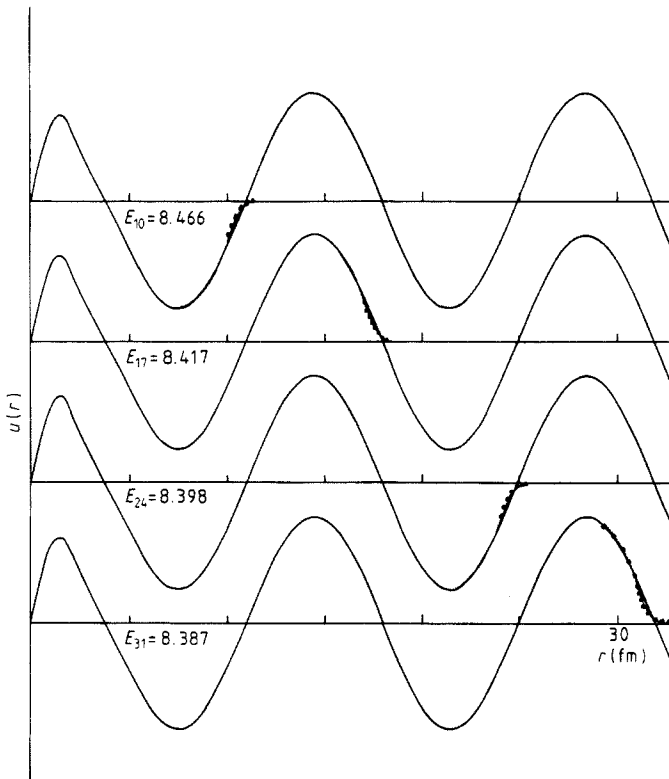


Figure 3. Comparison of off-resonance PB wavefunctions (dotted curves) of energy $E_N \approx 8.4$ MeV, where N is the dimension of the basis, with the exact scattering wavefunctions (full curves) at the same energies. The functions are normalised to be equal at their first maxima outside the potential.

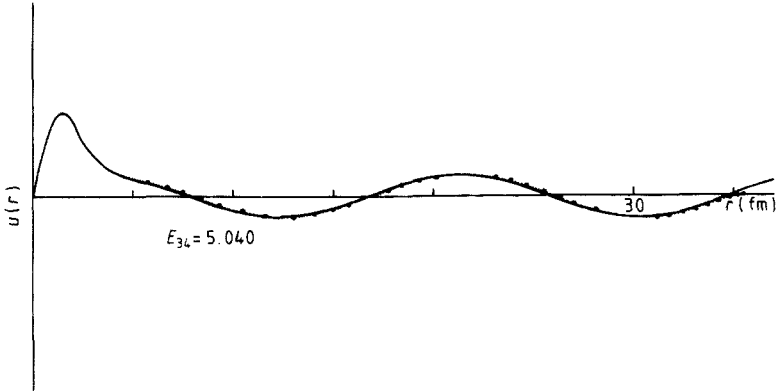


Figure 4. Comparison of a PB wavefunction (dotted curve) with the exact scattering wavefunction (full curve) at the same energy E_N in the resonance region. The functions are normalised to be equal at their first maxima outside the potential.

The fact that $u_n^{PB}(r)$ follows the scattering wavefunction well out in the asymptotic region offers a possibility of extracting from them the scattering phase shifts δ . This can be done, for instance, by assuming

$$u_n^{PB}(r) \sim \sin(k_n r + \delta) \quad (d \leq r \ll S_N) \quad (5)$$

where $k_n = (2\mu E_n / \hbar^2)^{1/2}$ with μ being the reduced mass, and determining δ by comparing this form with the $u_n^{PB}(r)$ calculated at some $r = r_1$ and r_2 ($r_1 \neq r_2$). The arbitrary choice of r_1 and r_2 can be avoided by using the integral representation (Hazi and Taylor 1970) of the K -matrix element $K = \tan \delta$, which reads as

$$K = - \frac{\langle u_n^{PB} | H - E_n | \mathcal{S}_{E_n} \rangle}{\langle u_n^{PB} | H - E_n | \mathcal{C}_{E_n} \rangle} = - \frac{\int_0^R u_n^{PB} (H - E_n) \mathcal{S}_{E_n} dr}{\int_0^R u_n^{PB} (H - E_n) \mathcal{C}_{E_n} dr} \quad (6)$$

Here $\mathcal{S}_{E_n}(r)$ and $\mathcal{C}_{E_n}(r)$ are arbitrary functions that satisfy $\mathcal{S}_{E_n}(0) = 0$, $\mathcal{C}_{E_n}(0) = 0$ and behave like $\sin k_n r$ and $\cos k_n r$, respectively, for $r \in (R, \infty)$, where $d < R < S_N$. The second equality holds because, for $r > R$, $(H - E_n)\mathcal{S}_{E_n}(r) = 0$ and $(H - E_n)\mathcal{C}_{E_n}(r) = 0$. An alternative formula is

$$K = - \int_{R_0}^R u_n^{PB} (H - E_n) \mathcal{S}_{E_n} dr / \int_{R_0}^R u_n^{PB} (H - E_n) \mathcal{C}_{E_n} dr \quad (7)$$

where $R_0 < R$ and the condition at the origin is replaced by $\mathcal{S}_{E_n}(R_0) = \mathcal{C}_{E_n}(R_0) = \mathcal{S}'_{E_n}(R_0) = \mathcal{C}'_{E_n}(R_0) = 0$. (The prime stands for the r derivative.) An obvious choice for \mathcal{S}_{E_n} and \mathcal{C}_{E_n} is

$$\begin{aligned} \mathcal{S}_{E_n}(r) &= \left[1 - \exp\left(-\rho \frac{(r - R_0)^2}{(R - R_0)^2}\right) \right] \sin k_n r, \\ \mathcal{C}_{E_n}(r) &= \left[1 - \exp\left(-\rho \frac{(r - R_0)^2}{(R - R_0)^2}\right) \right] \cos k_n r, \end{aligned} \quad (8)$$

with $\rho \approx 10-30$.

To derive (7), let us integrate the kinetic energy terms by parts twice. Denoting the Wronskian by W , we have

$$\int_{R_0}^R u_n^{\text{PB}} (H - E_n) \mathcal{S}_{E_n} dr = \frac{\hbar^2}{2\mu} [W(\mathcal{S}_{E_n}, u_n^{\text{PB}})]_{R_0}^R + \int_{R_0}^R [(H - E_n) u_n^{\text{PB}}] \mathcal{S}_{E_n} dr \quad (9)$$

and an analogous formula for the denominator. Equation (7) now follows from the assumption that $(H - E_n) u_n^{\text{PB}}(r) = 0$ for $r < R$, which implies that

$$u_n^{\text{PB}}(r) \sim \sin k_n r + K \cos k_n r \quad \text{for } r \approx R, \quad (10)$$

where \sim is the sign of proportionality, and from the identity $W(f, f) \equiv 0$. This derivation shows that formulae (6) and (7) are exact, and hence the K value they yield is independent of the choice of \mathcal{S}_{E_n} and \mathcal{C}_{E_n} , if $u_n^{\text{PB}}(r)$ is an exact solution up to $r = R$.

Apart from pathological choices for r_1 and r_2 , the δ extracted from equation (5) agrees with the exact δ within 0.005 for the non-resonant cases, and there is a systematic difference of about 0.07 in the resonance region. As table 2 shows, the use of (7) reduces even the slight staggering of the δ obtained from (5). It was found that with $\rho = 20$ and $R \approx S_N$ the prediction of (7) hardly depends on R . Its dependence on R_0 , which is notable only for the case of the smallest basis, is due to the 'graininess' of the basis. For the non-resonant cases the accuracy of the estimates is very satisfactory, but in the resonance region the discrepancy survives.

Table 2. Off- and on-resonance phase shifts calculated with N -dimensional bases using equation (7).

N	E_n (MeV)	δ (radian)				
		$R_0 = 0$	$R_0 = 2$ fm	$R_0 = 5$ fm	Exact	
10	8.466	1.3405	1.3435	1.3416	1.3429	
17	8.417	1.3429	1.3432	1.3424	1.3454	
24	8.398	1.3437	1.3438	1.3435	1.3464	
31	8.387	1.3442	1.3442	1.3440	1.3469	
†	33	5.157	0.5978	0.5978	0.5972	0.6699
	34	5.040	0.3850	0.3850	0.3845	0.4654
	35	4.931	0.1729	0.1728	0.1725	0.2537
	$33 + 2^1$	5.147	0.6086	0.6086	0.6081	0.6547

¹ This basis was obtained by augmenting the $N = 33$ basis with two elements centred around 1 and 2 fm, respectively.

† The last four rows corresponding to $N = 33, 34, 35$ and $33 + 2$ refer to the resonance state.

This discrepancy is explained by the fact that, due to the incompleteness of the basis in the region of the potential, the resonance energy is $\Delta E = 0.037$ MeV too high. (This is known from the calculation with the outgoing wave, see § 3.2.) According to the Breit-Wigner formula, this displacement shifts δ by $\Delta\delta = -0.077$, which is consistent with our finding. If this is the cause of the disagreement, it can, of course, be cured by increasing the density of the discretisation points. The inclusion of just two more points (at 1 and 2 fm) reduces ΔE to 0.023 MeV, and that implies $\Delta\delta = -0.048$. The last line of table 2 does show an agreement with this estimate.

4. Discussion

4.1. Working mechanism of the pseudo-bound state method

The way the PBSM works can be understood as follows. The choice of the basis defines an 'expansion length' $\Lambda \geq S_N + b$ beyond which the wavefunction must tend to zero rapidly. Thus the problem with a fixed basis closely resembles one in which the system is closed in a box of radius Λ . The diagonalisation then works like a bound-state variational method for the discrete energies at which the box boundary condition is satisfied. Some of the 'normal modes' generated in this way are plotted in figure 5. It is obvious that at energies at which the exact scattering solution $u(r)$ has a node at Λ , for $r \leq \Lambda$ the exact box solution $u_B(r)$ coincides with $u(r)$. If $u_B(r)$ is well approximated by the PB diagonalisation of expansion length Λ , the PB solution is a good approximation to the scattering problem as well.

With the expansion length increased, the nodes go farther apart, thus the energies E_n belonging to a fixed node number n go to zero. In the asymptotic region the spacing of the nodes is uniform just as within the potential well if there are several nodes there. But the distance between the nodes at the junction of the internal and external regions strongly depends on the energy. Therefore, the $E_n(S_N)$ curves are

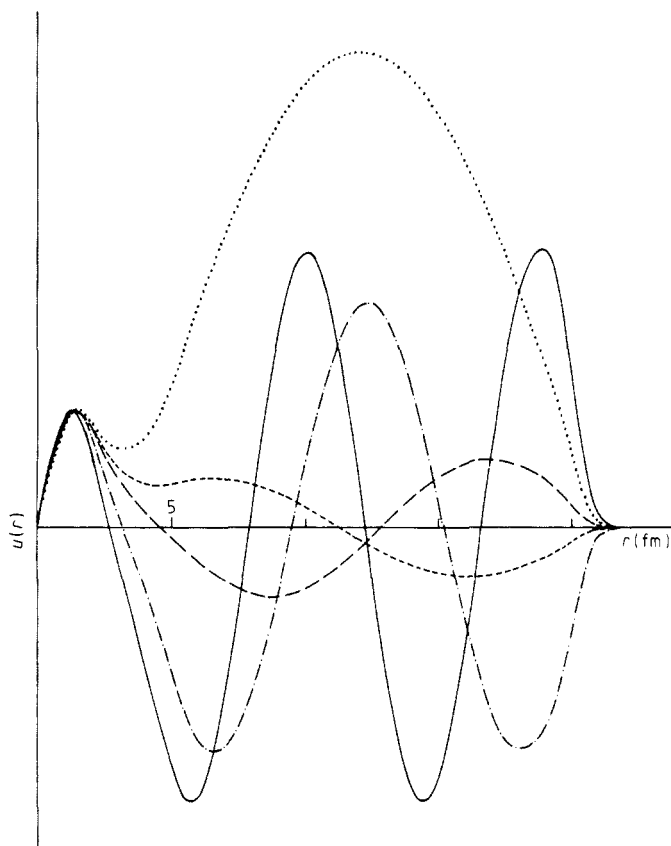


Figure 5. The $N = 20$ ($S_N = 19.5$ fm) PB wavefunctions normalised to be equal at their first maxima.

not smooth. They are flatter at energies where a long neck of the wavefunction is building up and steeper otherwise. The scattering wavefunction has a long neck just at resonances, and that explains the shape of the $E_n(S_N)$ curves.

Any inadequacy of the PB basis has a direct and an indirect effect: it makes the wavefunction (locally) inaccurate and displaces the PB energy. The former, if it occurs locally, can usually be eliminated from the extracted phase shift by suitably choosing R_0 , R and ρ (cf formulae (7) and (8)). The latter, however, is persistent as it causes the phase shift extracted to correspond to another energy.

There seem to be two critical regions where a PB basis may prove to be unsuitable: inside the potential and around $r = \Lambda$. In the inner region it is the rapid oscillation of the wavefunction, while around Λ it is the box boundary condition that tries the pliability of the basis. The greater the number of elements, around a certain point, that differ significantly from the $f(r) \equiv 0$ function, the more pliable is the basis there. While for an N -dimensional oscillator basis this characteristic grows with decreasing r up to N , for an equidistant GCM-like basis it is nearly uniform and usually low compared with N . It is therefore advisable, as we have seen, to choose the discretisation points to be more densely spaced in the interaction region. It is less important to make $\{S_i\}$ more dense around S_N since the PB energy hardly depends on the accuracy of the PB function there. But the R and ρ values are to be chosen, as we did, to cut off the vicinity of Λ .

Since the PBSM transforms the scattering problem to an energy eigenvalue problem, the phase shift at a given energy cannot be calculated directly. Such a method is practical if $\delta(E)$ is to be calculated for a range of energy. Then $\delta(E)$ can be computed at any particular E by interpolation. If, however, we need the solution sharp at a certain energy, we can always find it by varying $\{S_i\}$ (e.g. just S_N). The $\delta(E)$ can be extracted with reasonable accuracy if the PB solution covers at least half a wavelength outside the potential. Further increase of the expansion length (in half wavelength quanta) does not yield a substantially more accurate δ .

The relationship between the single-channel PB and scattering solutions is so simple because any positive-energy solution of the radial Schrödinger equation describes an elastic scattering process. However, if there are several open channels, a solution obtained by fixing the expansion length in each channel will generally contain incoming and outgoing waves in each channel. Just as in any coupled-channels method, the solution with the appropriate asymptotics can be obtained by a linear combination of linearly independent solutions of the same energy. These can be generated by changing the expansion length in each channel.

4.2. Variational background

The PBSM can be considered not only as a bound state but also as a scattering variational method. This was already pointed out by Hazi and Taylor (1970) by producing the same formula (equation (6)) for the K -matrix as the expansion method of Harris (1967), which had been shown to give the same K -matrix as Hulthén's variational method at the eigenenergy E_n (Nesbet 1968). In the GCM, however, it is not the Hulthén but the Kohn version of the Kohn-Hulthén variational approach (Moiseiwitsch 1966, pp 245-56) which has been adopted (Beck *et al* 1975, Mihailović *et al* 1976, Mito and Kamimura 1976); therefore, it is desirable to relate the PBSM to this method as well. For simplicity, we use the notation of the model case, but its generalisation to the realistic elastic scattering case is trivial.

Following Mihailović *et al* (1976), one can solve the scattering problem at any energy E by taking the trial function

$$\chi_E(r) = \sum_{j=1}^N \alpha_j u_j(r) + \mathcal{S}_E(r) + K \mathcal{C}_E(r), \quad (11)$$

where α_j and K are variational parameters and $u_j(r)$ are given in equation (3). Alternatively, the Hamiltonian may be pre-diagonalised in the subspace $\{u_j(r)\}$, to obtain $\{u_m^{\text{PB}}(r)\}$ of (4), and the scattering problem may then be attacked with the trial function of the type proposed by Harris (1967),

$$\phi_E(r) = \sum_{m=1}^N \beta_m u_m^{\text{PB}}(r) + \mathcal{S}_E(r) + K \mathcal{C}_E(r) \quad (12)$$

with β_m and K being the variational parameters. Since the bases (11) and (12) span the same subspace, any variational principle must be satisfied by the same χ_E and ϕ_E .

The Kohn variational principle states that, for functions $\psi_E(r)$ that have the asymptotic form $\psi_E \rightarrow \sin kr + K \cos kr$ (cf equation (10)), the functional

$$\mathcal{L}[\psi_E] = K - (2\mu/\hbar^2 k) \langle \psi_E | H - E | \psi_E \rangle \quad (13)$$

is stationary at $\psi_E = \omega_E$, the exact solution of the scattering problem, against any variations of ψ_E that obey the same boundary condition, and

$$\mathcal{L}[\omega_E] = K_{\text{exact}}.$$

By integration by parts of the kinetic energy term in the right-hand side of (13), one can show that the condition $\delta\mathcal{L}[\omega_E] = 0$ may be written as

$$\delta\mathcal{L}[\omega_E] = -(2\mu/\hbar^2 k) \langle \delta\omega_E | H - E | \omega_E \rangle = 0. \quad (14)$$

If ψ_E results from solving (14) on a truncated space, then $\mathcal{L}[\psi_E] \neq K$ in general; $\mathcal{L}[\psi_E]$ is then an improved approximation to the exact K -matrix. The Kohn method consists in solving (14) with a restricted trial function and calculating the corrected K -matrix, $\mathcal{L}[\psi_E]$.

By substitution of (12) into ω_E , equation (14) takes the form

$$\sum_{m=1}^N \langle u_n^{\text{PB}} | H - E | u_m^{\text{PB}} \rangle \beta_m = -(\langle u_n^{\text{PB}} | H - E | \mathcal{S}_E \rangle + \langle u_n^{\text{PB}} | H - E | \mathcal{C}_E \rangle K) \quad (15)$$

$(n = 1, \dots, N),$

$$\sum_{m=1}^N \langle \mathcal{C}_E | H - E | u_m^{\text{PB}} \rangle \beta_m = -(\langle \mathcal{C}_E | H - E | \mathcal{S}_E \rangle + \langle \mathcal{C}_E | H - E | \mathcal{C}_E \rangle K). \quad (16)$$

The same variational principle would produce similar equations for α_j , but with u_j^{PB} replaced by u_j . In either case, (15) can be formally solved for β_m (or α_j), and the solution substituted into (16) to produce K (Mihailović *et al* 1976), provided that

$$\text{Det}\{\langle u_n^{\text{PB}} | H - E | u_m^{\text{PB}} \rangle\} \neq 0,$$

which is satisfied if $E \neq E_n$. Since, however, the $\{u_m^{\text{PB}}\}$ basis, assumed to be orthonormal, has the property

$$\langle u_n^{\text{PB}} | H - E | u_m^{\text{PB}} \rangle = (E_n - E) \delta_{nm}, \quad (17)$$

at $E = E_n$ equation (15) immediately reduces to (6), whereas for $E \neq E_n$

$$\beta_n = (E - E_n)^{-1} \langle u_n^{\text{PB}} | H - E | \mathcal{S}_E + K \mathcal{C}_E \rangle \quad (18)$$

holds, which, substituted in (16), results in†

$$K = - \frac{\langle \mathcal{C}_E | H - E | \mathcal{S}_E \rangle + \sum_{m=1}^N \langle \mathcal{C}_E | H - E | u_m^{\text{PB}} \rangle (E - E_m)^{-1} \langle u_m^{\text{PB}} | H - E | \mathcal{S}_E \rangle}{\langle \mathcal{C}_E | H - E | \mathcal{C}_E \rangle + \sum_{m=1}^N \langle \mathcal{C}_E | H - E | u_m^{\text{PB}} \rangle (E - E_m)^{-1} \langle u_m^{\text{PB}} | H - E | \mathcal{C}_E \rangle}. \quad (19)$$

In the limit $E \rightarrow E_n$ this also reproduces (6). Because of the equivalence of bases (11) and (12), this also implies that (6) gives the limiting value of the K produced by (11) as well. Thus the PBSM is the common limiting case of the scattering formalisms based on (11) and (12) in the limit $E \rightarrow E_n$.

The application of Hulthén's method on the same trial function ϕ_E consists in determining β_m and K using equations (15) and, instead of (16), the equation

$$\langle \phi_E | H - E | \phi_E \rangle = 0. \quad (20)$$

With (15) adopted, equations (17) and (18) are also implied. As a consequence of (17) and (18), $\langle u_m^{\text{PB}} | H - E | \phi_E \rangle = 0$ holds for all m ; thus the condition (20) can be rewritten as

$$\sum_{m=1}^N \frac{\langle u_m^{\text{PB}} | H - E | \mathcal{S}_E + K \mathcal{C}_E \rangle^2}{E - E_m} + \langle \mathcal{S}_E + K \mathcal{C}_E | H - E | \mathcal{S}_E + K \mathcal{C}_E \rangle = 0, \quad (21)$$

which is to be solved for K . Letting E tend to E_n , we again arrive at equation (6).

Although at $E = E_n$ the Kohn and Hulthén methods give the same $K(E_n)$ of equation (6), and the same $\beta_m(E_n)$ for $m \neq n$, as defined by equation (18), they produce different $\beta_n(E_n)$ and hence totally different wavefunctions. The quantity $\beta_n(E_n)$ is defined by equation (18) as an energy limit, which depends on the energy behaviour of $K = K(E)$ in the vicinity of E_n . The Kohn value of $\beta_n(E_n)$ is obtained by inserting (19) in (18) and taking the limit $E \rightarrow E_n$:

$$\begin{aligned} \beta_n(E_n) = & - \langle \mathcal{C}_{E_n} | H - E_n | u_n^{\text{PB}} \rangle^{-1} \left(\langle \mathcal{C}_{E_n} | H - E_n | \mathcal{S}_{E_n} + K(E_n) \mathcal{C}_{E_n} \rangle \right. \\ & \left. + \sum_{m \neq n} \langle \mathcal{C}_{E_n} | H - E_n | u_m^{\text{PB}} \rangle (E_n - E_m)^{-1} \langle u_m^{\text{PB}} | H - E_n | \mathcal{S}_{E_n} + K(E_n) \mathcal{C}_{E_n} \rangle \right). \end{aligned} \quad (22)$$

This is a well defined finite number just as $\beta_m(E_n)$ and $K(E_n)$. In the Hulthén method the energy dependence of K around E_n is determined by equation (21):

$$\langle u_n^{\text{PB}} | H - E | \mathcal{S}_E + K(E) \mathcal{C}_E \rangle = \xi(E) (E - E_n)^{1/2},$$

where $\xi(E)$ varies slowly around $E = E_n$. Inserting this in (18), we find that β_n diverges:

$$\beta_n(E) \xrightarrow{E \rightarrow E_n} \xi(E) (E - E_n)^{-1/2}.$$

Renormalising the Hulthén wavefunction by multiplying it by β_n^{-1} , we get u_n^{PB} itself, which agrees with the conclusion of Hazi and Taylor (1970).

But from among the two methods, it is only Kohn's that is guaranteed by the Kohn principle to produce a stationary K -matrix. Using (18), (22) and (6) for the coefficients in ϕ_{E_n} , one can easily confirm that ϕ_{E_n} indeed satisfies the variational

† In a different context, Beck *et al* (1975) also discussed this equation.

principle (14). But in $\mathcal{L}[\phi_{E_n}]$ the correction term does not vanish automatically:

$$\mathcal{L}[\phi_{E_n}] = K(E_n) - \frac{2\mu}{\hbar^2 k} \left(\sum_{m \neq n} \frac{\langle u_m^{\text{PB}} | H - E_n | \mathcal{S}_{E_n} + K(E_n) \mathcal{C}_{E_n} \rangle^2}{E_n - E_m} + \langle \mathcal{S}_{E_n} + K(E_n) \mathcal{C}_{E_n} | H - E_n | \mathcal{S}_{E_n} + K(E_n) \mathcal{C}_{E_n} \rangle \right).$$

Thus, in general, $K(E_n)$ itself is not a stationary value of the functional \mathcal{L} . Nor is, of course, the Hulthén functional

$$\mathcal{K}[u] = -\langle u | H - E_n | \mathcal{S}_{E_n} \rangle / \langle u | H - E_n | \mathcal{C}_n \rangle$$

stationary in general at the Hulthén wavefunction u_n^{PB} :

$$\delta \mathcal{K}[u] |_{u_n^{\text{PB}}} = -\langle \delta u | H - E_n | \mathcal{S}_{E_n} + K(E_n) \mathcal{C}_{E_n} \rangle / \langle u_n^{\text{PB}} | H - E_n | \mathcal{C}_{E_n} \rangle.$$

This fact contradicts the statement of Hazi and Taylor (1970) on this matter. Both $\mathcal{L} + (2\mu/\hbar^2 k) \langle \phi_{E_n} | H - E_n | \phi_{E_n} \rangle$ and \mathcal{K} are, however, stationary in the exceptional case when $\mathcal{S}_{E_n} + K(E_n) \mathcal{C}_{E_n} = \omega_{E_n}$. In this trivial case equation (6) gives the exact K -matrix independent of u_n^{PB} , and thus both \mathcal{K} and \mathcal{L} are constant functionals. In practical cases we do not know $K(E_n)$ beforehand; it is nevertheless useful to know that the closer ω_{E_n} approaches by $\mathcal{S}_{E_n} + K(E_n) \mathcal{C}_{E_n}$ the more accurate $K(E_n)$ will be. Several of the conclusions of this section can be found in a discussion of the variational principle by Burke (1977).

5. Application in realistic calculations

In the preceding sections we have shown that the PBSM works well in a model imitating the GCM. Its applicability in realistic GCM calculations, however, depends largely upon how equations (6) and (7) can be adapted to that formalism. Now we shall answer this question.

In the basis functions (2) of the GCM the angular momentum projection can in general be performed as given in Nagarajan and Lovas (1980). To avoid inessential complications, we now confine ourselves to clusters of zero spin and positive parity. In this case $J = L$, $\pi = (-1)^L$, where L is the relative orbital momentum, and

$$\Phi^{JM\pi}(\mathbf{S}_i) = \Phi^{JM\pi}(\mathbf{S}_i) Y_{LM}^*(\hat{\mathbf{S}}_i) = \mathcal{A} \left[\exp\left(-\frac{r^2 + S_i^2}{2b^2}\right) i_L\left(\frac{rS_i}{b^2}\right) Y_{LM}(\hat{\mathbf{r}}) \Phi_A \Phi_B \right] Y_{LM}^*(\hat{\mathbf{S}}_i),$$

where i_L is a modified spherical Bessel function of the first kind (Abramowitz and Stegun 1964). With such a basis it is straightforward to calculate the normalisation and Hamiltonian kernels

$$N^{JM\pi}(S, S') = \langle \Phi^{JM\pi}(S) | \Phi^{JM\pi}(S') \rangle, \quad H^{JM\pi}(S, S') = \langle \Phi^{JM\pi}(S) | H | \Phi^{JM\pi}(S') \rangle \quad (23)$$

provided Φ_A and Φ_B as well as the internucleon force are simple enough. If the energy E_n resulting from the diagonalisation is such that $E_n - \epsilon_A - \epsilon_B > 0$, ϵ_A and ϵ_B being the cluster internal energies, the state is PB. By analogy with equation (10), it is plausible that for values of the intercluster separation r that are large enough for the

clusters not to overlap but are still smaller than S_N , the function

$$u_n^{\text{PB}}(r) = \sum_{i=1}^N c_i \exp\left(-\frac{r^2 + S_i^2}{2b^2}\right) r i_L\left(\frac{rS_i}{b^2}\right) \quad (24)$$

behaves like

$$u_n^{\text{PB}}(r) \sim F_L(k_n r) + K_L G_L(k_n r),$$

where F_L and G_L are the regular and irregular Coulomb function and $k_n = [(2\mu/\hbar^2)(E_n - \varepsilon_A - \varepsilon_B)]^{1/2}$.

Let $\mathcal{F}_L(k_n r)$ and $\mathcal{G}_L(k_n r)$ and their first r -derivatives be zero at $r = R_0$ and be close to $F_L(k_n r)$ and $G_L(k_n r)$, respectively, for $r \in (R, \infty)$, where R is larger than R_0 and the nuclear interaction radius of the two clusters but smaller than S_N . If we choose R_0 to be in the asymptotic region where the nuclear forces as well as the intercluster antisymmetrisation effects are negligible, and the Coulomb potential can be represented by a two-body term, V_C , then u_n^{PB} of (24) obeys

$$H_0 u_n^{\text{PB}}(r) = (E_n - \varepsilon_A - \varepsilon_B) u_n^{\text{PB}}(r) \quad \text{for } R_0 \leq r \leq R,$$

where

$$H_0 = -\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} \right) + V_C(r).$$

Since H_0 is a two-body Hamiltonian, equation (9) and the similar equation for the cosine-like function apply to it if \mathcal{S} and \mathcal{C} are replaced with \mathcal{F}_L and \mathcal{G}_L . Consequently,

$$K_L = -\frac{\int_{R_0}^R u_n^{\text{PB}}(r) [H_0 - (E_n - \varepsilon_A - \varepsilon_B)] \mathcal{F}_L(k_n r) dr}{\int_{R_0}^R u_n^{\text{PB}}(r) [H_0 - (E_n - \varepsilon_A - \varepsilon_B)] \mathcal{G}_L(k_n r) dr}.$$

This formula is indeed simple to apply.

6. Conclusions

We have seen that the PBSM with GCM-like bases works remarkably well. The way it works is that the basis defines an expansion length Λ , and the GCM diagonalisation is tantamount to approximately solving the energy eigenvalue problem in a box of radius Λ . The wavefunction produced is a good approximation within the box to the exact one of the same energy. This makes it possible to use the PBSM to describe scattering events and resonances. The energy of the system is a result of the diagonalisation, and the application of the method usually requires the scanning of a range of energy by a set of calculations with different bases.

The resonances not only manifest themselves in the phase shift but also by producing inflexion points in the $E(\Lambda)$ curve. This lends itself to determining the resonance energy and width. Though for broad resonances these quantities are determined more reliably by finding the corresponding Gamow states, yet, especially if the resonance wavefunction is needed in subsequent calculations, it is convenient to resort to the PBSM.

The application of the PBSM to scattering is supported by the fact that its K -matrix is equal to that resulting from the Hulthén variational method. This K -matrix coincides with the uncorrected K -matrix of the Kohn method at the PB energies. The Hulthén wavefunction becomes singular at the PB energies, and the PBSM may be viewed as

an eigenvalue problem, non-singular itself, to find these singularities. Although the Hulthén K -matrix is well defined at the PB energies, its definition in the Hulthén formalism involves an infinity-over-infinity type limit; thus its computation in this formalism is unstable around the PB energies (Nesbet 1968). In the PBSM this difficulty does not appear. In other versions of the Kohn–Hulthén approach there are further singularities appearing systematically. These are due to some coincidences in the choice of the square-integrable basis elements on the one hand and the incoming or outgoing waves on the other (Nesbet 1968). Since in the PB diagonalisation there are no incoming or outgoing waves, the PBSM is free of these singularities, too.

The only slight inconvenience of the PBSM as compared with any proper scattering calculation is that we cannot specify the energy *a priori*. But we emphasise that in most practical cases in the field of low energy collisions of light nuclei, to which the GCM scattering model is tailored, the phase shift is needed in a range of energy. If so, the exact choice of the points at which the energy is discretised is, to some extent, arbitrary. But the PBSM helps to optimise this choice. With equidistant discretisation of the generator coordinate, the steeper $\delta(E)$ is, the denser the resulting energy discretisation points are. The PB diagonalisation works like the discretisation involved in a Gaussian type quadrature (Reinhardt 1979). On the other hand, by changing the basis, any particular energy value can be approximated with arbitrary accuracy if needed.

The only extra care to be taken when applying the PBSM concerns the Coulomb potential, which must be accurate throughout the long expansion region.

The main advantage of the PBSM over conventional scattering calculations is that having a bound-state GCM code one can carry out scattering calculations without any change, and the extraction of the phase shift is also simple. It seems straightforward to generalise it to a multichannel problem, and there this advantage may be more important.

The numerical examples shown may be of some interest apart from the GCM. They show how suitable the shifted Gaussian basis is when applied to PBSM. The approximation involved in the use of such a basis is very transparent, because of the direct correspondence between the last basis element and the expansion length covered on the one hand, and between the density of the elements and the goodness of this coverage as well. Furthermore, since there is no reason for sticking to equidistant steps, it is easy to optimise the basis size. Hence the numerical difficulties caused by the use of almost linearly dependent bases never occur in practice.

Acknowledgments

We would like to thank Professor P G Burke for a careful reading of the manuscript, many valuable suggestions and for bringing to our attention the work of Temkin. We also wish to thank Dr D M Brink and Professor M Kawai for stimulating criticism.

References

- Abramowitz M and Stegun I A (ed) 1964 *Handbook of Mathematical Functions* (Washington: National Bureau of Standards) p 443
Barz H-W, Bunakov V E and El-Naiem A M 1973 *Nucl. Phys. A* **217** 141

- Beck R, Borysowicz J, Brink D M and Mihailović M V 1975 *Nucl. Phys. A* **244** 45
- Burke P G 1977 *Potential Scattering in Atomic Physics* (London: Plenum) pp 86–7
- Coester F and Schlessinger L 1973 *Ann. Phys.* **78** 90
- Cole B J, Huby R and Mines J R 1970 *Phys. Lett.* **33B** 320
- Csernai L P, Zimányi J, Gyarmati B and Lovas R G 1978 *Nucl. Phys. A* **294** 41
- Filippov G F and Okhrimenko I P 1980 *Yad. Fiz. (USSR)* **32** 932 (Engl. transl. *Sov. J. Nucl. Phys.* **32** 480)
- Fortune H T, Gray T J, Trost W and Fletcher N R 1969 *Phys. Rev.* **179** 1033
- Giraud B G, Mihailović M V, Lovas R G and Nagarajan M A 1981 *Daresbury Laboratory preprint* DL/NUC/P 134T (to be published in *Ann. Phys.*)
- Harris F E 1967 *Phys. Rev. Lett.* **19** 173
- Hazi A U and Taylor H S 1970 *Phys. Rev. A* **1** 1109
- Hird B and Huang K H 1973 *Can. J. Phys.* **51** 956
- Huby R 1970 *Phys. Lett.* **33B** 323
- Lovas R G 1974 *Acta Phys. Hung.* **36** 165
- 1977 *Nucl. Phys. A* **285** 198
- Mihailović M V, Goldfarb L J B and Nagarajan M A 1976 *Nucl. Phys. A* **273** 207
- Mihailović M V and Poljšak M 1978 *Nucl. Phys. A* **311** 377
- Mihailović M V and Rosina M (ed) 1973 *Generator Coordinate Method for Nuclear Bound States and Reactions (Fizika 5 Suppl.)*
- Mito Y and Kamimura M 1976 *Prog. Theor. Phys.* **56** 583
- Moisewitsch B L 1966 *Variational Principles* (London: Interscience)
- Nagarajan M A and Lovas R G 1980 *Daresbury Laboratory preprint* DL/NUC/P107 T
- Nesbet R K 1968 *Phys. Rev.* **175** 134
- Reinhardt W P 1979 *Comp. Phys. Comm.* **17** 1
- Schlessinger L and Payne G L 1972 *Phys. Rev. C* **6** 2047
- Temkin A 1966 *Autoionization* (Baltimore: Mono Book Corporation)