Three and Four Centre Oscillators and Their Application in Nuclear Physics

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The extension of the nuclear two-centre-oscillator to three and four centres is investigated. Some special symmetry-properties are required. In two cases an analytical solution of the Schrödinger equation is possible. A numerical procedure is developed which enables the diagonalization of the Hamiltonian in a non-orthogonal basis without applying Schmidt's method of orthonormalization. This is important for calculations of arbitrary two-dimensional arrangements of the centres.

1. Introduction

The wellknown inability of the liquid drop model to describe satisfactorily complicated fission processes [1] led to the suggestion [2, 3] that shell structure effects may play an important role. To discuss the shell effect of nuclear shapes appearing during an asymmetric fission of a nucleus Maruhn and Greiner [4] extended the two-center shell model of Scharnweber et al. [5, 6] which is based on the double oscillator model.

In all these cases one can handle only nuclear fissions into two fragments. To calculate multiple fission as well as cluster structures of light nuclei, it is necessary to consider general arrangements of more than two harmonic oscillators. They may be situated along a line, in a plane, or in space.

The most general ansatz of such a potential is

$$V_i(\mathbf{r}) = \tfrac{1}{2}\, m\, \{\omega_{xi}^2\,(x-x_i)^2 + \omega_{yi}^2\,(y-y_i)^2 + \omega_{zi}^2\,(z-z_i)^2\} \quad i = 1, \ldots, N \qquad (1)$$

(N = number of centres).

As one can see immediately, we have to restrict the functions $V_i(\mathbf{r})$ such that they match continuously in those planes joining neighbouring centres. In what follows, several cases are discussed.

2. Linear Arrangements of Three and Four Centres

The cylindrical symmetry and the continuity of $V(\mathbf{r})$ require to make the following ansatz

$$V(\varrho, z) = \tfrac{1}{2}\, m\, (\omega_\varrho^2\, \varrho^2 + \omega_{zi}^2\,(z-z_i)^2)\,. \qquad (2)$$

The resulting nuclear shapes given by equipotential surfaces are shown in Figure 1.

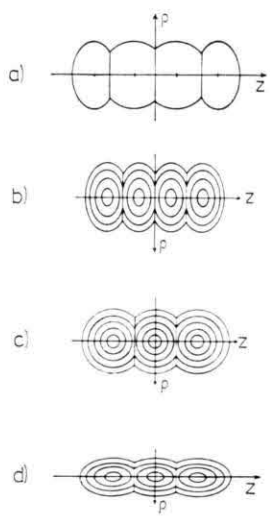


Fig. 1. Nuclear shapes and equipotential surfaces. In a) a general form for nuclear shapes treated here is shown. In b), c), and d) all fragments are equal but each one is either oblate (b), spherical (c), or prolate (d). The number of fragments is three or four respectively.

Clearly $V(\varrho, z)$ is not continuous along the z-axis, but has sharp edges at the matching planes between the centres.

For mathematical convenience we choose equal ω_{zi} as an additional symmetry, which means equal deformation for all fragments, but we note that also in the more general case of unequal ω_{zi} analytic solutions are obtained. The Schrödinger equation is then given by

$$\left\{-\frac{\hbar^2}{2\,m}\,\Delta + \tfrac{1}{2}\, m\,(\omega_\varrho^2\,\varrho^2 + \omega_z^2\,(z-z_i)^2) - E\right\} \cdot \psi_E(\varrho, \varphi, z) = 0\,. \qquad (3)$$

The separation of variables according to

$$\Psi_E(\varrho, \varphi, z') = \vartheta(\varphi)\cdot\chi(\varrho)\cdot\psi(z') \quad \text{with} \quad z' = z - z_i \qquad (4)$$

yields the solution

$$\begin{aligned}
&\nu(\varphi) = (2\pi)^{-1/2}\exp\{i\, n_\varphi\, \varphi\}\ ;\ n_\varphi \varepsilon N^0\,,\\
&\chi(\varrho) = C\left[\frac{m\,\omega_\varrho}{\hbar}\right]^{(|1+|n}} \exp\left\{-\frac{m\,\omega_\varrho}{2\,\hbar}\,\varrho^2\right\}\cdot {}_1F_1\left(-n_\varrho\,;\,1+|\,n_\varphi\,|\,;\,\frac{m\,\omega_\varrho}{\hbar}\,\varrho^2\right);\ n_\varrho \varepsilon N^0\,,\\
&\psi(z') = \exp\left\{-\frac{m\,\omega_z}{2\,\hbar}\,z'^2\right\}\cdot\left\{C_{1i}\sqrt{\frac{m\,\omega_z}{\hbar}}\,z'\,{}_1F_1\left(\frac{1-n_z}{2}\,;\,\frac{3}{2}\,;\,\frac{m\,\omega_z}{\hbar}\,z'^2\right)+C_{2i}\,{}_1F_1\left(-\frac{n_z}{2}\,;\,\frac{1}{2}\,;\,\frac{m\,\omega_z}{\hbar}\,z'^2\right)\right\}.
\end{aligned}\tag{5}$$

The single particle energies are given by

$$E_{n_z n_s n_\psi} = \hbar\,\omega_z(n_z+\tfrac{1}{2}) + \hbar\,\omega_\varrho(2\,n_\varrho+|\,n_\varphi\,|+1)\,. \tag{6}$$

The wave function $\psi(z)$ contains $2N$ constants of integration (C_{1i} and C_{2i}) which have to be chosen such that $\psi(z)$ is a quantum mechanically acceptable wave function. The following requirements have to be fulfilled:

a) continuity and differentiability,

b) square integrability,

c) definite symmetrical behaviour under the transformation $z \to -z$ (because of H being symmetric under reflection at $z=0$) (parity quantum number π). With the abbreviations

$$\begin{aligned}
F^0 &= {}_1F_1\left(-\frac{n_z}{2}\,;\,\frac{1}{2}\,;\,k\,a^2\right),\\
U_0 &= U\left(-\frac{n_z}{2}\,;\,\frac{1}{2}\,;\,k\,a^2\right),\\
F^1 &= {}_1F_1\left(\frac{1-n_z}{2}\,;\,\frac{3}{2}\,;\,k\,a^2\right),\\
F^2 &= {}_1F_1\left(\frac{2-n_z}{2}\,;\,\frac{3}{2}\,;\,k\,a^2\right),\\
U^2 &= U\left(\frac{2-n_z}{2}\,;\,\frac{3}{2}\,;\,k\,a^2\right),\\
F^3 &= {}_1F_1\left(\frac{3-n_z}{2}\,;\,\frac{3}{2}\,;\,k\,a^2\right),\\
k &= m\,\omega/\hbar
\end{aligned}\tag{7}$$

for the hypergeometrical functions we obtain in the cases of three (four) centres for the two possible symmetries $\pi = \pm 1$ homogenous systems of equations for the C-coefficients:

a) Case $N=3$ yields:

$\alpha)$ $\pi = 1$, $C_{2,0} = 0$:

$$(1-k\,a^2)F^1 + 2\,k\,a^2\,\frac{1-n_z}{3}\,F^3\,C_{1,0} - a\sqrt{k}(U^0 - n_z\,U^2)\cdot C_2 = 0\,,$$

$$a\sqrt{k}\,F^1\,C_{1,0} - U^0\,C_2 = 0\,;$$

$\beta)$ $\pi = +1$, $C_{1,0} = 0$:

$\psi'(z=a)$ continous

$$(F^0 + 2\,n_z\,F^2)\,C_{2,0} + (U^0 - n_z\,U^2)\,C_2 = 0\,,$$

$\psi'(z=a)$ continous $\qquad F^0\cdot C_{2,0} - U^0\cdot C_2 = 0\,.$

b) Case $N=4$ yields:

ψ continous at $z = 2\,a$

$$a\sqrt{k}\,F^1\,C_{1,1} + F^0\cdot C_{2,1} - U^0\cdot C_3 = 0\,,$$

$\psi'(2\,a)$ continous $\sqrt{k}\left((1-k\,a^2)F^1 + 2\,k\,a^2\,\dfrac{1-n_z}{3}\,F^3\right)$

$$\cdot C_{1,1} - k\,a(F^0 + 2\,n_z\,F^2)\,C_{2,1} - k\,a(U^0 - n_z\,U^2)\,C_3 = 0\,;$$

$\alpha)$ $\pi = +1$:

$\psi'(0)$ continous $\sqrt{k}\left((1-k\,a^2)F^1 + 2\,k\,a^2\,\dfrac{1-n_z}{3}\,F^3\right)$

$$\cdot C_{1,1} + k\,a(F^0 + 2\,n_z\,F^2)\,C_{2,1} = 0\,,$$

$\beta)$ $\pi = -1$:

$$\psi(0)\text{ continous } a\sqrt{k}\,F^1\cdot C_{1,1} - F^0\cdot C_{2,1} = 0\,.$$

Eigenvalue equations can now be obtained by setting the determinant of the above systems equal to zero. This yields in both cases:

a) $N=3$:

$\alpha)$ $\pi = +1$: $F^0(U^0 - n_z\,U^2) + U^0(F^0 + 2\,n_z\,F^2) = 0\,.$

$\beta)$ $\pi = -1$:

$$k\,a^2\,F^1(U^0 - n_z\,U^2) - U^0\left((1-k\,a^2)F^1 + 2\,k\,a^2\,\frac{1-n_z}{3}\,F^3\right) = 0\,; \tag{8}$$

b) $N=4$:

$\alpha)$ $\pi = +1$:

$$\begin{aligned}
&(U^0 - n_z\,U^2)\,(1-2\,k\,a^2)F^0\,F^1 - 2\,k\,a^2\left(n_z\,F^1\,F^2 - \frac{1-n_z}{3}\,F^0\,F^3\right)\\
&+ 2\,U^0(F^0 + 2\,n_z\,F^2)\cdot\left((1-k\,a^2)F^1 + 2\,k\,a^2\,\frac{1-n_z}{3}\,F^3\right) = 0\,,
\end{aligned}\tag{9}$$

$\beta)$ $\pi = -1$:

$$(1-4\,k\,a^2)F^0\,F^1\,U^0 + 2\,k\,a^2\cdot\left[\frac{1-n_z}{3}\,F^0\,F^3\,U^0 + n_z\,F^1(F^0\,U^2 - F^2\,U^0)\right] = 0\,.$$

If k is known the solutions of the equations above can be found by applying Newton's method. As usual in nuclear shell theory, k is evaluated from the relation

$$\hbar\,\omega_0 = 41\,A^{-1/3}\,[\mathrm{MeV}] \qquad (10)$$

(see Ref. 6) and from the constraint of volume conservation (incompressibility of nuclear matter) when the deformation varies. In this work the most simple prescription for volume conservation, namely the surface-volume-conservation is used [7]. It yields

$$k(a) = 1.226\,r^{-1}(a)\,. \qquad (11)$$

Here $r(a)$, the cluster radius, is the solution of the cubic equation

$$2\,r^3 + 3\,(N-1)\,a\,r^2 = 2\,R^3 + (N-1)\,a^3 \qquad (12)$$

when $a < R\cdot N^{-1/3}$, elsewhere [the case of separated fragments $(a > R\cdot N^{-1/3})$] it is $r = R\cdot N^{-1/3}$. In the above formulas R means the radius of the undeformed nucleus: $R = 1.256\,\mathrm{A}^{1/3}[\mathrm{fm}]$ and the assumption of spherical clusters $(\omega_\varrho = \omega_z)$ is made.

The generalization to ellipsoidal deformations of the nuclear fragments is done by introducing an additional deformation parameter β. As suggested by the nuclear shapes occurring in this case (Fig. 1), we choose β equal to the ratio of the main axis, which gives $\beta = \omega_z/\omega_\varrho$. A straightforward calculation shows that we have only to substitute

$$r(\beta, a) = \beta^{2/3}\,r(a) \qquad (14)$$

in Equation (12).

Now the quantum numbers $\{n_z\}$ can be obtained from the eigenvalue equations. They are plotted in Figs. 2, 3 against a for the model cases of C^{12} and O^{16}. So are the single-particle-energies in Figures 4, 5. The development of the single oscillator spectrum of the original compound nucleus into a threefold respectively fourfold degenerate oscillator spectrum for the separated fragments is noticed. As a consequence of volume conservation the oscillator spacing is smaller in the former case than in the latter case. By adding the single-particle energies up to the Fermi-level, we obtain a rough estimate of the binding energy-depending on the deformation parameter a. This is shown for some light nuclei, for which the neglect of ls-forces makes some sense in Figs. 6 to 9. Obviously there occur quasistable triple- and quadriple cluster configurations. Their precise location and also their stability will be modified when ls-forces and fragment deformations

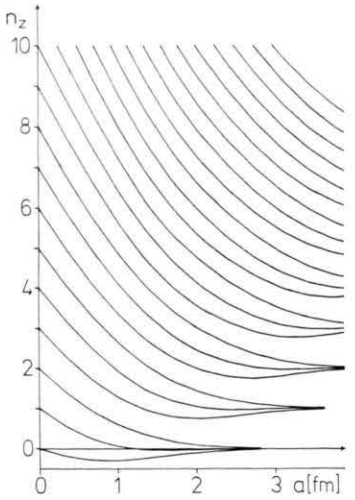


Fig. 2. n_z-eigenvalues for a ^{12}C-nucleus composed of three fragments. The threefold degeneration for large separations is obviously.

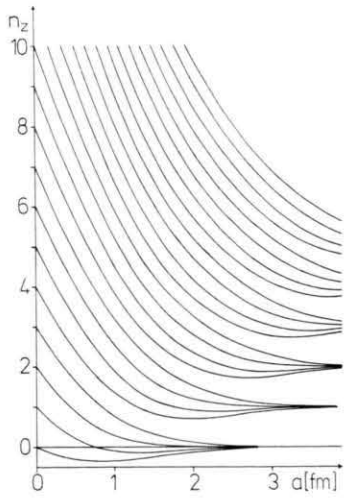


Fig. 3. n_z-eigenvalues for a ^{16}O-nucleus composed of four fragments. Here a fourfold degeneration occurs.

are included in a more realistic calculation, which also have to be renormalized in the sense of Strutinsky. Nevertheless, these results give a qualitative impression of the importance of the multiple cluster-structures in light nuclei.

3. Clover-Leaf Arrangements of Three and Four Fragments

In the previous section it was shown that an analytical solution of the Schrödinger equation exists if several restrictions on the potential are assumed. In more general cases numerical methods have to be

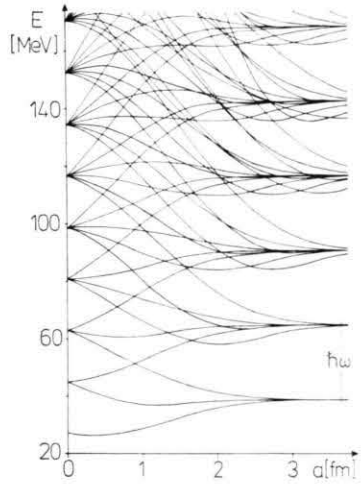


Fig. 4. Single particle energies for three fragments forming a ^{12}C-nucleus. These energies were calculated using the eigenvalues shown in Figure 2. The rearrangement to three equivalent shells for large separations is clearly to be seen.

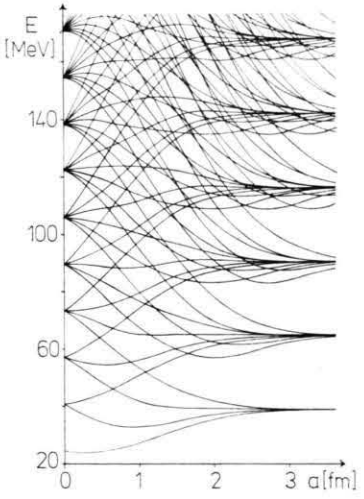


Fig. 5. Single particle energies for four fragments forming a ^{16}O-nucleus with fourfolg degeneration for large separations.

used. Usually the single particle wave functions of a harmonic oscillator, or of a more-center-oscillator composed of harmonic potentials are used as a basis for diagonalization. But this usually means involved calculations of matrix elements with complicated basis functions, especially if considering two or three-dimensional arrangements. In these latter cases an analytic solution may not be given even for harmonic potentials as the Schrödinger equation

Fig. 8. Total single particle energy of a ^{36}Ar-nucleus composed of three fragments.

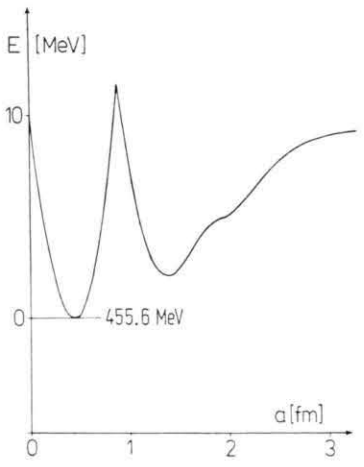


Fig. 6. Total single particle energy for ^{12}C. The single particle energies of Fig. 4 were added up to the fermi level without taking into consideration coulomb energy. The sharp peak is due to level crossing and probably will disappear when shell corrections are taken into consideration.

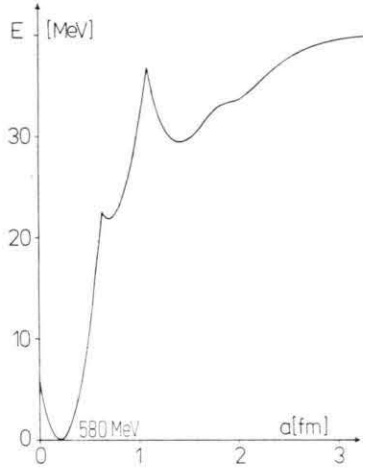
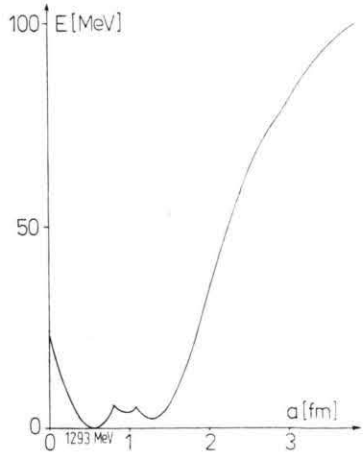


Fig. 7. Total single particle energy of a ^{16}O-nucleus composed of four fragments.



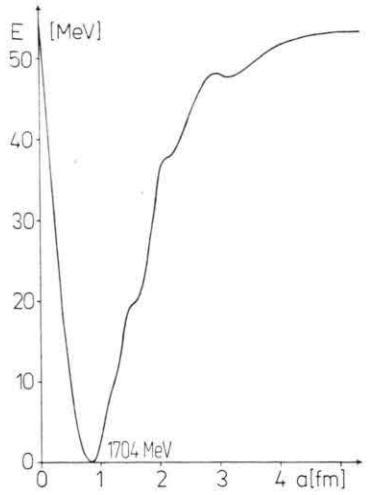


Fig. 9. Total single particle energy of a ^{48}Cr-nucleus composed of four fragments.

does not separate. Hence we propose to look for a basis consisting of simple functions with good convergence properties for a wide variety of deformed potentials. The potentials to be considered are those occurring in fission processes or clustesr structures in nuclei. They may be thought of as several harmonic oscillators nearly having the shape of the desired potentials.

An only slightly deformed nucleus may be treated excellently in the basis of the harmonic oscillator. Thus in the limits of one compound nucleus and of several fully separated fragments one can use the eigenfunctions of one or more harmonic oscillators respectively. The orthogonal basis wave functions within the i'th oscillator are

$$|\varphi_k{}^i\rangle = H_k(x-x_i) \times \exp\{-\tfrac{1}{2}(x-x_i)^2\}\, N_k\,. \quad (15)$$

Here x_i denotes the positions of the centre of the i^{th} oscillator and H_k are Hermite polanomials. It is obvious that potentials of fragments not totally separated or cluster structures may be described equally well in this basis. Low states coincide with the properly symmetrized eienfunctions of the oscillators which are already separated in energies; high states coincide with the eigenfunctions of all n-oscillators which are nearly identical for high energies. So the intermediate levels of the potential ought to be a superposition of the intermediate levels of the n-oscillators.

When actually treating problems in this basis, difficulties arise from the fact that the basis vectors $\varphi_k{}^i$ are not orthonormal (over completeness of the basis): Sets belonging to different centres i, j overlap. Indeed,

$$\int_{-\infty}^{+\infty} \exp[-\tfrac{1}{2}\{(x-x_i)^2+(x-x_j)^2\}] \cdot N_k N_l H_k(x-x_i)\, H_l(x-x_j)\,\mathrm{d}x \neq \delta_{kl}\,\delta_{ij}\,. \quad (16)$$

Furthermore, the eigenfunctions of the different oscillators are nearly colinear for higher states

$$\int_{-\infty}^{+\infty} \exp[-\tfrac{1}{2}\{(x-x_i)^2+(x-x_j)^2\}] \cdot N_k{}^2 H_k(x-x_i)\, H_k(x-x_j)\,\mathrm{d}x \approx 1\,. \quad (17)$$

Thus the basis becomes overcomplete, especially for a small separation of the centers. Because common numerical methods suppose the basis to be orthonormal one has either to orthogonalize according to Schmidt's method, or a numerical procedure has to be provided allowing to treat the eigenvalue problem directly in the nonorthonormal basis. To avoid the time-consuming orthonormalization and to take advantage of the simple form of the basis functions when calculating the matrix elements, we have chosen the second method.

Generally, the matrix H representing the Hamiltonian in the basis $|\varphi^l\rangle$ has to be calculated and a nonunitary transformation T has to be found such that H is diagonalized. However, the calculations may be considerably reduced by treating the modified eigenvalue problem instead:

$$A\,|\psi\rangle = B\,|\psi\rangle\,, \quad (18)$$

A and B being matrices. It must be remembered here that the matrix representing a self-adjoint operator is hermitean if it is represented in an orthonormal basis, which is not the case here. Thus especially $\langle\varphi^l|\,H\,|\varphi^k\rangle$ is not the matrix representing the Hamiltonian in this nonorthonormal basis!

We start with the Schrödinger equation

$$\mathcal{H}\,\psi = E\,\psi \quad (19)$$

in the basis $|\varphi^l\rangle$

$$|\psi\rangle = \sum_l a_l\,|\varphi^l\rangle \quad (20)$$

and obtains

$$\mathcal{H}\sum_l a_l\,|\varphi^l\rangle = E\,\sum_l a_l\,|\varphi^l\rangle\,. \quad (21)$$

Multiplying with the associated bra $\langle\varphi^k|$ we obtain

$$\sum_l \langle\varphi^k|\,\mathcal{H}\,|\varphi^l\rangle\, a_l = E\,\sum_l \langle\varphi^k|\,\varphi^l\rangle\, a_l\,. \quad (22)$$

This may be regarded as a matrix equation

$$\hat{A}\,|\psi\rangle = E\cdot\hat{S}\,|\psi\rangle \quad (23)$$

with
$$A_{kl} = \langle \varphi^k \,|\, \mathcal{H} \,|\, \varphi^l \rangle \,,$$
$$S_{kl} = \langle \varphi^k \,|\, \varphi^l \rangle \,, \quad |\, \psi \rangle_l = a_l \,. \tag{24}$$

The matrix representing the Hamiltonian in this basis may now be calculated easily

$$\hat{H} = \hat{S}^{-1}\, \hat{A} \tag{25}$$

but is, however, not hermitean.

To obtain the eigenvalues and eigenvectors we firsts diagonalize S. As its elements are scalar products, it is hermitean according to the property of the scalar product

$$\langle \varphi^k \,|\, \varphi^l \rangle = \langle \varphi^l \,|\, \varphi^k \rangle^* \,. \tag{26}$$

Hence there exists an unitary transformation U diagonalizing S

$$\hat{U}\, \hat{A}\, \hat{U}^+ \cdot \hat{U} \,|\, \psi \rangle = E\, \hat{U}\, \hat{S}\, \hat{U}^+ \cdot U \,|\, \psi \rangle$$
$$\hat{A'} \cdot |\, \psi \rangle' = E \cdot \hat{S'} \cdot |\, \psi \rangle' \,. \tag{27}$$

This is the same eigenvalue problem in the basis $|\, \varphi'^l \rangle = U^+ \,|\, \varphi^l \rangle$. As the scalar product is positive definite the elements of S' are positive. Thus there exists a regular matrix X with

$$\hat{X} \cdot \hat{X} = \hat{S'} \,. \tag{28}$$

Transforming (27) with X yields

$$\hat{X}\, \hat{A'}\, \hat{X}^{-1} \cdot \hat{X} \,|\, \psi \rangle' = E\, \hat{S'} \cdot \hat{X} \,|\, \psi \rangle' \tag{29}$$

as S and S' commute. Multiplying by S'^{-1} we obtain

$$\hat{X}^{-1}\, \hat{A'}\, \hat{X}^{-1} \cdot \hat{X} \,|\, \psi \rangle' = E\, \hat{X} \,|\, \psi \rangle' \,,$$
$$\hat{A''} \,|\, \psi \rangle'' = E \,|\, \psi \rangle'' \,. \tag{30}$$

X transforms the eigenvalue equation to an orthonormal basis, and in this representation A'' now actually is the matrix representing the Hamiltonian. Equation (30) may now be treated by standard methods.

Up to now the basis vectors were supposed to be linearly independent. Generally this is true, but as already mentioned, for small separations and large eigenvalues some of the corresponding eigenvectors may become collinear, and the basis is then overcomplete. For further calculations, the superfluous basis vectors have to be eliminated. Usually it is rather complicated to test a set of vectors for linear independence. Therefore it is advantageous to diagonalize the matrix S first and then to eliminate the linearly dependent vectors. If two basis vectors are linearly dependent, the matrix S is not regular. The matrix S' being similar to S is not regular either and thus contains at least one zero in its main diagonal. Therefore no inverse matrix S^{-1} exists and the procedure fails, but the problem may be solved at this step by simply eliminating the rows and columns containing the zeros of S' and A' respectively.

4. Calculation of Matrix Elements

The elements of the matrix $\hat{S}$ can be calculated analytically

$$\langle \varphi^k \,|\, \varphi^l \rangle = \int_{-\infty}^{+\infty} N_k\, N_l \exp\left[-\tfrac{1}{2} \left\{ (x - x_i)^2 + (x - x_j)^2 \right\} \right] H_k(x - x_i)\, H_l(x - x_j) \,. \tag{31}$$

Using the transformation

$$u = x - \tfrac{1}{2}(x_i + x_j) \,, \delta = x_i - x_j \tag{32}$$

and expanding H_k and H_l into a series by means of

$$\mathrm{d}H_n(x)/\mathrm{d}x = 2\, n\, H_{n-1}(x) \,, \tag{33}$$

we obtain

$$\langle \varphi^k \,|\, \varphi^l \rangle = \sqrt{\pi} \exp\{ -\delta^2/4 \}\, \delta^{k-l}\, k!\, l!\, 2^k \cdot \sum_{\alpha=0}^{k} \frac{(-1)^\alpha \cdot \delta^{2\alpha}}{2^\alpha\, \alpha!\, (l-\alpha)!\, (k-l+\alpha)!} \tag{34}$$

The elements of the matrix A are of the form

$$\langle \varphi^k \,|\, \mathcal{H} \,|\, \varphi^l \rangle = \langle \varphi^k \,|\, \partial^2/\partial x^2 \,|\, \varphi^l \rangle + \langle \varphi^k \,|\, \mathcal{V} \,|\, \varphi^l \rangle \,. \tag{35}$$

The first term, the kinetic part of the operator, can also be given analytically. It reads

$$\langle \varphi^k \,|\, \partial^2/\partial x^2 \,|\, \varphi^l \rangle = \int_{-\infty}^{+\infty} N_k\, N_l \exp\left\{ -\tfrac{1}{2}(x - x_i)^2 \right\} \cdot H_k(x - x_i)\, \frac{\partial^2}{\partial x^2} \exp\left\{ -\tfrac{1}{2}(x - x_j)^2 \right\} H_l(x - x_j) \,. \tag{36}$$

By means of (33) and

$$x\, H_n = n\, H_{n-1} + \tfrac{1}{2}\, H_{n+1} \tag{37}$$

we may reduce this expression to a combination of scalar products

$$\left\langle \varphi^k \left| \frac{\partial^2}{\partial x^2} \right| \varphi^l \right\rangle = -\frac{\sqrt{k\, l}}{2} \langle \varphi^{k-1} \,|\, \varphi^{l-1} \rangle - \frac{\sqrt{(k+1)\,(l+1)}}{2} \langle \varphi^{k+1} \,|\, \varphi^{l+1} \rangle + \frac{\sqrt{k(l+1)}}{2} \langle \varphi^{k-1} \,|\, \varphi^{k+1} \rangle + \frac{\sqrt{l(k+1)}}{2} \langle \varphi^{k+1} \,|\, \varphi^{l-1} \rangle \,. \tag{38}$$

The matrix elements of the potential energy $\langle \varphi^k \,|\, V(x) \,|\, \varphi^l \rangle$ can be calculated analytically only

for a few simple forms of the potential. If one considers more complicated forms or a two- or three-dimensional problem where the potential cannot be separated into independent terms for x, y and z, no analytical calculations are possible. It is advantageous, in this case, to calculate some matrix elements numerically and to derive the others from these by means of recursion relations [8]. As $V(x)$ is a scalar these formulas are independent of the potential and it is sufficient to give them for the product of two basic functions. Any potential may be then be treated.

Using the recursion relation

$$H_{k+1} = 2\,x\,H_k - 2\,k\,H_{k-1} \tag{39}$$

we obtain

$$H_{k+1}(x-x_i)H_l(x-x_j) = H_k H_{l+1} + 2\,l\,H_k H_{l-1} - 2\,k\,H_{k-1}H_l - 2\,(x_i-x_j)H_k H_l\,. \tag{40}$$

So it is only necessary to calculate the main diagonal and the few off-diagonal elements with $k=l$.

5. Test of the Accuracy of the Numerical Method

The following table (Tab. 1) shows the results obtained with the numerical method and the exact solution of the eigenvalues of a harmonic two-oscillator of excentricity 1.5 (dimensionless coordinates). The dimension of the matrix diagonalized was twenty. As the Schrödinger equation separates for an harmonic more-centre-oscillator, only the eigenvalues in z-direction were considered. As the separation of the Schrödinger equation was made in cartesian coordinates for the numerical treatment, but in cylindrical coordinates for the analytic calculations the eigenvalues may not be compared immediately: Hermite's differential equation yields only odd positive integers while Kummer's equation yields all positive integers. However, the calculation to be performed for comparing the results is straightforward.

Table 1. Comparison between the results of analytical and numerical calculation. The dimension of the matrix diagonalized was 20, the excentricity 1.5.

Analytic	Numeric	Error (%)
.8015	.8015	.004
1.1575	1.1600	.217
2.6487	2.6491	.015
3.6469	3.6574	.305
5.1040	5.1044	.008
6.4168	6.4192	.037
7.9298	7.9243	.005
9.3733	9.3736	.003
10.9287	10.9295	.007
12.4549	12.4557	.007
14.0492	14.0513	.015
15.6263	15.6280	.011
17.2516	17.2597	.047
18.8657	18.8986	.174
20.5163	20.7690	1.232
22.1590	.0000	
23.8304	.0000	
25.4960	.0000	
27.1851	.0000	
28.8697	.0000	

As can be seen from the table the difference between the two results is very small. Of course, similar comparisons were made for other excentricities and different dimensions of the matrices. All results were equally excellent, but for larger matrices attention must be paid to the accuracy of the integration over polynomials of higher degree. The convergence generally is excellent, nearly all eigenvalues obtained by diagonalization may be used. Actually in the example shown in the table only the last eigenvalue shows an error of more than .5 percent.

6. Conclusion

The methods developed in this paper are very useful especially for a treatment of multiple fission processes and cluster structures of light nuclei. Only recently, triple fission with the emission of an α-particle in addition to two heavy fragments has become more interesting [9]. In this field a large amount of experimental data exists without an appropriate theory, and the method developed here may be appropriate for these problems after some mathematical generalization.

A critical parameter is here the fission mass, but first calculations were done to solve the current discrepancies with the aid of the two centre shell model [10]. The treatment of cluster-structures using different centres for the α- or d-clusters will also be interesting [11, 12], even if shell-model calculations are not of such importance here because they may be treated explicitly by single-particle coordinates. However, since the interaction between nucleons and clusters are easier to treat in collective coordinates, a many-centre-ansatz may be an adequate starting point.

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