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Orthogonality condition model for bound and resonant states with a separable expansion of the potential

K F Pál†

Institute of Nuclear Research of the Hungarian Academy of Sciences, H-4001 Debrecen, PO Box 51, Hungary

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Abstract. We show a very efficient solution of the equation of Saito's orthogonality-condition model (OCM) for bound and resonant states by means of a separable expansion of the potential (PSE method). We derive some simplifications of the published formulae of the PSE method, which facilitate its application to the OCM and may be useful in solving the Schrödinger equation as well.

1. Introduction

It is firmly established that the microscopic two-cluster models can successfully describe many levels in light nuclei and they can also provide good results for the elastic scattering of light nuclei (for example, Fujiwara *et al* 1980, Furutani *et al* 1980). Unfortunately, even the simplest microscopic model, which substitutes the wavefunctions of the internal nucleonic motion in both clusters by harmonic oscillator (HO) wavefunctions with equal oscillator parameters, needs lengthy calculations.

The calculations can be greatly simplified by using Saito's orthogonality-condition model (OCM) (Saito 1968, 1969), which has proved to be a good approximation to the microscopic model. In this model the equation of motion is a Schrödinger-like equation for the intercluster relative motion with an effective local cluster-cluster interaction. The Pauli principle is taken into account by a projection operator that forces the solution to be orthogonal to the Pauli-forbidden (or redundant) states, which give rise to vanishing many-body wavefunctions.

The OCM equation is an integro-differential equation because of the presence of the projector. To avoid the difficulties of the direct numerical integration of this equation, Saito (1969, 1977) proposed a simple numerical method, which has been applied to scattering problems. However, for bound or resonant states this method does not seem easily applicable. Another fully numerical method for the OCM problem is the so-called inverse-iteration method. This method can easily be used not only for scattering states but also for the bound states belonging to the lowest energy for each set of quantum numbers in a given potential well. To find states above the ground state for the same set of quantum numbers is more involved. For resonant states this method is also much more complicated.

The OCM equation is frequently solved for bound states by a wavefunction expansion (WFE) (Fujiwara *et al* 1980). Since the redundant states are elements of an HO basis,

† Present address: SERC Daresbury Laboaratory, Daresbury, Warrington WA4 4AD, UK.

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by expanding the solution in terms of this basis, the effect of the projector is reduced to the omission of the redundant states. A very nice feature of this method is that if the potential is some sum of Gaussian and modified Gaussian functions—these are very common forms in the OCM—almost all the calculations can be carried out analytically. A shortcoming of this method is that the asymptotic behaviour of the wavefunction will be incorrect even if a large basis is used.

In this paper we use a powerful method, which was recently proposed for solving the Schrödinger equation (Révai 1975, Gyarmati *et al* 1979) and is free of this deficiency. Nevertheless, it has the same analytical feature as the WFE method. The method is based on a separable expansion of the potential (PSE method). It is very easily applicable not only for bound states but for resonant states as well (Gyarmati *et al* 1984, Kruppa and Papp 1984) and it will be shown that it is well suited to the OCM problem. For some applications the method has definite advantages over any fully numerical methods even for bound states. For example, the overlap functions, which is needed for the theoretical description of direct-transfer reactions (Lovas and Pàl 1984) or decay, and the wavefunction in momentum representation can be calculated in a very straightforward way. The method is also applicable without any modification if the potential has an explicit non-locality.

In § 2 the PSE method for the Schrödinger equation is reviewed and some necessary formulae are presented. In § 3 some simplifications are introduced, which make the method well suited for the OCM problem. Then the PSE method is applied to the OCM problems (§ 4). Finally, our bound-state results are compared to those of the WFE method, an example for the resonant-state solution is given and conclusions are drawn (§ 5).

2. The PSE method for the Schrödinger equation

In the PSE method the solution of the Schrödinger equation

$$(T+V)|\phi\rangle = E|\phi\rangle$$

is achieved as the limit of the solutions of the auxiliary problems

$$(T+\tilde{V}_N)|\phi_N\rangle = E_N|\phi_N\rangle, \tag{1}$$

where the truncated potential $\tilde{V}_N$ is a sum of separable terms:

$$\tilde{V}_N = P_N V P_N \tag{2}$$

with

$$P_N = \sum_{\lambda,\mu} \sum_{i=0}^{N} |i\lambda\mu\rangle\langle i\lambda\mu|. \tag{3}$$

In (3) $|i\lambda\mu\rangle$ denotes an element of a complete set of orthonormal functions. We choose $|i\lambda\mu\rangle$ to be HO functions, with i and $\lambda\mu$ denoting the radial node number and the orbital momentum respectively. If V satisfies rather weak conditions, the PSE solution converges to the exact one (Gyarmati *et al* 1979). Therefore, if N is large enough, $|\phi\rangle$ can be approximated by $|\phi_N\rangle$ very well. The PSE as an approximate method consists of solving (1) for an appropriate N.

This method has been applied with success to various problems and has proved superior to the WFE, especially in problems where the asymptotic part of the wavefunction is important. Moreover, unlike the WFE, the PSE is applicable for resonant states.

A formal analogy between the WFE and PSE methods is that both involve truncated forms of the Schrödinger equation. The difference is that while in the WFE method both the potential and kinetic energy operators are truncated, in the PSE the kinetic energy operator remains untruncated. The truncation of T is responsible for the wrong tail behaviour of the WFE wavefunction mentioned in the introduction. Obviously, the PSE does not suffer from this deficiency. Nevertheless, the WFE is a variational method, whose convergence is necessarily monotonic, and this is not true for the PSE even for bound states. This shortcoming is compensated for, however, by the fact that the PSE usually converges faster than the WFE (Révai 1975, Bang *et al* 1978). Moreover, the convergence of the PSE method is much less sensitive to the choice of the oscillator parameter than that of the WFE method.

If V is spherical and $|\phi\rangle$ is a bound or resonant state that belongs to a particular orbital momentum lm, (1) is equivalent to the Lippmann-Schwinger equation

$$|\phi_N\rangle = G_0(E_N) \sum_{i,j=0}^{N} |ilm\rangle V_{ij}^l \langle jlm|\phi_N\rangle \tag{4}$$

where G_0 is the free Green operator and

$$V_{ij}^l = \langle ilm|V|jlm\rangle.$$

By introducing the notation

$$c_i = \langle ilm|\phi_N\rangle \tag{5}$$

(4) takes the form

$$|\phi_N\rangle = \sum_{i=0}^{N} G_0(E_N)|ilm\rangle \sum_{j=0}^{N} V_{ij}^l c_j. \tag{6}$$

From (6) we can see that the first $N+1$ coefficients c_i $(0 \leqslant i \leqslant N)$ determine the wavefunction uniquely. If we multiply (6) by $\langle klm|(k=0 \ldots N)$, we get a system of homogeneous linear equations:

$$\sum_{j=0}^{N} \left(\delta_{kj} - \sum_{i=0}^{N} G_{ki}^l V_{ij}^l \right) c_j = 0. \tag{7}$$

Here the notation

$$G_{ij}^l = \langle ilm|G_0(E_N)|jlm\rangle \tag{8}$$

is used. The matrix elements G_{ij}^l can be calculated through recurrence relations (Kruppa and Papp 1984). For the indices i and j these are

$$G_{i+1,j}^l = (W_i^l G_{ij}^l - Q_{i-1}^l G_{i-1,j}^l - \delta_{ij})/Q_i^l \tag{9}$$

$$G_{i,j+1}^l = (W_j^l G_{ij}^l - Q_{j-1}^l G_{i,j-1}^l - \delta_{ij})/Q_j^l \tag{10}$$

where

$$W_i^l = \langle ilm|E - T|ilm\rangle = E - \frac{\hbar^2\beta}{2m}(2i + l + \tfrac{3}{2}) \tag{11}$$

$$Q_i^l = \langle i+1\, lm|T|ilm\rangle = \langle ilm|T|i+1\, lm\rangle$$

$$= \frac{\hbar^2\beta}{2m}[(i+1)(i+l+\tfrac{3}{2})]^{1/2} \tag{12}$$

$\beta = m\omega/\hbar$ is the oscillator parameter and m is the reduced mass. As $Q^l_{-1} = 0$, the second term of the right-hand side of (9) vanishes for $i = 0$, and the same applies to (10) for $j = 0$. Therefore for the recurrence relations to be used, it is sufficient to know G^l_{00}. This can be calculated via a simple recurrence relation from G^0_{00}, which is expressible with the error function (Kruppa and Papp 1984).

The system of equations (7) has a non-trivial solution if and only if its determinant is zero. This condition yields the energy eigenvalue or the depth of the potential for a given energy. Solving (7) we obtain the PSE wavefunction from (6) as a linear combination of the functions $G_0(E_N)|ilm\rangle$. These functions can be calculated from $G_0(E_N)|0lm\rangle$ by means of the relation (Kruppa and Papp 1984)

$$G_0(E)|i+1\,lm\rangle = \left(W^l_i G_0(E)|ilm\rangle - Q^l_{i-1} G_0(E)|i-1\,lm\rangle - \frac{2m}{\hbar^2\beta}|ilm\rangle \right) \Big/ Q^l_i . \tag{13}$$

Kruppa and Papp (1984) have also given a recurrence relation for $G_0(E)|0lm\rangle$ and the explicit forms for $l = 0$ and $l = 1$. Of course, if the wavefunction in momentum representation is to be calculated, these relations need not be used, because G_0 is a simple multiplicative factor.

It can easily be derived from (6) that the normalisation condition for the wavefunction is

$$\sum_{i,j=0}^{N} d_i \langle ilm|G_0^2(E_N)|jlm\rangle d_j = 1$$

where

$$d_i = \sum_{j=0}^{N} V^l_{ij} c_j$$

and the matrix elements of the $G_0^2(E_N)$ operator can be calculated from $\langle 00m|G^2(E)|00m\rangle$ by the aid of recurrence relations similar to the ones used in calculating the matrix elements of $G_0(E_N)$ (Kruppa and Papp 1984).

Gyarmati *et al* (1979) introduced a 'smoothing procedure', which can speed up the convergence of the PSE method. Instead of P_N an operator

$$P'_N = \sum_{\lambda\mu} \sum_{i=0}^{N} |i\lambda\mu\rangle \sigma_i^N \langle i\lambda\mu|$$

is used in (2) with the property of $\lim_{N\to\infty} P'_N = 1$. In the formulae the only modification implied is to replace V^l_{ij} by $V^{l'}_{ij} = V^l_{ij}\sigma^N_i\sigma^N_j$. The choice

$$\sigma_i^N = \frac{1 - \exp\{-[\alpha(N+1-i)/(N+1)]^2\}}{1 - \exp(-\alpha^2)} \qquad (i = 0, 1, \ldots, N)$$

with $\alpha = 6$ has proved to be very successful in practical applications.

3. Simplification of the PSE equations

The formalism of § 2 is already suitable for practical calculations. It is based on the general formalism used in the code of Kruppa and Papp (1984), but is specialised to spherical potentials. It is, however, possible to exploit further the particular properties of the HO basis and make the formulae simpler. The first step is a re-arrangement of

equations (7). If we multiply the kth ($k = N-1, N-2, \ldots, 1$) equation (this contains index $k-1$) by Q^l_{k-1}/Q^l_k and the $(k+1)$th equation by W^l_k/Q^l_k and then we subtract them from the $(k+2)$th equation, using (9), we arrive at the new $(k+2)$th equation:

$$\left(Q^l_{k-1}c_{k-1} - W^l_k c_k + Q^l_k c_{k+1} + \sum_{j=0}^{N} V^l_{kj}c_j\right) \Big/ Q^l_k = 0. \tag{14}$$

As $Q_{-1} = 0$, an equation of the form of (14) can be written for $k = 0$ as well. Then, multiplying equations (14) by $G^l_{0k}Q^l_k$ and adding them to the first of equations (7), using relation (9) again, we get the following expression:

$$\left(-Q^l_{N-1}c_{N-1} + \frac{G^l_{0N-1}Q^l_{N-1}}{G^l_{0N}}\, c_N - \sum_{j=0}^{N} V^l_{Nj}c_j\right) G^l_{0N} = 0.$$

Putting this equation into the last place and multiplying it by -1, we obtain the new system of equations:

$$\frac{1}{Q^l_k}\sum_{j=0}^{N}\left(Q^l_{k-1}\delta_{k-1j} - W^l_k\delta_{kj} + Q^l_k\delta_{k+ij} + V^l_{kj}\right)c_j = 0 \qquad (k = 0, \ldots, N-1) \tag{15}$$

$$G^l_{0N}\sum_{j=0}^{N}\left(Q^l_{N-1}\delta_{N-1j} - \frac{G^l_{0N-1}Q^l_{N-1}}{G^l_{0N}}\,\delta_{Nj} + V^l_{Nj}\right)c_j = 0. \tag{16}$$

These equations contain only two elements of the Green matrix G^l_{ij}, both of them from the first row, and the time-consuming matrix multiplication has disappeared. Nevertheless, this system of equations is equivalent to the original one and its determinant is also the same.

The evaluation of the wavefunction can also be simplified. As the coefficients contained in the recurrence relation (13) are numbers, it can easily be seen that $G_0(E_N)|ilm\rangle$ is a linear combination of the $G_0(E_N)|0lm\rangle$ and the HO states $|jlm\rangle$ ($j \leqslant i-1$). The wavefunction being a linear combination of $G_0(E_N)|ilm\rangle$ ($i \leqslant N$), can be written as

$$|\phi_N\rangle = AG_0(E_N)|0lm\rangle + \sum_{j=0}^{N-1} B_j|jlm\rangle. \tag{17}$$

The multiplication of (16) by $\langle ilm|(i = 0, 1, \ldots, N)$ and the use of the definitions (5) and (8) yield expressions for the combination coefficients A and B_j:

$$A = c_N/G^l_{N0} \qquad B_j = c_j - G^l_{j0}c_N/G^l_{N0}. \tag{18}$$

Equation (17) shows that we can calculate the wavefunction in coordinate representation without actually calculating $G_0(E_N)|ilm\rangle$ for $i > 0$ from (13).

An alternative form for the normalisation condition for the wavefunction is

$$1 = \sum_{i=0}^{\infty} c_i^2. \tag{19}$$

This condition is consistent with the usual convention for resonant states and also good for bound states. The c_i are defined by (5) and, for $i \leqslant N$, their values are provided by (15) and (16). Let i be greater than N. Multiplying (17) by $\langle ilm|$, using (18), (5) and (8) we end up with

$$c_i = \langle ilm|G_0(E_N)|0lm\rangle c_N/G^l_{N0} = G^l_{i0}c_N/G^l_{N0} \qquad (i > N).$$

If we substitute it into (19), the normalisation condition takes the form

$$1=\sum_{i=0}^{N} c_i^2+(c_N/G^l_{N0})^2 \sum_{i=N+1}^{\infty} \langle 0lm|G_0(E_N)|ilm\rangle\langle ilm|G_0(E_N)|0lm\rangle$$

$$=\sum_{i=0}^{N} c_i^2+(c_N/G^l_{N0})^2\left(\langle 0lm|G_0^2(E_N)|0lm\rangle-\sum_{i=0}^{N}(G^l_{i0})^2\right). \tag{20}$$

Equations (15)-(18) and (20) show that we need only one row of the Green matrix and a single element of the matrix of the $G_0^2(E_N)$ operator. This is a substantial simplification of the formulae of § 2; it allows a more economical computation. We emphasise that the formalism so far is not specified to the OCM. We shall see, however, that these re-arrangements will be especially useful in the case of the OCM equation.

4. The OCM equation and the PSE method

In the OCM model the wavefunction $|\phi\rangle$ of the intercluster relative motion satisfies the OCM equation

$$\Lambda(T+V)|\phi\rangle=E|\phi\rangle. \tag{21}$$

Here E is the energy of the relative motion, T is the relative kinetic energy operator, V is an effective cluster-cluster interaction and Λ is the projection operator projecting out of the subspace of the redundant states. From the microscopic cluster model that the OCM is based on, it can be shown that the redundant states are elements of a HO basis (Zaikin 1971, Horiuchi 1977) and they have the smallest quantum numbers.

We shall apply the PSE method with the basis defined by the redundant states. As we need a sound operator T, we re-arrange the OCM equation (21) as

$$[T-(1-\Lambda)T+\Lambda V]|\phi\rangle \tag{22}$$

and then, just as in the case of the Schrödinger equation, we approximate it with (1). Here the 'truncated potential' is

$$\tilde{V}_N=P_N[-(1-\Lambda)T+\Lambda V]P_N. \tag{23}$$

Denoting the number of forbidden states belonging to an orbital momentum λ by n_λ, and using the definition (3), we can cast (23) into the form

$$\tilde{V}_N=\sum_{\lambda\mu}\sum_{i=0}^{n_\lambda-1}\sum_{j=0}^{N}|i\lambda\mu\rangle\langle i\lambda\mu|-T|j\lambda\mu\rangle\langle j\lambda\mu|+\sum_{\lambda\mu}\sum_{i=n_\lambda}^{N}\sum_{j=0}^{N}|i\lambda\mu\rangle\langle i\lambda\mu|V|j\lambda\mu\rangle\langle j\lambda\mu|. \tag{24}$$

We note that if the expansion contains at least one non-forbidden state for every λ ($N\geqslant\max(n_\lambda)$), the first triple sum is exactly equal to the untruncated operator $-(1-\Lambda)T$ because $\langle i\lambda\mu|T|j\lambda\mu\rangle=0$ if $|i-j|>1$. Therefore only the operator V is truncated by P_N just as in the case of the Schrödinger equation. From (24) it follows that solving the OCM problem we have to change the matrix elements of V to the matrix elements of $-T$ at the first n_l row of V^l_{ij}. Using this new matrix V^l_{ij}, we can solve the OCM equation with the formulae of the preceding sections.

We can reduce the problem to the subspace of the non-redundant states if we use the PSE equations in their re-arranged form, (15) and (16). As the first n_l rows of the matrix V^l_{kj} contain the matrix elements of $-T$, with the notations (11) and (12) they

can be written as

$$V^l_{kj} = -Q^l_{k-1}\delta_{k-1,j} + (W^l_k - E)\delta_{kj} - Q^l_k\delta_{k+1,j} \qquad (k = 0, \ldots, n_l - 1).$$

With this expression the first n_l equations of (18) reduce to

$$-(E/Q_k)c_k = 0 \qquad (k = 0, \ldots, n_\lambda - 1). \tag{25}$$

These equations only express that the solution is orthogonal to the redundant states, as it should be. We note that this requirement cannot be seen explicitly from the original form (7) of the PSE equations.

Since our first n_l equations (25) are trivial, we have to solve only a reduced problem. We can also notice that we need only the matrix elements of the potential between non-redundant states; any other matrix elements are multiplied by $c_i = 0$ $(i = 0, \ldots, n_l - 1)$ everywhere.

The smoothing procedure can be used in the case of the OCM equations as well. A possible choice for σ_i^N is

$$\sigma_i^N = \begin{cases} 1 & (i = 0, \ldots, n_l - 1) \\ \dfrac{1 - \exp\{-[\alpha(N + 1 - i)/(n + 1 - n_l)]^2\}}{1 - \exp(-\alpha^2)} & (i = n_l, \ldots, N). \end{cases}$$

An important quantity, the overlap function U, can be calculated in a very straightforward manner from the PSE solution. As $|U\rangle = A^{1/2}|\phi\rangle$, where the operator A is diagonal on the basis and its eigenvalues a_i tend to 1 when i increases, we can get a very good approximation to U if N is large enough:

$$|U\rangle = |\phi\rangle + (A^{1/2} - 1)|\phi\rangle \approx |\phi\rangle + \sum_{i=0}^{N} (a_i^{1/2} - 1)c_i|i\rangle.$$

5. Results and conclusions

In this section we show some examples for the solution of the OCM equation with the PSE method. For the bound-state cases we also provide some comparisons between the PSE and WFE methods. The bound-state examples to be shown are calculations for the ground state of the $^{16}O + \alpha$ system. This state belongs to a relative orbital momentum $l = 0$. The number of the $l = 0$ forbidden states is $n_0 = 4$. We have used an effective cluster-cluster interaction of the Gaussian form $V(r) = -V_0 \exp[-(r/a)^2]$ with $V_0 = -126.5$ MeV and $a = 2.7031$ fm. In figure 1(a) we compare the energies E_N of the intercluster relative motion obtained from the PSE and WFE methods as functions of the maximum radial node number N of the basis. It can be seen that the PSE converges faster than the WFE in the case of OCM as well. Figure 1(a) also shows that the smoothing procedure can speed up the convergence appreciably, so it is worthwhile to use it. The energies of this PSE method for a fixed N are usually closer to the exact one by two to three orders of magnitude than the WFE energies. (In our example the 'exact energy' $E = -4.724\,790$ has been determined by extrapolation.)

It may be important to determine not only the energy but also the wavefunction with some accuracy. In figure 2(a) we compare the two methods from this point of view. We show the PSE and WFE wavefunctions that belong to the $N = 11$ and $N = 33$ calculations of figure 1(a). While the $N = 11$ WFE wavefunction is unacceptable, the corresponding PSE wavefunction is very good everywhere, even in the asymptotic

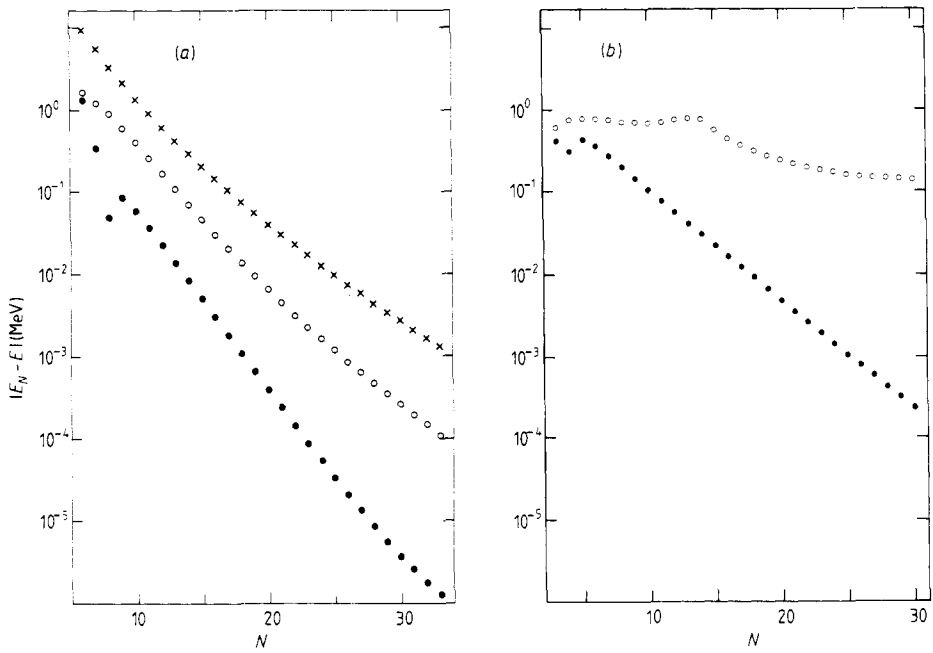

Figure 1. $|E_N - E|$ values as the function of the maximum radial node number N of the basis for (a) the ground state and (b) the 6^+ state of the $^{16}O+\alpha$ system. The energies E_N of the relative motion have been calculated with WFE (×) and PSE (○, without smoothing; ●, with smoothing $\alpha = 6$) methods. The ground-state energy $E = -4.724\,790$ and the 6^+ state energy $E = 6.99212 - 0.63490\ i$ have been obtained by extrapolation. The strange behaviour of the PSE method with smoothing in the first few points of figure 1(a) is a consequence of the change of sign of $E_N - E$.

region. The $N = 33$ WFE wavefunction is also very good within ~8 fm, but its tail behaviour is wrong. In fact, the region where a WFE wavefunction is good grows as slowly as $\sim N^{1/2}$.

We can conclude that the PSE method is superior to the WFE for the bound-state OCM problem in cases when the WFE is applicable at all. Moreover, if we use the simplified formulae of § 3, the practical solution is hardly more difficult. In fact the first N of the PSE equations (18) are the same as the WFE equations, and the last one, (19), differs only in that W^l_N is replaced by $G^l_{0N-1}Q^l_{N-1}/G^l_{0N}$. For this reason, the PSE does not seem more difficult than any of the fully numerical methods.

To prove the applicability of the PSE method to resonant states, we also show some results for the lowest $l = 6$ state of the $^{16}O+\alpha$ system. In this example there is one forbidden state. We have used the same potential as in the bound-state case. In figure 1(b) we plot the values $|E_N - E|$ as functions of N. It can be seen that the smoothing procedure is even more important here than for the bound state. The convergence is slower—but at least when the smoothing procedure is used it is satisfactory. Nevertheless, for a very narrow resonance the imaginary part of the energy may be relatively inaccurate. The comparison of the resonant wavefunctions calculated with two different N (figure 2(b)) also shows the slower convergence: the agreement is worse than for the bound-state case. (The wavefunctions in figure 2(b) correspond to that of in figure 2(a) in the number of the allowed states.) However, our examples show that with a

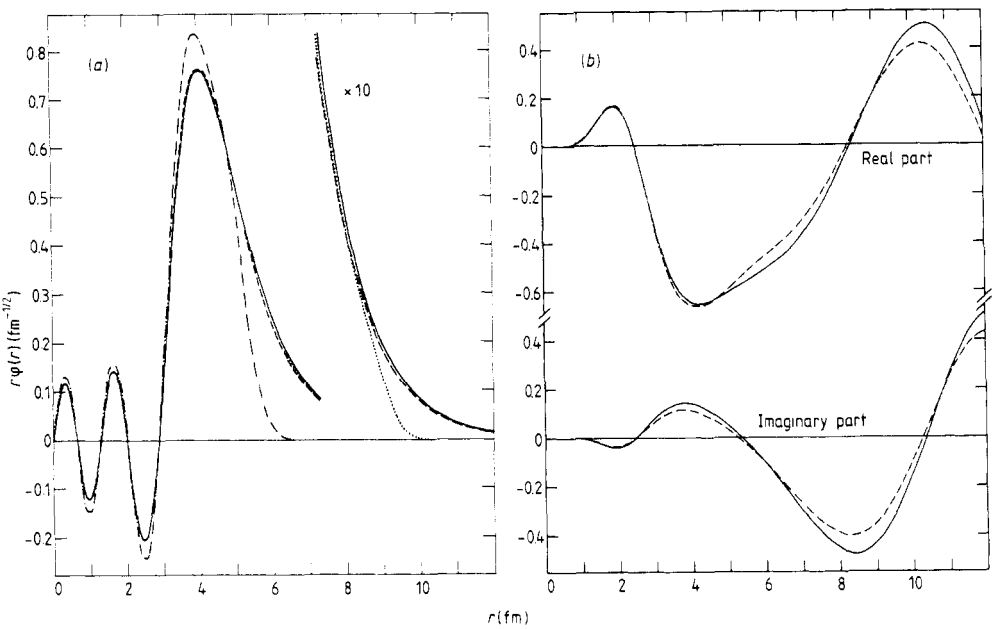

Figure 2. Radial OCM functions $r\phi(r)$ for (a) the ground state and (b) the 6^+ state of $^{16}O+\alpha$. The dependence of these functions on the size of the basis is shown. In (a): ——, PSE ($N=33$); · · ·, WFE ($N=33$); - - - PSE ($N=11$); — · — WFE ($N=11$). In (b): ——, PSE ($N=30$); - - - PSE ($N=8$). The parameters are the same as in figure 1. The smoothing procedure is used with $\alpha=6$ for the PSE.

large enough basis the PSE method provides a possibility for an easy calculation of the quasi-bound states of cluster nuclei†.

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