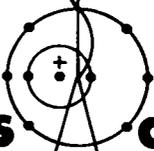


LA-4735-MS

C. 3

CIC-14 REPORT COLLECTION
**REPRODUCTION
COPY**

Finite-Difference Solution of
Axially Symmetric Nuclear
Single-Particle Potentials



los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

UNITED STATES
ATOMIC ENERGY COMMISSION
CONTRACT W-7405-ENG. 36

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

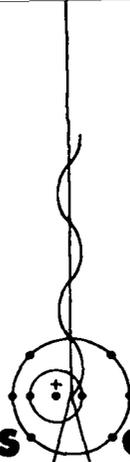
This report, like other special-purpose documents in the LA. . .MS series, has not been reviewed or verified for accuracy in the interest of prompt distribution.

Printed in the United States of America. Available from
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151
Price: Printed Copy \$3.00; Microfiche \$0.95

LA-4735-MS

UC-34

ISSUED: August 1971



los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

Finite-Difference Solution of Axially Symmetric Nuclear Single-Particle Potentials

by

E. O. Fiset

J. R. Nix

M. Bolsterli



FINITE-DIFFERENCE SOLUTION OF AXIALLY
SYMMETRIC NUCLEAR SINGLE-PARTICLE POTENTIALS

by

E. O. Fiset, J. R. Nix, and M. Bolsterli

ABSTRACT

We have investigated an implicit finite-difference method for solving Schrödinger's equation for axially symmetric static nuclear single-particle potentials. The method used is an improved version of the procedure outlined by Dickmann. The finite-difference equations are obtained in prolate spheroidal coordinates by use of a variational principle. The eigenvalues and eigenvectors of the resulting band matrix are found by use of inverse iteration, with the linear system of equations solved directly. The method works satisfactorily, but requires approximately 25 times as much computing time as an expansion of the wave function in deformed harmonic-oscillator basis functions, for comparable accuracy in the eigenvalues.

I. INTRODUCTION AND CONCLUSION

Many studies in nuclear physics involve solving Schrödinger's equation for axially symmetric static nuclear single-particle potentials. Such equations arise for slightly deformed potentials in connection with various ground-state properties of deformed nuclei, and for more highly deformed potentials in connection with the influence of single particles on the fission process and on heavy-ion reactions.

There are two general methods for solving these equations: expanding the wave function in a set of basis functions and finite-difference methods. Expansion methods traditionally have been used for small deformations, but at the beginning of this study serious questions had been raised regarding the convergence of these methods for the large distortions encountered in fission and in heavy-ion reactions (see, for example, Ref. 1). We therefore decided to investigate the accuracy and speed with which the equations could be solved by means of a finite-difference method.

The approach that we have followed is an improved version of the procedure outlined by Dickmann.² This is an implicit method, in which all the values of the wave function are connected

simultaneously through a system of linear equations. For small deformations Rost³ and Tarp⁴ have considered an explicit finite-difference method, in which the potential itself is expanded in a sum of functions separable in the spherical coordinates r and θ ; this leads to a set of coupled differential equations to be solved simultaneously. However, it appears that for large deformations so many terms would be required in such an expansion of the potential to make this approach impractical from the outset.

In the meantime, expansion methods using deformed harmonic-oscillator basis functions have also been developed for large deformations.⁵⁻⁷ This permits a direct comparison to be made between the expansion and finite-difference methods. It turns out that for fairly smooth potentials, such as generalized Woods-Saxon potentials⁵ or folded Yukawa potentials,^{6,7} the convergence of the deformed harmonic-oscillator expansion is much faster than we had originally anticipated, even for very large deformations. For comparable accuracy, the single-particle energies can be computed for such potentials roughly 25 times as rapidly by use of the expansion method as by use of the finite-difference method (for a

general reflection-asymmetric axially symmetric shape).

Although of limited usefulness for calculating single-particle energies for smooth potentials, there are two areas where a finite-difference method could still conceivably be preferable to an oscillator-expansion method. The first is in connection with less smooth potentials, such as those containing cusps in the equipotential surfaces. For example, the convergence of a deformed (one-center) oscillator expansion is very slow for a generalized two-center oscillator potential.⁸ Although this particular potential is efficiently treated in terms of a deformed two-center oscillator expansion, other potentials containing strong cusps might be solved advantageously by a finite-difference method.

The second area where a finite-difference method might be useful is in calculating the asymptotic behavior of bound-state wave functions for very deformed potentials. The asymptotic behavior of wave functions calculated in an oscillator expansion is Gaussian, whereas the true asymptotic behavior of the bound-state wave functions is not (for realistic potentials that approach zero at large distances). To obtain the proper asymptotic behavior in the expansion method would require replacing the calculated wave function at large distances by the known asymptotic solution. On the other hand, the proper asymptotic solution is given automatically in the finite-difference method.

Since our primary interest is in calculating the energies for smooth potentials, we have not seriously investigated either of these areas.

For the benefit of anyone who would like to pursue either these or other aspects of a finite-difference method of solution, we describe briefly in the remainder of this report the method that we have studied. Some of the details and relevant formulas have already been given by Dickmann² and will not be repeated here. Reference 7 discusses the specific single-particle potential that we have used, as well as some physical applications of the results. The present report is not intended for further publication, and is purposefully brief and informal.

II. SELECTION OF GRID POINTS

In the finite-difference approach the single-particle wave functions are calculated at only a finite number of spatial grid points, and the differential Hamiltonian is replaced by a finite-difference matrix which couples the values of the wave function at neighboring points. Because of the limitation to axially symmetric shapes, our potentials are functions only of ρ and z , where ρ and z are the usual cylindrical coordinates. Consequently the z -component of total angular momentum is a constant of the motion.

Since only a finite number of grid points are used, it is desirable to distribute them advantageously, with most of the points concentrated in regions where the wave functions change rapidly. This is accomplished in two steps. First, we make a coordinate transformation to prolate spheroidal coordinates, which is given by

$$\begin{aligned}\rho &= a \sinh \eta \sin \theta , \\ z &= a \cosh \eta \cos \theta , \\ \psi &= \psi .\end{aligned}$$

The coordinate surfaces are prolate spheroids ($\eta = \text{constant}$), hyperboloids of revolution of two sheets ($\theta = \text{constant}$), and half planes ($\psi = \text{constant}$). The quantity a is the distance between the origin and the focus common to the spheroids and hyperboloids. The shape of the coordinate system is changed by varying a , which is selected so that the eccentricity of the coordinate spheroids approximates that of the given nuclear shape.

The second step in distributing the grid points advantageously is to use a nonuniform spacing in η , with the points spaced more closely for small values of η than for large values. Since in practice it is more convenient to make finite-difference approximations in terms of constant step sizes, we make a further nonlinear transformation to the variable t , defined by

$$\sinh \eta = \frac{bt}{(1-t^2)^\alpha(1+ct^2)}, \quad 0 \leq t < 1 .$$

The constants b , α , and c determine the distribution

of points. In particular, the number of points distributed near the $\rho = 0$ axis is determined largely by the choice of b , the rate at which η approaches infinity (i.e., the number of points in the large ρ region) is determined by the choice of α , and the distribution of points in the intermediate range depends largely upon c . In most of our studies we have used the values $\alpha = 0.5$, $c = 1.5$, and $b = 2R_0/a$, where R_0 is approximately the nuclear radius.

At this point we could also consider a nonuniform spacing in the angular coordinate θ , but have found that a uniform spacing is adequate. However, for convenience we choose to change the range of the variable so that it runs from -1 to 1 . This is accomplished by the transformation

$$\theta = \pi(1 - s)/2, \quad -1 \leq s \leq 1.$$

For setting up the finite-difference matrix we have used 20 intervals in t and 40 intervals in s (20 for positive and 20 for negative s). This gives a step size of 0.05 both in t and in s . Because the wave functions vanish both at $\rho = \infty$ and at $|z| = \infty$ the points at $t = 1$ need not be considered explicitly. In addition, the symmetry or antisymmetry of the wave functions is used to eliminate the points at $\rho = 0$. [These are the $t = 0$ points which lie between the two foci, and the $s = \pm 1$ ($\theta = 0$ or π) points which lie outside the foci.] Thus we are left with 19 points in t and 39 points in s . The distribution of these points is shown in Fig. 1.

The corresponding distribution of points in the original ρ - z space is shown in Fig. 2 for the case of ^{240}Pu at the deformation $y = 0.24$, which is the shape indicated by the solid curve. (See Ref. 7 for a precise definition of y .)

To make the following discussion more general, we denote the number of points in the t and s directions by n_t and n_s , respectively. The total number of spatial grid points is then given by $n_t n_s = 741$, but because of spin-orbit coupling we have to calculate a spin-parallel and a spin-antiparallel component at each spatial point. Thus the dimension of matrices we consider is $N \equiv 2n_t n_s = 1482$.

III. DERIVATION OF FINITE-DIFFERENCE EQUATIONS

There are two standard methods used to obtain finite-difference equations for eigenvalue problems.

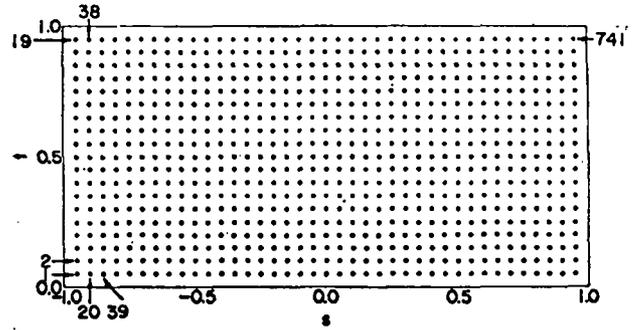


Fig. 1. Location of finite-difference points in the s - t plane. The numbers indicate the ordering of the spatial grid points in the finite-difference matrix. Since we used nearest-neighbor finite-difference approximations it is clear from the figure that point 1 is coupled only to points 2 and 20; point 2 is coupled to points 1, 3, and 21; point 21 is coupled to points 2, 20, 22, and 40; etc. Because of spin-orbit coupling there are spin-parallel and spin-antiparallel components associated with each point. This leads to a matrix of dimension $2 \times 19 \times 39 = 1482$ and bandwidth $2 \times (2 \times 19 + 1) + 1 = 79$.

In the most common method, finite-difference approximations for the various derivatives that enter are applied directly to the differential equation, in our case the Schrödinger equation. In the second method, the finite difference approximations are made inside the expression for the eigenvalue, in our case $\langle \Psi | H | \Psi \rangle$. The former method has the disadvantage of yielding nonsymmetric matrices whose eigenvalues are

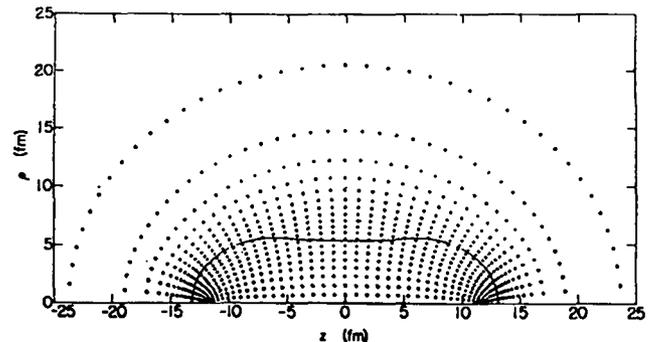


Fig. 2. Location of finite-difference points in the ρ - z plane for ^{240}Pu at the deformation $y = 0.24$. Also shown is the outline of the equivalent sharp-surface potential for this shape. Cross sections of the spheroids and hyperboloids corresponding to constant η and θ are easily discernible.

not necessarily real. Although this problem can be removed by a technique used by Dickmann, we chose to use the latter method, where the bilinear appearance of Ψ enables a symmetric finite-difference matrix to be identified.

In the latter method, the eigenvalue equation is obtained directly from a finite-difference approximation to the variational equation

$$\delta \langle \Psi | (H - E) | \Psi \rangle = \delta \int_{-1}^1 ds \int_0^1 dt w(s,t) \Psi^\dagger(s,t) (H - EI) \Psi(s,t) = 0 .$$

The wave function $\Psi(s,t)$ is a two-component column vector representing the spin-parallel and spin-anti-parallel components, $\Psi^\dagger(s,t)$ is its complex-conjugate transpose, H is a 2×2 Hamiltonian matrix which couples the two spin components, and I is the 2×2 identity matrix. The azimuthal dependence of the wave function has been eliminated explicitly. The weight function $w(s,t)$ is given by the product of the volume element in prolate spheroidal coordinates and the Jacobian for the transformation to s and t , namely

$$w(s,t) = 2\pi a^3 (\sinh^2 \eta + \sin^2 \theta) \sinh \eta \sin \theta \left| \frac{d\eta}{dt} \frac{d\theta}{ds} \right| .$$

In the above integral, terms that involve second derivatives are integrated by parts before the finite-difference approximations are made. This transforms the second derivatives into first derivatives, which are then approximated by means of a two-point finite-difference rule (whose error is proportional to the square of the grid-point step size). A two-dimensional trapezoidal rule (whose error is consistent with the error in the finite-difference approximation) is used to evaluate the integral. Taking the variation of this result then leads to the matrix equation

$$\sum_{j=1}^N H_{ij} \Psi_j = E w_i \Psi_i , \quad i = 1, \dots, N ,$$

where the finite-difference Hamiltonian matrix H is symmetric. (In several instances we use the same

symbol to denote different forms of a given quantity.) The subscripts i and j each refer to the N spatial-spin grid points used in the calculation. The weight factor w_i in the right-hand side of this equation is removed by the transformation

$$\psi_i = \Psi_i \sqrt{w_i} .$$

This converts the equation into the standard form

$$\sum_{j=1}^N H_{ij} \psi_j = E \psi_i , \quad i = 1, \dots, N ,$$

where the elements of the symmetric matrix H are given by

$$H_{ij} = H_{ij} / \sqrt{w_i w_j} .$$

The ordering of points in the s - t plane for the purpose of constructing the Hamiltonian matrix is in principle arbitrary. The system we have used is shown in Fig. 1. Since the finite-difference approximation couples only nearest-neighbor points, the wave function at point number n is coupled to the wave function at points $n + 1$, $n - 1$, $n + n_t$, and $n - n_t$, provided that point n is not on any of the edges of the s - t plane.

The spin-orbit term requires that the wave functions have two components, which correspond to the spin being parallel to and antiparallel to the total angular momentum. That is, the two ℓ_z values $\Omega + \frac{1}{2}$ and $\Omega - \frac{1}{2}$ are coupled because ℓ_z is not a good quantum number in the presence of spin-orbit forces. Such a two-component wave function is commonly written as

$$\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} ,$$

where Ψ_1 is the spin-parallel component and Ψ_2 is the spin-antiparallel component. However, if written in this way, the spin-orbit coupling between Ψ_1 and Ψ_2 would lead to nonzero elements far off the diagonal, which would make a direct diagonalization of the matrix more difficult. It is far more convenient to reorder the various elements of Ψ according to

$$\Psi = \begin{pmatrix} \Psi_1(1) \\ \Psi_2(1) \\ \Psi_1(2) \\ \Psi_2(2) \\ \vdots \\ \Psi_1(741) \\ \Psi_2(741) \end{pmatrix},$$

where, e.g., $\Psi_1(n)$ refers to Ψ_1 at the n th spatial point. With this ordering the n th (spatial-spin) component of Ψ is coupled to at most the $n \pm (2n_t + 1)$ components of Ψ . These couplings result in a finite-difference Hamiltonian matrix that has a band structure with nonzero elements off the diagonal only as far as $2n_t + 1$ elements on either side. Of course, many of the elements within the band are also zero, reflecting the fact that the finite-difference approximation does not couple, for example, the 13th and 18th points. The actual structure of the resulting band matrix is shown in Fig. 3, where nonzero elements are indicated by black dots.

IV. DETERMINATION OF EIGENVALUES AND EIGENVECTORS

For each value of Ω there are N (1482) eigenvalues of the finite-difference Hamiltonian matrix. However, we are interested in obtaining only a relatively few of them, in particular the bound states. Therefore, we use the method of inverse iteration, which picks out particular solutions. The method involves making an initial guess for a particular eigenvalue and eigenvector, and then successively improving the eigenvector. For example, to find

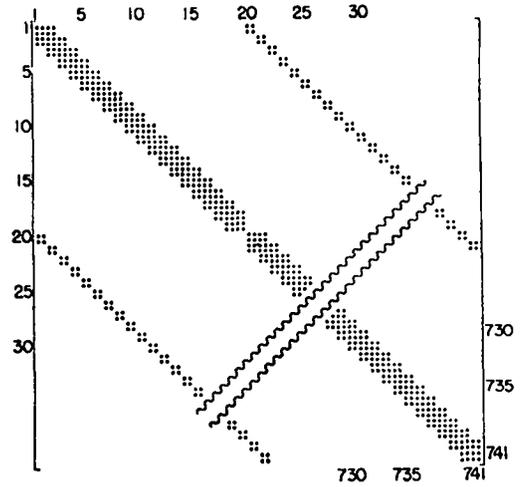


Fig. 3. Structure of finite-difference Hamiltonian. Dots indicate nonzero matrix elements. Numbers along the axes indicate the numbers of the spatial points as shown in Fig. 1. The number of the row or column of the matrix is given by twice the number shown minus one. The numbers on the top and left refer to the upper left-hand portion of the matrix, and the numbers on the bottom and right refer to the lower right-hand portion.

the eigenvalue closest to λ , we let λ be our eigenvalue guess. The initial guess ϕ_0 to the eigenvector can be taken to be an N -element column vector whose elements are all equal. We generate a new (unnormalized) guess ϕ_1 to the eigenvector from the equation

$$(H - \lambda I)\phi_1 = \phi_0,$$

or

$$\phi_1 = (H - \lambda I)^{-1}\phi_0,$$

where H is the finite-difference band matrix, and I is the $N \times N$ identity matrix. In general, a j th guess can be generated from the $(j-1)$ st guess by

$$(H - \lambda I)\phi_j = \phi_{j-1},$$

or

$$\phi_j = (H - \lambda I)^{-1}\phi_{j-1} = (H - \lambda I)^{-j}\phi_0.$$

To demonstrate that ϕ_j is a better approximation to the wave function corresponding to λ than

is ϕ_0 , it is convenient to use completeness to write ϕ_0 as a linear combination of the N eigenvectors of H . Then the preceding equation becomes

$$\phi_j = (H - \lambda I)^{-j} \sum_{i=1}^N a_i \psi^{(i)} = \sum_{i=1}^N \frac{a_i}{(E_i - \lambda)^j} \psi^{(i)}.$$

By virtue of the factor $1/(E_i - \lambda)^j$, the j th guess has greatly accentuated that eigenvector in the expansion of ϕ_0 corresponding to the eigenvalue nearest to λ .

The general procedure that we have followed involves selecting a λ and a ϕ_0 and then obtaining the inverse of the matrix $(H - \lambda I)$. The inverse is then raised to the j th power (where $j \approx 5$ in practice), and the result is dotted into ϕ_0 to give a new wave function ϕ_j . The quantity $E_1 = \langle \phi_j | H | \phi_j \rangle / \langle \phi_j | \phi_j \rangle$ is formed, and if it is sufficiently close to λ , we stop. If it differs from λ by more than a certain amount we start over again using ϕ_j as ϕ_0 , but still using the original λ . We calculate a new ϕ_j and a new E_1 . We continue the process until the new E_1 is sufficiently close to the previous one. When this occurs we say the process has converged to the eigenvalue E_1 , and the final ϕ_j (after normalization) is the corresponding eigenvector $\psi^{(1)}$. The value of λ is not changed to E_1 in subsequent iterations because the inverse of $(H - \lambda I)$ has already been obtained whereas the inverse of $(H - E_1 I)$ has not. Since the process of taking inverses is the most time-consuming part of the calculation, it is desirable to minimize the number of inverses required.

The inverse of $(H - \lambda I)$ can in general also be used to find the second closest eigenvalue to λ once the closest has been found. This is accomplished by using as the initial wave-function guess a vector that is orthogonal to the previously found eigenvector. Once the second eigenvector and eigenvalue have been found, a third can in general be obtained by using a guess that is orthogonal to both previously found eigenvectors. In principle this process could be continued and all desired eigenvectors found with just the one inverse, $(H - \lambda I)^{-1}$. However, in practice a point is reached where λ is sufficiently far from the eigenvalue being sought that the number of iterations required

is too large, and it becomes more economical to use a new λ and compute a new inverse. With the use of any one λ , it is necessary to continually subtract out from a newly generated ϕ_j components of previously found eigenvectors that are generated because of numerical errors.

The inversion of the band matrix was performed by the standard procedure of first factoring the band matrix into upper and lower triangular factors and then inverting the two factors. The use of a direct method for inverting the band matrix was found to be roughly 100 times as fast as the Kaczmarz iterative method used by Dickmann.² However, the direct method requires substantially more storage space than the iterative method, which makes some form of extended-core storage imperative for implementing the direct method.

V. NUMERICAL ACCURACY

The computer program that we have written finds all eigenvalues and eigenvectors between two input energies. (For example, all bound states are calculated if these two energies are the bottom of the potential well and 0.) The accuracy with which the eigenvalues of the Hamiltonian matrix (which are only approximations to the eigenvalues of the true Hamiltonian) are found is an input quantity, which we have taken to be 10^{-5} MeV. With this accuracy requirement and the number of grid points that we used, the program averages about 30 sec of CDC 6600 computing time per level. The program has no problem resolving very nearly degenerate states because of the orthogonalization procedure described above; it has resolved states that are as close together as 10^{-5} MeV.

The program was used to obtain the eigenvalues and eigenvectors for ^{240}Pu for symmetric deformations ranging from $y = 0$ to $y = 0.4$ and for the superheavy nucleus $^{298}_{114}$ for deformations from $y = 0$ to $y = 0.2$. (See again Ref. 7 for a definition of y .) In addition, the program was tested extensively for ^{240}Pu for the spherical shape, for $y = 0.24$, for the case of two equal tangent spheres, and for a very asymmetric shape corresponding to the $x = 0.8$ Businaro-Gallone saddle point.⁹

The finite-difference approximation introduces an error which is to be distinguished from the accuracy of the inverse-iteration solution mentioned

above. This finite-difference error depends upon how rapidly the wave function is varying and upon the magnitude of the step size. If the wave function is a smooth function of ρ and z (and therefore of s and t), the solution is quite accurate. However, for more oscillatory wave functions there is a degradation of the accuracy. We found in practice that nodes (or oscillations) in the radial direction caused more serious degradation than did nodes in the angular direction.

The accuracy of the solutions could be checked by comparing the eigenvalues obtained for a sphere with exact spherical solutions obtained with a one-dimensional program, and for general shapes with solutions obtained by use of deformed harmonic-oscillator expansions.⁵⁻⁷ For superheavy nuclei like $^{298}_{114}$, the accuracy for the number of grid points used ranged from several thousandths of an MeV for the ground-state level up to almost 1 MeV for highly oscillatory levels that are nearly unbound. The accuracy was somewhat better for lighter nuclei. For almost every level, we found that the finite-difference result was lower than the exact results. (This is not a contradiction of the variational principle, which applies only when an exact Hamiltonian is used; in our case the Hamiltonian has been replaced by a finite-difference approximation.)

The single-particle energies can be computed with comparable accuracy for a general reflection-asymmetric axially symmetric shape in about 1.2 sec of CDC 6600 computing time per level by use of deformed harmonic-oscillator expansions,⁵⁻⁷ which is

approximately 25 times as fast as the finite-difference method. Expansion methods are therefore to be preferred when the main interest is in calculating the single-particle energies of relatively smooth potentials. It is possible that a finite-difference method could be useful in connection with less smooth potentials and for calculating the asymptotic behavior of bound-state wave functions. However, we have not pursued either of these areas.

ACKNOWLEDGMENTS

We would like to thank B. L. Buzbee for writing the initial version of the computer program we have used for finding the eigenvalues and eigenvectors of a band matrix, and P. Concus, G. Ehrling, G. H. Golub, and S. Wahlborn for useful communications regarding numerical techniques.

REFERENCES

1. J. Houvriez, Saclay Report CEA-R-3645 (1968).
2. F. Dickmann, Z. Physik 203, 141 (1967).
3. E. Rost, Phys. Rev. 154, 994 (1967).
4. R. L. Tarp, Livermore Report UCRL-50430 (1968).
5. J. Damgaard, H. C. Pauli, V. V. Pashkevitch, and V. M. Strutinsky, Nucl. Phys. A135, 432 (1969).
6. G. Ehrling and S. Wahlborn, Phys. Letters 34B, 369 (1971).
7. M. Bolsterli, E. O. Fiset, J. R. Nix, and J. L. Norton, Los Alamos Preprint LA-DC-12817 (1971); submitted to Phys. Rev. C.
8. U. Mosel, private communication (1970).
9. J. R. Nix, Nucl. Phys. A130, 241 (1969).