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A NEW METHOD OF CALCULATING WAVE
FUNCTIONS ON HARMONIC
OSCILLATOR BASIS

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INTRODUCTION

The expansion of unknown wave functions in terms of harmonic oscillator wave functions (HOWF) is one of the oldest and most widely used approximations in nuclear physics. The main attractive feature of such an approach is the simplicity of calculations due to

- the simple form of the HOWF themselves;
- the possibility of a direct analytical calculation of many integrals involving them;
- the unique possibility of performing coordinate transformations on them in closed form using linear transformations in a finite dimensional function space (Talmi-Moshinsky-Smirnov coefficients).

On the other hand the HOWF have certain well-known disadvantages, too, connected with their incorrect asymptotic behaviour which, in the cases where the peripheral part of the wave function is important, either lead to incorrect results or necessitate taking into account a large number of terms in the expansion. The method proposed in this work is an attempt to avoid the above-mentioned difficulties still retaining the calculational simplicity of HOWF.

DESCRIPTION OF THE METHOD

We will be looking for the bound-state solutions of the Schrödinger-equation:

$$(E^\alpha - H_0 - V)|\Psi_\alpha\rangle = 0 \quad (1)$$

(the notations are obvious). Introducing a complete ortho-

normal set of state-vectors $|i\rangle$ the usual way of solving (1) by expansion is to write

$$|\Psi_\alpha\rangle \approx \sum_{i=0}^N c_i^\alpha |i\rangle \quad (2)$$

and the approximate energies $E_{(N)}^\alpha$ and the coefficients c_i^α are obtained as eigenvalues and eigenvectors of the $N \times N$ Hamiltonian matrix:

$$H_{ij} = \langle i | H_0 + V | j \rangle, \quad i, j = 0, \dots, N. \quad (3)$$

(In the following we shall refer to this procedure as the wave function expansion (WFE) method). The WFE method corresponds to considering the problem in a truncated function space spanned by the first N functions of the basis $|i\rangle$. The truncation is complete in the sense that *both* operators H_0 and V are replaced by PH_0P and PVP , respectively, where P is the projection operator onto the chosen subspace:

$$P = \sum_{i=0}^N |i\rangle \langle i|. \quad (4)$$

While the operator PVP can be thought of as the interaction operator of an auxiliary physical problem, PH_0P does not correspond to the quantum-mechanical kinetic energy operator of any system. This is essentially the reason why the wave functions of the type (2) show unphysical behaviour in the regions, where the potential is negligible and the form of the true wave function is determined by the kinetic energy only. As is well known, in the asymptotic region the true wave function must have an exponentially decaying shape, the decay rate depending on the energy eigenvalue, and a correct representation of such a shape over a wide range requires a great number of terms if functions, having a different asymptotic behaviour (e.g., HOWF), are used. To overcome this difficulty we propose to consider the Hamiltonian

$$\tilde{H} = H_0 + \tilde{V} = H_0 + PVP = H_0 + \sum_{i,j=0}^N |i\rangle V_{ij} \langle j| \quad (5)$$

with $V_{ij} = \langle i | V | j \rangle$ and to approximate the eigenvalues and eigenfunctions of H by those of \tilde{H} . This choice corresponds to truncating the potential V in the same way as in (3) but leaving the kinetic energy H_0 unchanged. The auxiliary problem defined by the Hamiltonian \tilde{H} can be solved exactly using the familiar techniques developed for separable potentials - therefore we call this method the potential separable expansion (PSE) method. We rewrite the Schrödinger-equation

$$(\epsilon^\alpha - H_0 - \tilde{V}) |\tilde{\Psi}_\alpha\rangle = 0 \quad (6)$$

in the form of the Lippman-Schwinger equation, appropriate for the bound-state solution:

$$|\tilde{\Psi}_\alpha\rangle = G^\circ(\epsilon^\alpha) \tilde{V} |\tilde{\Psi}_\alpha\rangle, \quad (7)$$

where $G^\circ(z) = (z - H_0)^{-1}$ is the Green-operator of the non-interacting system. Using (5) eq. (7) can be put in the form

$$|\tilde{\Psi}_\alpha\rangle = G^\circ(\epsilon^\alpha) \sum_{i,j=0}^N |i\rangle V_{ij} \langle j | \tilde{\Psi}_\alpha\rangle. \quad (8)$$

Multiplying of eq. (8) from the left by $\langle k |$ leads to the following equation for the coefficients $\tilde{c}_j^\alpha = \langle j | \tilde{\Psi}_\alpha\rangle$

$$\sum_{j=0}^N M_{kj}(\epsilon^\alpha) \tilde{c}_j^\alpha = 0 \quad (9)$$

with

$$M_{kj}(z) = \delta_{kj} - \sum_{i=0}^N G_{ki}^\circ(z) V_{ij}, \quad (10)$$

where the obvious notation

$$G_{ki}^\circ(z) = \langle k | G^\circ(z) | i \rangle \quad (11)$$

has been used.

To solve the homogeneous eq. (9) for the coefficients \tilde{c}_j^α first we have to find those values ϵ^α for which the determinant $|M_{ij}(\epsilon^\alpha)|$ vanishes. These are the exact

eigenvalues of the Hamiltonian (5). Having ϵ^α eq. (9) and the normalization requirement uniquely define the coefficients \tilde{c}_j^α . It can be easily shown, that - excluding the case of pathologically strong potentials - the asymptotic behaviour of the coordinate-space wave function $\langle \vec{r} | \tilde{\Psi}_\alpha \rangle$ satisfies the relation

$$\langle \vec{r} | \tilde{\Psi}_\alpha \rangle \xrightarrow{|\vec{r}| \rightarrow \infty} A_\alpha \exp \left\{ -\sqrt{\frac{2m|\epsilon^\alpha|}{\hbar^2}} |\vec{r}| \right\} \quad (12)$$

as it should be for physical solutions of problems with short-range potentials.

From computational point of view the PSE method involves essentially one new element as compared with the WFE method, the calculation of the matrix elements $\langle i | G^\circ(z) | k \rangle$. This task is greatly simplified if the complete set of states $|i\rangle$ consists of harmonic oscillator states, since the operator $G^\circ(z)$ is diagonal in the momentum representation and the HOWF have identical forms both in the coordinate and momentum representation. Thus, the computation of the matrix elements is reduced to calculation of a single integral involving two HOWF and the

propagator $(z - \frac{p^2}{2m})^{-1}$ and can be easily performed.

There is another computational method used along with the PSE which is worth mentioning. The method is similar to that of σ -factors known from the theory of applied Fourier-analysis^{* 1/}. It is essentially a way to regularize (or to smooth) the oscillations (Gibbs phenomenon) which always arise when a smooth function is expanded in terms of a complete orthonormal set of functions and the expansion is truncated at a finite number of terms. Let us give a brief sketch of the method. We consider the expansion

* The author acknowledges the assistance of I. Borbely, who pointed out the existence of this method and helped to apply it to the present problem.

$$f(x) \approx f_N(x) = \sum_{i=0}^N c_i g_i(x), \quad (13)$$

where $g_i(x)$ form a complete orthonormal set:

$$\int g_i(x) g_j(x) dx = \delta_{ij}. \quad (14)$$

In this case the Fourier-coefficients c_i are given by

$$c_i = \int f(x) g_i(x) dx. \quad (15)$$

These coefficients ensure that for a given N $f_N(x)$ is the best approximation of $f(x)$ (in the sense of the norm following from (14)). The oscillations in $f_N(x)$ are connected with the poor convergence of the derivative series $f'_N(x)$ in which the high- i terms have a non-desirable increased role. The idea of the σ -factor method consists in modifying the coefficients c_i in such a way that the convergence of $f'_N(x)$ should be improved at the price of certain loss in accuracy in the approximation of the function itself. This can be achieved by damping the higher order terms in the expansion using the σ -factors as

$$\tilde{c}_i = c_i \sigma_i^{(N)}; \quad f(x) \approx \tilde{f}_N(x) = \sum_{i=0}^N \tilde{c}_i g_i(x). \quad (16)$$

The factors $\sigma_i^{(N)}$ should fulfill the requirements

$$0 \leq \sigma_i^{(N)} \leq 1; \quad \sigma_0^{(N)} = 1; \quad \sigma_{N+1}^{(N)} = 0 \quad (17)$$

otherwise their detailed i -dependence is arbitrary and is chosen to fit the actual problem best. In our case the σ -factors enter the PSE method via eq. (5) which can be considered as a truncated double expansion of an operator on the basis $|i\rangle$, the expansion coefficients being the V_{ij} . The modified eq. (5) should read as

$$\tilde{V} = \sum_{i,j=0}^N |i\rangle \sigma_i^{(N)} V_{ij} \sigma_j^{(N)} \langle j|. \quad (5a)$$

We have used for $\sigma_i^{(N)}$ the form

$$\sigma_i^{(N)} = \frac{1 - \exp[-(a \frac{i-N-1}{N+1})^2]}{1 - \exp(-a^2)} \quad (18)$$

with an "experimentally" determined value $a=5$. The result of using eq. (5a) instead of eq. (5) is a considerably greater stability of the results against the increase of N ; both the energies and the wave functions tend towards their exact limits almost without oscillations.

NUMERICAL EXAMPLE

In order to demonstrate the usefulness of the described method we considered the problem of single-particle bound states in a Woods-Saxon potential. The potential parameters were chosen as

$$V(r) = -V_0 \left(1 + \exp\left(\frac{r-R}{a}\right)\right)^{-1}$$

$$V_0 = 51.3 \text{ MeV}; \quad a = 0.6829 \text{ fm}$$

$$R = 3.1426 \text{ fm} (=1.24 \text{ fm} \cdot 16^{1/3})$$

(it resembles the shell-model potential of ^{16}O). There is a $1s$ and $2s$ bound state in this potential* with the binding energies: $E_{1s} = 31.1002 \text{ MeV}$; $E_{2s} = 3.2084 \text{ MeV}$. The exact eigenvalues E_i and wave-functions $\phi_{\text{ex}}^i(r)$ of these states were obtained by careful numerical integration of the radial Schrödinger equation. We compared the quality of reproduction of these exact quantities by the two methods as a function of the number of terms N in the expansions (2) and (5a). Following the usual

* For the sake of simplicity we considered $\ell=0$ states for the present test.

practice we tried to fix the oscillator parameter b from the requirement of the most rapid convergence. For the WFE method it turned out, as it was to be expected, that the optimal oscillator parameters for the strongly bound $1s$ state and for the weakly bound $2s$ state are strongly different (1.55 fm and 2.25 fm , respectively). In the PSE method, on the other hand, we were able to find one single value ($b = 1.35 \text{ fm}$) for which the convergence for both states was optimal. If in a calculation both s -states are needed, their orthogonality is important and the use of different oscillator parameters in their expansion is not permissible. Therefore in the WFE case sometimes an intermediate b value has to be chosen. In our case the intermediate value is $b = 1.90 \text{ fm}$ and we included into results the calculations made with this value, too. The obtained results are shown in Tables 1 and 2. In order to characterize the quality of the approximate wave functions we calculated their overlaps $\int \phi^i \phi_{\text{ex}}^i$ with the exact ones, and the quantities

$$\Delta = 1 - \int \phi^i \cdot \phi_{\text{ex}}^i = \frac{1}{2} \int (\phi^i - \phi_{\text{ex}}^i)^2$$

are shown in the tables.

CONCLUSION

The results show that while for the strongly bound states the two methods can be applied equally well, in the case of a weakly bound state the superiority of the PSE method is evident. Another important point is, that if weakly and strongly bound states are needed simultaneously in a certain problem, in the WFE method an intermediate non optimal oscillator parameter must be chosen strongly reducing the convergence rate, while in the PSE method optimal convergence can be achieved for both states with the same parameter. This feature of the PSE may be due to the fact that in this case the object of expansion is not one or another physical state but rather the potential itself - which is the same for all states. In general we can say, that in the cases when the long-distance behaviour of the wave function is impor-

Table 1

Results for the 1s state. The exact binding energy is $E_{1s} = 31.1002$ MeV.
The non-filled columns mean, that the values do not change any more with

N	WFE b = 1.55 fm		WFE b = 1.90 fm		PSE b = 1.35 fm	
	E_{1s} , MeV	$\Delta \cdot 10^6$	E_{1s} , MeV	$\Delta \cdot 10^6$	E_{1s} , MeV	$\Delta \cdot 10^6$
1	31.0788	191	31.0476	498	31.3456	440465
2	31.0791	173	31.0861	81	31.1379	38
3	31.0997	4	31.0911	49	31.0955	6
4	31.0999	2	31.0968	18	31.0966	1
5	31.1000	1	31.0996	3	31.1001	<.5
6	31.1002	<.5	31.1001	<.5	31.1002	<.5
7			31.1001	<.5		
8			31.1001	<.5		
9			31.1001	<.5		
10			31.1002	<.5		
11						
12						
13						
14						
15						

Table 2

Results for the 2s state. The exact binding energy is: $E_{2s} = 3.2084$ MeV

N	WFE b = 2.25 fm		WFE b = 1.90 fm		PSE b = 1.35 fm	
	E_{2s} , MeV	$\Delta \cdot 10^6$	E_{2s} , MeV	$\Delta \cdot 10^6$	E_{2s} , MeV	$\Delta \cdot 10^6$
1	.9968	53177	2.1578	37522	-	-
2	1.4268	42168	2.1759	40475	4.1457	850
3	2.9681	4108	3.0258	12625	3.4128	278
4	3.0620	5008	3.0909	7798	3.1632	27
5	3.1949	620	3.1301	4853	3.2055	2
6	3.1949	640	3.1772	2328	3.2123	1
7	3.1990	326	3.1834	1664	3.2073	<.5
8	3.2039	99	3.1968	879	3.2080	<.5
9	3.2040	113	3.2001	572	3.2083	<.5
10	3.2072	17	3.2033	353	3.2083	<.5
11	3.2072	22	3.2052	213	3.2084	<.5
12	3.2082	14	3.2061	134		
13	3.2082	15	3.2070	74		
14	3.2083	26	3.2074	48		
15	3.2084	29	3.2078	20		

tant (weakly-bound states, reactions involving the nuclear periphery, asymptotic normalization constants) the PSE is much better suited to the problem than the WFE method.

REFERENCES

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