ENERGY LEVELS OF A SPHEROIDAL NUCLEUS

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This is to certify that the

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ENERGY LEVELS OF A SPHEROIDAL NUCLEUS

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CONTENTS

I. INTRODUCTION

Within the last two years there has been a renewal of theoretical interest in the single particle model of the nucleus. The lack of comprehensive experimental data makes the justification for any model somewhat arbitrary. The single particle model assumes that the nucleon interaction produces a uniform potential so that each nucleon may be thought of as a single particle in a square well potential. Variations of this potential are discussed by Feenberg and Hammack[1] but we shall not be concerned with them in this thesis. A shell structure in the nucleus in many ways similar to that in atomic structure is strongly indicated[2] by the stability of nuclei possessing the "magic number" values for N or Z of 2, 8, 20, 50, 82, and 126 which appear to be the values for closed shells. Stability is assumed on the relative abundance in nature of isotones and isotopes characterized by these "magic numbers". This stability for particular N and Z values as well as the marked occurence of isomers among odd-mass nuclides with nearly closed shells led to several closely related explanations[3] among which that of M. G. Mayer[4] was perhaps the most successful.

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[1]See references 1-6 in the bibliography at the end of this thesis.

[2]Ibid.

[3]Ibid.

[4]Ibid.

In Mayer's interpretation a strong spin-orbit coupling is assumed which increases with the angular momentum. The energy levels are obtained from a quantum mechanical treatment on the basis of the single particle model. Assuming that the spins of paired nucleons cancel and that the total nuclear spin of odd-mass nuclei is just that resulting from the odd nucleon, Mayer predicted correctly the spins of all odd nuclei up to Z = 83 encountering only two exceptions. The occurence of isomerism near the closed-shell state results from the fact that at this point there are closely spaced energy levels with very different spins. The immediate shortcoming of this theory was noted by Rainwater[5] who pointed out that on the assumption of an approximately spherical charge distribution the quadrapole moment is much lower than the observed one. To overcome the difficulty he suggested an oblate spheroidal potential well. Feenberg and Hammack[6], by an approximation method based on a spherical nucleus, determined the m, ℓ-dependent change in the energy levels for small distortions. The purpose of this thesis is to show the resulting change for appreciably larger distortions.

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[5] Ibid.

[6] Ibid.

II. THEORY AND COMPUTATIONAL METHODS

We assume an ordinary uniform potential distributed throughout the volume of the spheroid. It is further assumed that the volume is not changed by the distortion. The Schrodinger equation in the usual time-independent form is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi . \tag{1}$$

The potential energy of the square well potential is

$$V = -V_0 \qquad \text{inside the spheroid,} \tag{2a}$$

$$V = 0 \qquad \text{outside the spheroid.} \tag{2b}$$

We then have for the Schrodinger equation

$$\nabla^2\psi + \frac{2m}{\hbar^2}(V_0 + E)\psi = 0 , \tag{3}$$

Letting $$K^2 = \frac{2m}{\hbar^2}(V_0 + E) , \tag{4}$$

we obtain the ordinary scalar Helmholtz equation

$$\nabla^2\psi + K^2\psi = 0 . \tag{5}$$

Eisenhart[7] has shown that there are eleven coordinate systems in which this equation is separable. The oblate spheroidal system is one of them and our problem is that of obtaining solutions for the equation in this system.

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[7] L. P. Eisenhart, Annals of Mathematics 35, pp. 284-304 (1934).

The oblate spheroidal coordinates, ξ, η, and φ, are related to the rectangular system by the following transformations:

$$x = a\,[\,(1-\eta^2)(1+\xi^2)\,]^{1/2}\cos\varphi\,, \tag{6a}$$

$$y = a\,[\,(1-\eta^2)(1+\xi^2)\,]^{1/2}\sin\varphi\,, \tag{6b}$$

$$z = a\,\eta\,\xi\,, \tag{6c}$$

where a is the semi-focal distance. The wave equation in this system is

$$\frac{\partial}{\partial\xi}\left[(1+\xi^2)\frac{\partial\psi}{\partial\xi}\right] + \frac{\partial}{\partial\eta}\left[(1-\eta^2)\frac{\partial\psi}{\partial\eta}\right] + \left[\frac{1}{1-\eta^2} - \frac{1}{1+\xi^2}\right]\frac{\partial^2\psi}{\partial\varphi^2} + c^2(\xi^2+\eta^2)\psi = 0, \tag{7}$$

where c represents the product ka. Upon separation of variables we obtain the three ordinary differential equations

$$\frac{d^2}{d\varphi^2}(\Phi) + m^2\Phi = 0, \tag{8a}$$

$$\frac{d}{d\eta}\left[(1-\eta^2)\frac{dS}{d\eta}\right] - \left[\frac{m^2}{1-\eta^2} - A_{\ell m} + c^2(1-\eta^2)\right]S = 0\,, \tag{8b}$$

$$\frac{d}{d\xi}\left[(1+\xi^2)\frac{dR}{d\xi}\right] + \left[\frac{m^2}{1+\xi^2} - A_{\ell m} + c^2(1+\xi^2)\right]R = 0, \tag{8c}$$

where m and $A_{\ell m}$ are separation constants.

Comprehensive, although slightly different, treatments of this problem have been carried out, both by Leitner and Spence[8], and Stratton et al[9]. As the latter includes tables of coefficients

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[8]A. Leitner, and R. D. Spence, The Oblate Spheroidal Wave Functions, Journal of the Franklin Institute. 249; 299 (1950).

[9]J. A. Stratton, P.M. Morse, L. J. Chu, and R. A. Hutner, Elliptic Cylinder and Spheroidal Wave Functions. John Wiley, New York, 1941.

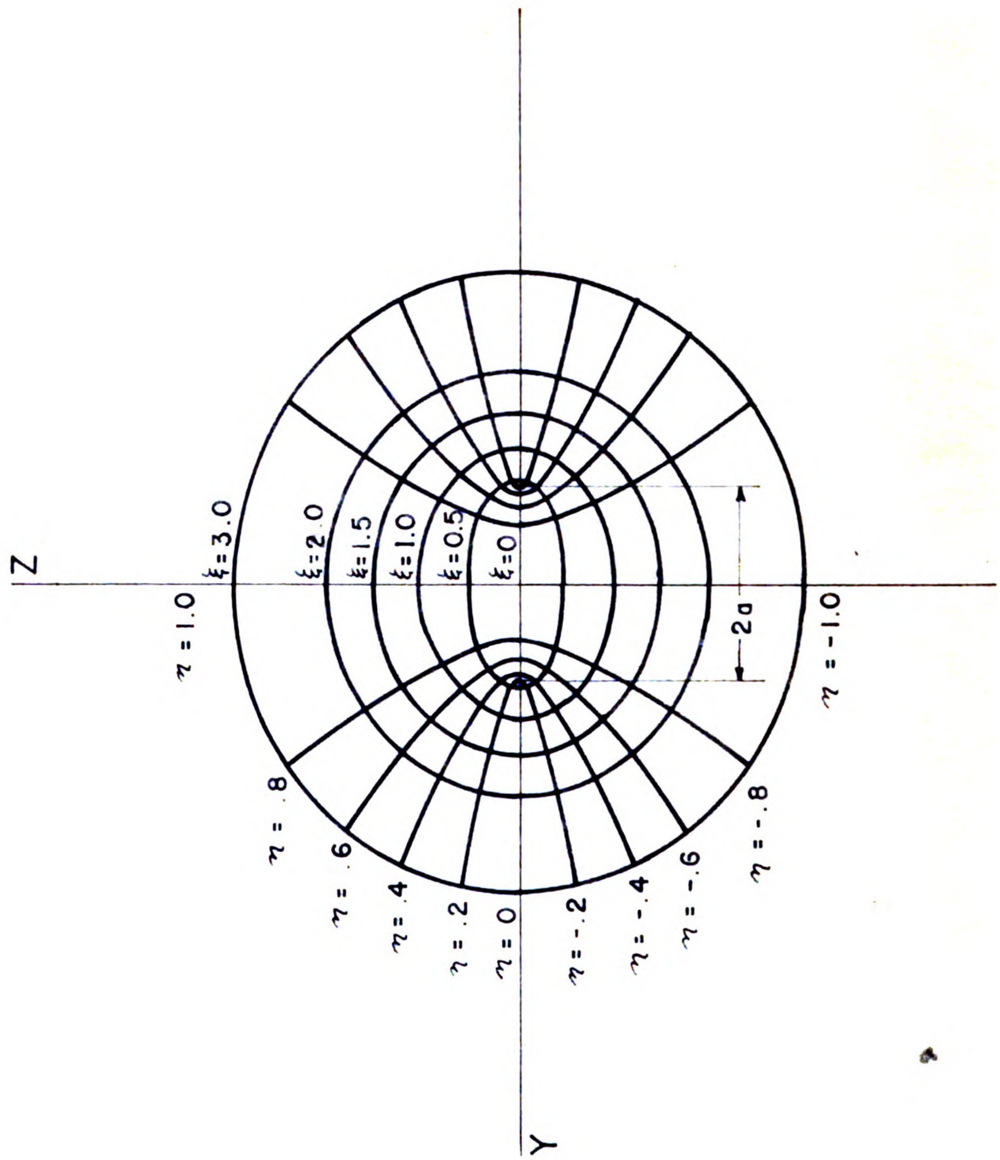

Figure 1. Cross section of the oblate spheroidal coordinates.

which are particularly useful in the computational work it is used throughout the discussion.

If a physical situation is to be represented by a wave function it is necessary that the function and its derivative be continuous, finite, and single-valued at every point in space. This of course limits the acceptable solutions. Obviously the solution of the equation in Φ is of the form $e^{im\varphi}$. In order that the wave function be single-valued m must be restricted to positive or negative integers. Solutions of the angular equation (8b) are series of associated Legendre polynomials, P^{m}_{m+n} , with a consequent restriction on m that it be less than or equal to ℓ . In determining the energy eigenvalues we require only the radial solutions.

The radial equation is put in a form differing only slightly from the equation of the associated Legendre functions by the substitution $\xi = iz$. The resulting equation is

$$\frac{d}{dz}\left[(1-z^2)\frac{dF_{\ell m}}{dz}\right] - \left[\frac{m^2}{1-z^2} - A_{\ell m} + c^2(1-z^2)\right]F_{\ell m} = 0. \qquad (9)$$

This equation has a regular singular point at $z=\pm 1$, that is at $\xi = \pm i$. It differs from the associated Legendre equation in that it has an irregular singular point at infinity. As the equation is of second order it has two indenendent solutions. One of these, the radial function of the first kind, remains finite at $z=\pm 1$; the other, the radial function of the second kind, contains logarithmic singularities at these points. This occurs for imaginary values of ξ .which are not in its physical range. However the logarithmic term becomes the arc tangent when its argument becomes iz, i.e. ξ .

The arc tangent of ξ has a branch point at $\xi = 1$; consequently the condition that the wave function be single-valued eliminates the radial function of the second kind in regions which include $\xi = 1$, in our case the interior of the spheroid.

The boundary condition of the continuity of the wave function and its derivative is applied at the potential boundary. Here the radial function of the first kind should be joined to a proper linear combination of radial functions of the first and second kind. The argument of the solution outside the spheroid will be pure imaginary. This results from the fact that the new k defined must be imaginary as V_0 becomes zero in equation (4). The radial functions of the second kind are considerably more difficult to obtain and to evaluate than are functions of the first kind. If the potential V_0 is considered quite large the amplitude of the wave function inside the spheroid is large compared to the exponentially decreasing function outside the spheroid. With the assumption of a large potential then, to a first approximation, the boundary condition may be altered to a requirement that the wave function vanish at the potential boundary, i. e. at some value of ξ , hereafter designated ξ_0 . This approximation is particularly good for the lower lying energy levels. The justification for such an approximation decreases markedly for increasing ℓ and n.

In a few cases $\xi = 1$ lies outside the potential boundary. However the fact that the radial solution of the second kind oscillates only in regions outside $\xi = 1$, combined with our boundary conditions eliminates the function of the second kind for this case as well.

The radial function of the first kind is

$$R^{(1)}_{m,l}(c\xi) = \frac{(\xi^2+1)^{m/2}}{\xi^m \sum\limits_{n=0,1}^{\infty}{}' f_n^{l-m} \frac{(n+2m)!}{n!}} \sum_{n=0,1}^{\infty}{}' i^{l-n} f_n^{l-m} \frac{(n+2m)!}{n!} j_{n+m}(c\xi), \tag{10}$$

where

$$j_{n+m}(c\xi) = \sqrt{\frac{\pi}{2c\xi}}\; J_{n+m+\frac{1}{2}}(c\xi) \tag{11}$$

is a spherical Bessel function. In the notation of Stratton et al, ℓ is used to designate $l - m$ as used here where l and m follow the ordinary notation of quantum mechanics. The prime denotes summation over even values of the summation index n when $l - m$ is even; over odd n when $l - m$ is odd. The solution is normalized such that it reduces to the spherical case when c goes to zero or ξ becomes infinite.

With the assumption that the volume of the spheroid remains constant throughout the distortion we obtain an expression for the semi-focal distance a in terms of the radius a_0 of the undistorted sphere. The volume of the spherical nucleus is given by

$$v_0 = \frac{4}{3}\pi a_0^3, \tag{12}$$

and that of the spheroidal nucleus by

$$v_s = \frac{4}{3}\pi \alpha \beta \gamma, \tag{13}$$

where $\alpha = \beta$ represents the semi-major axis and γ the semi-minor axis of the spheroid. From the coordinate transformation, equations

(6), they are expressed in terms of a and ξ as

$$\alpha = \beta = a(\xi_0^2 + 1), \tag{14}$$

and

$$\gamma = a\xi_0 . \tag{15}$$

Equating the volumes it is evident that

$$a = \frac{a_0}{[\xi_0(\xi_0^2+1)]^{1/3}} . \tag{16}$$

Remembering that $c = ka$, we obtain for the eigenvalue

$$k^2 = \frac{c^2}{a_0^2}[\xi_0(\xi_0^2 + 1)]^{2/3} . \tag{17}$$

Under our assumptions the radial function must go to zero at the spheroidal boundary. Picking a c value we return to the radial function (10) and determine the value of the argument $c\xi$, and hence ξ_0, for which the series in spherical Bessel functions[10] goes to zero. The "total" quantum number n indicates the number of spheroidal nodes; $n = 1$ corresponding to the first zero, $n = 2$ to the second, etc. It should be noted that unlike the atomic case ℓ is not restricted to values less than n.

The eccentricity for a particular value of k is found from the defining equation,

$$\epsilon = \frac{(\alpha^2 - \gamma^2)^{1/2}}{\alpha} = \frac{1}{(\xi_0^2+1)^{1/2}} \tag{18}$$

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[10] Tables of Spherical Bessel Functions, Columbia University Press (1947).

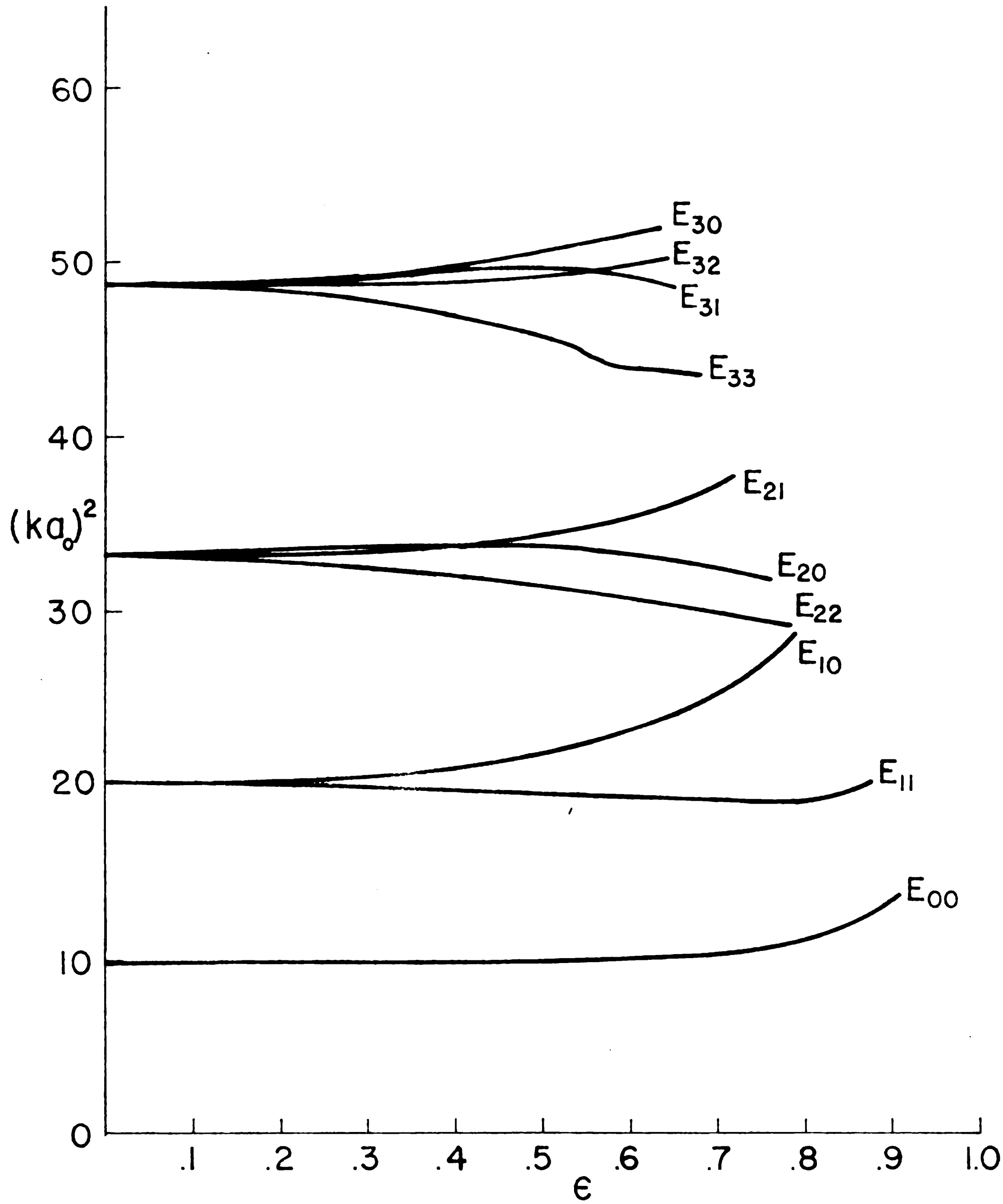
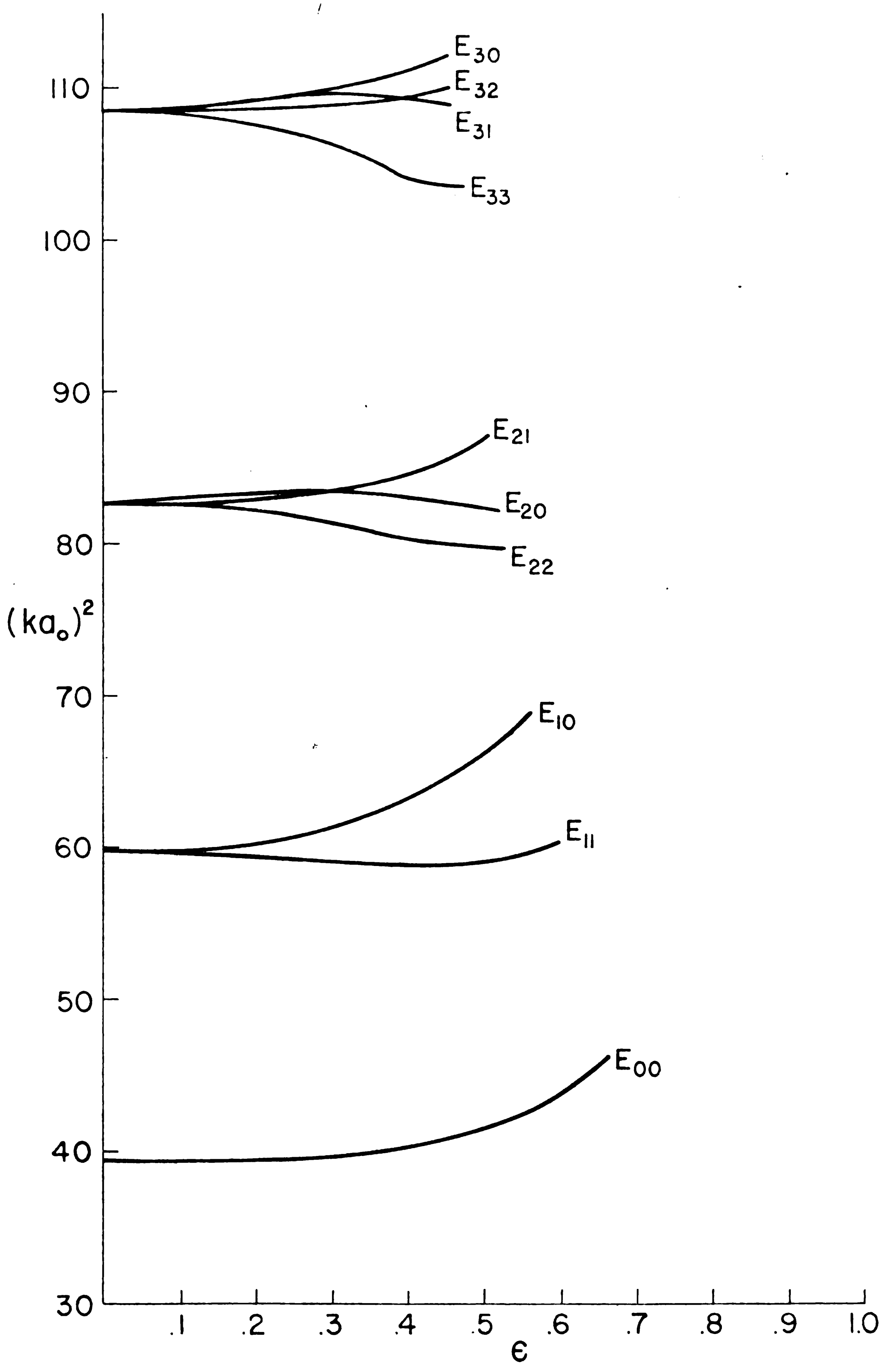


Figure 2. Variation in the energy levels [illegible]
versus the eccentricity for n = 1. [illegible]



E30
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III. EVALUATION OF THE DATA

Stratton et al tabulate the coefficients $f_m^{\ell-m}$ for ℓ values through three and for values of c through five. This necessarily restricted our computations to s, p, d, and f levels. We were able to obtain values for the first two closed shells on the Mayer scheme. The third shell contains a $1g_{9/2}$ term closing it which is just beyond our computational reach. The limit on c provided no problem as the values given permitted eccentricities sufficiently larger than those which seem physically probable. This would remain true for a fairly large range of n, although for a specified c value the eccentricity is reduced by increasing n.

In the computations c values were taken from zero to five, predominately at intervals of five-tenths. Where graphing indicated necessary this interval was shortened. Energy levels were computed for n equal to one and two. The limit on the ℓ values obtainable made higher values of n useless. The real limit on the n values which can be used lies in the tables of spherical Bessel functions available at the present time. Most of the points were found by successive approximations, although a graphical method was occasionally employed. The results are good to three significant figures. Consequently the data is given in graphical form, with the variation in the energy levels plotted against the eccentricity. As we are concerned only with the variation in the levels, the energy is expressed in terms of the dimensionless $(ka_0)^2$.

As may be seen from the graphs there is some crossing of the energy levels for a given ℓ. More important is the indication that for a slightly larger eccentricity we may expect a crossing of the E_{10} and E_{21} levels. Crossing of the levels is found experimentally, particularly for larger values of n. Our graphs indicate that for increasing n the rate of variation versus eccentricity increases quite sharply. Also the greatest variation seems to occur for s and p levels. Perhaps the crossing of levels which does occur could be at least partially explained on this basis.

The results obtained indicate that the previously mentioned perturbation method of Feenberg and Hammack which gives the variation in the energy levels is a fairly good approximation for eccentricities less than one-tenth and n equal to one, but for increasing n is reliable for a decreasing range of eccentricities.

IV. NOTE ON THE QUADRAPOLE MOMENT

As noted in the introduction, a spherical nucleus cannot adequately account for the relatively large quadrapole moments which are observed. Qualitatively it appears evident that the oblate spheroidal potential well results in an approximately prolate spheroidal distribution of the wave function. This result is indicated by the fact that in most instances maxima in the angular function occur at $\eta = 1$. This gives a larger positive quadrapole moment which is desired.

The ordinary expression for the quadrapole moment is

$$Q = \int_V \psi \bar{\psi}\,(3z^2 - r^2)\,d\tau_m\,, \tag{19}$$

where r is the radial distance from the center of the charge distribution and $d\tau_m$ is the element of nuclear volume.

Expressed in the oblate spheroidal system this becomes

$$Q = a^5 \int_{\xi=0}^{\xi_0} \int_{\eta=-1}^{1} \int_{\phi=0}^{2\pi} \psi \bar{\psi} \left[2\xi^2\eta^2 - (1-\eta^2)(1+\xi^2)\right](\eta^2+\xi^2)\,d\phi\,d\eta\,d\xi, \tag{20}$$

where

$$\psi = \frac{e^{im\phi}}{\sqrt{2\pi}} \sum_{n=0,1}^{\infty}{}' f_n^{l-m} P_{m+n}^m(\eta) \frac{(\xi^2+1)^{m/2}}{\xi^m \sum_{n=0,1}^{\infty}{}' f_n^{l-m} \frac{(n+2m)!}{n!}} \sum_{n=0,1}^{\infty}{}' i^{l-m} f_n^{l-m} \frac{(n+2m)!}{n!}\, j_{m+n}(c\xi)\,, \tag{21}$$

and

$$\bar{\psi} = \frac{e^{-im\phi}}{\sqrt{2\pi}} \sum_{n=0,1}^{\infty}{}' f_n^{l-m} P_{m+n}^m(\eta) \frac{(\xi^2+1)^{m/2}}{\xi^m \sum_{n=0,1}^{\infty}{}' f_n^{l-m} \frac{(n+2m)!}{n!}} \sum_{n=0,1}^{\infty}{}' (-i)^{l-m} f_n^{l-m} \frac{(n+2m)!}{n!}\, j_{m+n}(c\xi)\,. \tag{22}$$

The problem of computing the quadrapole moment is rather complicated due to the term $(\eta^2 + \xi^2)$ appearing in the integrand from the expression for the volume element in this system.

BIBLIOGRAPHY

1. Feenberg, E., and Hammack, K. C., Nuclear Shell Structure. Physical Review 75; 1877 (1949).

2. Mayer, M. G., Nuclear Configurations in the Spin-Orbit Coupling Model. I. Empirical Evidence. Physical Review 78; 16 (1950).

3. Feenberg, E., Hammack, K. C., and Nordheim, L. W., Note on Proposed Schemes for Nuclear Shell Models. Physical Review 75; 1968 (1949).

4. Mayer, M. G., Nuclear Configurations in the Spin-Orbit Coupling Model. II. Theoretical Considerations. Physical Review 78; 22 (1950).

5. Rainwater, J., Nuclear Energy Level Argument for a Spheroidal Nuclear Model. Physical Review 79; 432 (1950).

6. Feenberg, E., and Hammack, K. C., Note on Rainwater's Spheroidal Nuclear Model. Physical Review 81; 285 (1951).