Energy Eigenvalues for a Spherical Well with an Exponentially Diffuse Boundary*

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The discrete energy eigenvalues of a spherical well with an exponentially diffuse boundary are obtained to a good approximation for a range of well parameters of interest in nuclear physics. The method used involves replacing the centrifugal energy in the exponentially diffuse region by an approximate expression which leads to analytic solutions of the wave equation. The matching of the internal and external wave functions is then accomplished by the use of specially prepared graphs and tables. The eigenvalues and eigenfunctions are thought to be of interest in connection with studies of the independent particle model of the nucleus.

1. INTRODUCTION

A NUMBER of recent studies[1–3] have stimulated interest in the problem of a single particle in a central field with a diffuse boundary. While most of this interest has been in connection with the positive energy states of the continuum, nevertheless the bound states are also of considerable importance. In this paper, an approximate method is developed which appears to be adequate for the range of well parameters encountered in nuclear physics.

The solution of the square spherical well eigenvalue problem is an essential preliminary phase of the approximate method of solution of the diffuse boundary problem. Accordingly, this older problem, which has been solved earlier in the literature,[4] will be considered briefly first.

2. EIGENVALUES FOR THE SQUARE SPHERICAL WELL

The radial wave equation for the lth state of orbital angular momentum for a central field characterized by the potential $V(r)$ may be placed in the form

$$d^2G/dr^2+(2m/\hbar^2)[W-V(r)-\hbar^2l(l+1)/2mr^2]G=0, \quad (1)$$

where $G=rR$ and R is the radial wave function. For the study of the spherical well of depth V_0 and radius a, it is convenient to let a serve as a unit of length, $E_0=\hbar^2/2ma^2$ serve as a unit of energy and to define the dimensionless parameters:

$$\epsilon_w^2=-W/E_0, \quad (2)$$

$$\epsilon_0^2=V_0/E_0, \quad (3)$$

and

$$\epsilon'^2=\epsilon_0^2-\epsilon_w^2. \quad (4)$$

Letting $\rho=r/a$, the radial wave equation becomes

$$G''+[\epsilon'^2-l(l+1)\rho^{-2}]G=0, \quad \rho<1 \quad (5)$$

and

$$G''-[\epsilon_w^2+l(l+1)\rho^{-2}]G=0, \quad \rho>1, \quad (6)$$

where prime denotes differentiation relative to ρ. The internal solution which is well-behaved at $\rho=0$ is

$$G_i=A_i\rho^{\frac{1}{2}}J_{l+\frac{1}{2}}(\epsilon'\rho), \quad (7)$$

where J denotes the usual Bessel function and A_i denotes a normalization constant. The external solution which is well-behaved as $\rho\to\infty$ may be expressed in terms of modified Hankel functions. Denoting these functions by $K_{l+\frac{1}{2}}$ the external solution may be written as

$$G_e=A_e\rho^{\frac{1}{2}}K_{l+\frac{1}{2}}(\epsilon_w\rho). \quad (8)$$

The ϵ_w eigenvalues are obtained without consideration of the normalization constants by imposing the requirement that at the boundary,

$$\rho=1, \quad -G_i'/G_i=-G_e'/G_e \quad \text{or} \quad I_l(\epsilon')=E_l(\epsilon_w), \quad (9)$$

where $I_l(\epsilon')$ and $E_l(\epsilon_w)$ are defined as the negatives of the logarithmic derivatives of the internal and external radial wave functions.

To facilitate the solution of this transcendental equation subject to the condition imposed by Eq. (4), tables and graphs of I_l and E_l have been prepared. In this effort, use was made of the recurrence relations:

$$I_l(x)=l-(x^2/I_{l-1}+l), \quad (10)$$

$$E_l(x)=l+(x^2/E_{l-1}+l), \quad (11)$$

which follow from the usual recurrence relations between Bessel functions. Using Eq. (11) and

$$E_0(x)=x, \quad (12)$$

the higher integral order $E_l(x)$ were generated. To obtain higher order $I_l(x)$ including nonintegral orders which are needed in Sec. 3, tabulated Bessel functions for orders between $-\frac{1}{2}$ and $+\frac{1}{2}$ were first used to generate the corresponding I_l functions. Then Eq. (10) was used to generate the higher order functions. In Fig. 1 and Fig. 2 the values of various $I_l(x)$ and $E_l(x)$ are plotted at abscissas corresponding to x^2. These graphs

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[2] D. M. Chase and F. Rohrlich, Phys. Rev. **94**, 81 (1954).

[3] Feshbach, Porter, and Weisskopf, Phys. Rev. **96**, 448 (1954).

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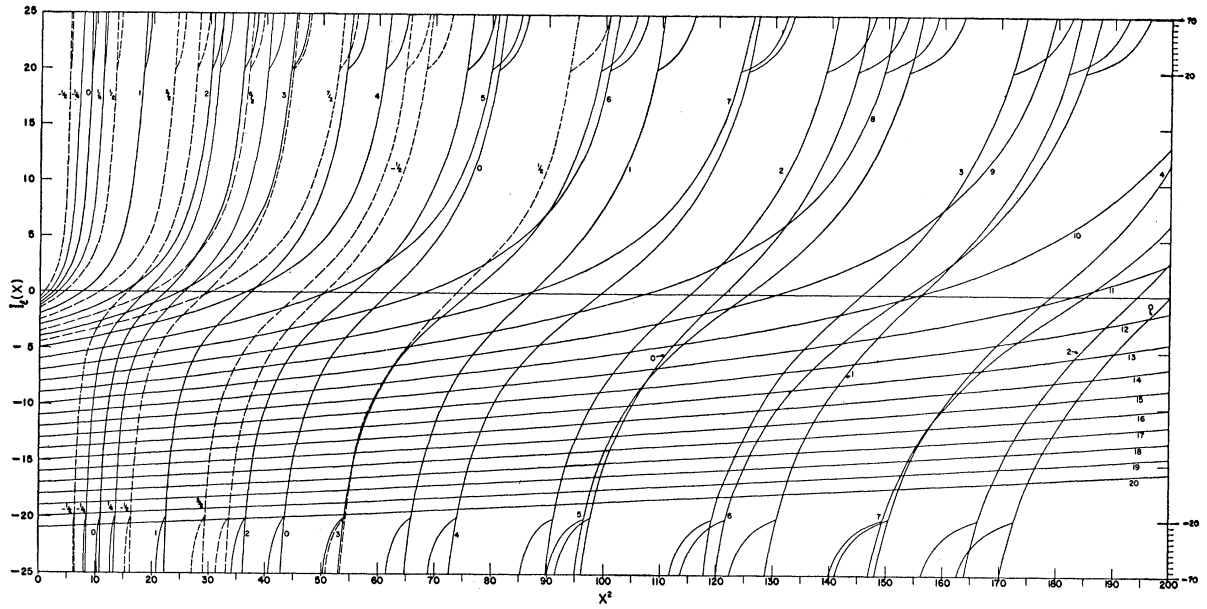

FIG. 1. The function $I_l(x)$ plotted against x^2. Labels within the graph denote l. The second set of curves which start at $I=\pm 20$ correspond to the right scales.

greatly facilitate the task of obtaining functional relations between ϵ_w^2 and ϵ_0^2 for various l's which simultaneously satisfy Eq. (4) and Eq. (9).

Figure 3 contains the results of the work with the square well potential. The form of presentation of the eigenvalues follows that of Moszkowski[5] who has prepared a similar graph for a somewhat narrower range of the well range parameter. Essentially, Fig. 3 represents the energy eigenvalue in units of E_0 measured relative to the bottom of the well. For a given state this parameter has a far smaller range of variation as ϵ_0^2 is changed than ϵ_w^2 which corresponds to the actual energy. Furthermore, these ϵ'^2 values go over to the results of the infinite spherical well as ϵ_0^2 goes to infinity. The ϵ'^2 eigenvalues for the infinite spherical well case are obtained simply by imposing the requirement that $J_{l+\frac{1}{2}}(\epsilon')=0$. These ϵ'^2 eigenvalues for the infinite case results are shown on the right side of Fig. 3. Some noteworthy points which are apparent in Fig. 3 are the $3s-1h$ and $1j-2g$ cross-overs as well as the fact that the approximate equality in spacing of the low-lying levels breaks down above the $1g$ state.

3. SPHERICAL WELL WITH AN EXPONENTIALLY DIFFUSE BOUNDARY

In this section, a continuous central potential is assumed which changes at $r=a$ from a constant $-V_0$ to

$$V(r)=-V_0\exp[(a-r)/\delta a]. \quad (13)$$

The dimensionless parameter δ characterizes the "shortness" of the exponential "tail". The case $\delta=0$ is simply the case discussed in the previous section. The form of the interior radial wave equation and its solutions are, of course, unaltered from those developed in the previous section; however, the dimensionless radial equation for $\rho>1$ in this case is

$$G''+[\epsilon_0^2\exp(1-\rho/\delta)-l(l+1)\rho^{-2}-\epsilon_w^2]G=0. \quad (14)$$

Because of the presence of both the exponential and ρ^{-2} terms, Eq. (14) cannot be reduced to any of the well-studied differential equations. It is, however, known that for s states, i.e., when the ρ^{-2} term vanishes, Eq. (14) can be transformed into Bessel's equation.[6] One approximate procedure which has been used[7] to overcome the difficulty for other than s states is equivalent to replacing ρ^{-2} by 1. The centrifugal energy can then be taken together with ϵ_w^2 and solutions can be obtained in terms of Bessel functions. This approximation, however, is fairly crude and the chief concern here shall be to improve upon it. The improvement considered here is based upon the assumption that

$$\rho^{-2}\approx\alpha^2+(1-\alpha^2)\exp[(1-\rho)/\delta], \quad (15)$$

where the constant α^2 is chosen to accomplish the best match of the function on the right to the function on the left over the external region of importance. Thus, the "centrifugal" energy in the external region is absorbed into the exponential tail and the total energy. The external radial wave equation now becomes

$$4\delta^2G''+\{k^2\exp[(1-\rho)/\delta]-n^2\}G=0, \quad (16)$$

[5] S. A. Moszkowski, Phys. Rev. **89**, 482 (1953).

[6] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Part II, Chap. 12.

[7] B. J. Malenka, Phys. Rev. **86**, 68 (1952).

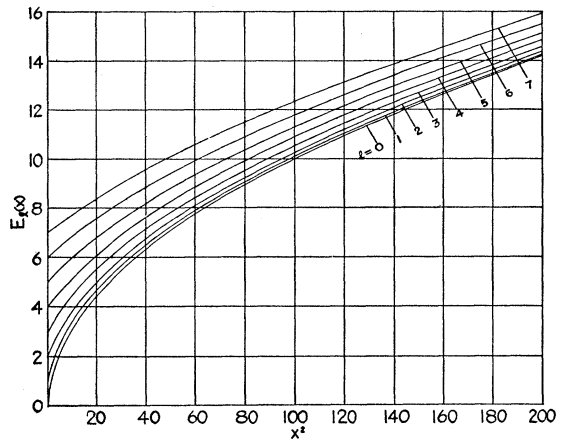

FIG. 2. The function $E_l(x)$ plotted against x^2. Labels within the graph denote l.

where

$$k^2=4\delta^2[\epsilon_0^2-l(l+1)(1-\alpha^2)], \tag{17}$$

$$n^2=4\delta^2[\epsilon_w^2+l(l+1)\alpha^2]. \tag{18}$$

Letting

$$x=\exp((1-\rho)/2\delta), \tag{19}$$

the radial equation becomes

$$x^2G''+xG'+(k^2x^2-n^2)G=0, \tag{20}$$

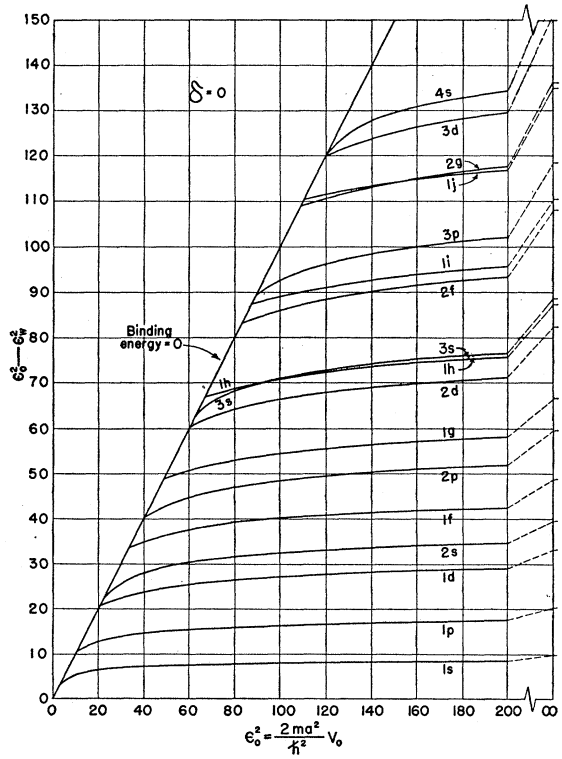

FIG. 3. Energy eigenvalues for the square spherical well (i.e., $\delta=0$). The right scale gives the infinite spherical well eigenvalues.

where the prime here denotes differentiation relative to x. The solution of this equation which is well behaved as $\rho\to\infty$, i.e., as $x\to 0$ is

$$G_e=A_eJ_n(kx)=A_eJ_n\{k\exp[(1-\rho)/2\delta]\}. \tag{21}$$

The negative of the logarithmic derivative of the exterior function at $\rho=1$ is thus

$$-G_e'/G_e=kJ_n'(k)/2\delta J_n(k)$$
$$=\tfrac{1}{2}[n-kJ_{n+1}(k)/J_n(k)]. \tag{22}$$

Introducing $\nu=n-\frac{1}{2}$, the negative of the external logarithmic derivative takes the form

$$E_\nu(k,\delta)=-I_\nu(k)/2\delta-1/4\delta, \tag{23}$$

where $I_\nu(k)$ is precisely the function introduced in Eq. (9). The eigenvalue equation for the present case thus becomes

$$I_l(\epsilon')=-[I_\nu(k)/2\delta]-(1/4\delta). \tag{24}$$

The parameters involved in this equation are subject to the requirements imposed by Eq. (4), Eq. (17), and Eq. (18). These may be combined into

$$\epsilon'^2=[k^2-(\nu+\tfrac{1}{2})^2]/4\delta^2+l(l+1). \tag{25}$$

For a given δ, l, and k^2, Eq. (24) and Eq. (25) may be regarded as two simultaneous equations for the determination of ϵ' and ν. Actually, for the application to which these solutions have been applied, δ and l are first chosen in accord with the states under study and ν is taken in accord with the orders of tabulated or graphed I functions. Then, Eq. (24) and Eq. (25) are solved simultaneously for ϵ'^2 and k^2. Since ν^2 fixes ϵ_w^2, and ϵ'^2 in conjunction with ϵ_w^2 determines ϵ_0^2, it is possible to generate the curves relating ϵ'^2 to ϵ_0^2 throughout the range of interest.

For the purposes of solving Eq. (24) and Eq. (25) for ϵ'^2 and k^2, the graph of the values of I functions may be utilized in the following way. According to Eq. (25), ϵ'^2 is a linear function of k^2 with the slope $(1/4\delta^2)$. If a compressed scale is prepared such that one unit on the ϵ'^2 scale corresponds to $(1/4\delta^2)$ units of ϵ'^2 on the compressed scale, then for chosen values of ν and l the compressed scale may be positioned so that any ϵ'^2 on the compressed scale corresponds directly to k^2 on the basic scale. This may be accomplished simply by aligning the value of $(\nu+\frac{1}{2})^2$ on the regular scale next to $l(l+1)$ on the compressed scale. Next, a compressed vertical scale is prepared with an offset index so that as the index point is slid along the center axis of the horizontal scale the readings of the curve correspond directly to $E_\nu(k,\delta)$ given by Eq. (23). Now to solve simultaneously for the values of ϵ'^2 and k^2 the special vertical scale is moved in relation to ϵ'^2 values listed on the horizontal scale and readings of the νth curve are taken. At the same time, values of $I_l(\epsilon')$ are read at the corresponding ϵ'^2 of the basic scale. Proceeding in this way, one finds readily the ϵ'^2 eigenvalues. Having

generated all the ϵ'^2 (and k^2) values for a given ν and l, one advances to the next ν for the same l and repeats the procedure. In this way, a series of relationships between ϵ'^2 *vs* ν^2 for each l is developed.

It is noteworthy that the values of ϵ'^2 so obtained do not depend upon the constant α^2. However, to translate from ϵ'^2 and k^2 into ϵ_0^2 and ϵ_w^2, a value of α^2 must be established.

4. ADJUSTMENT OF α^2

The form chosen for Eq. (15) insures the agreement of the right and left sides at $\rho=1$. Clearly, therefore, α^2 may be related to a second point at which agreement between these functions is imposed. Denoting this point by ρ_1, Eq. (15) may be placed in the form

$$\alpha^2=[\rho_1^{-2}-\exp(1-\rho_1/\delta)]/[1-\exp(1-\rho_1/\delta)]. \quad (26)$$

Thus, the adjustment problem has been reduced essentially to the problem of arriving at a prescription for the second cross over point between the functions characterized in Eq. (15).

The procedure used in this study takes advantage of the fact that the case $\delta=0$ can be solved exactly, as well as by the approximation method. Therefore, this case was studied carefully in an effort to find how best to accomplish the adjustment of α^2 for the small values of δ which may be of interest in nuclear physics.

Equation (17) and Eq. (18) indicate that as $\delta\rightarrow 0$ both the order, n, and the argument, k, of the external radial function vanish. Since $J_1(0)=0$ and $J_0(0)=1$, it follows immediately from Eq. (22) that

$$-G_e'/G_e=[\epsilon_w^2+l(l+1)\alpha^2]^{\frac{1}{2}}. \quad (27)$$

To obtain a reasonable value for α^2, the right side of this equation was equated to the function $E_l(\epsilon_w)$ derived in Sec. 2. When solved for α^2, Eq. (27) then becomes

$$\alpha^2=[E_l^2(\epsilon_w)-\epsilon_w^2]/l(l+1). \quad (28)$$

Substituting into this for a range of values for ϵ_w^2 and l it became clear that the values of α^2 so obtained varied only slightly (in the range from 0.8 to 0.9). The final constant,

$$\alpha^2=0.82645 \quad \text{for} \quad \delta=0, \quad (29)$$

was chosen as an appropriate one. This corresponds to a second cross-over point at

$$\rho=1.1=1+0.1 \quad \text{for} \quad \delta=0. \quad (30)$$

This choice was made not only because of its convenience but also because it works particularly well for small values of ϵ_w^2, the region for which Eq. (27) is most sensitive to α^2. This region of ϵ_w^2 values is particularly of interest in applications of these results to the study of particle binding energies and nuclear transitions. Accordingly, it would seem best to favor this region in an adjustment.

TABLE I. The values of $\alpha^2(\delta)$.

δ	0	0.1	0.2	0.3	0.4	0.5
α^2	0.8264	0.6466	0.4744	0.3349	0.2214	0.1280

For nonzero values of δ, the rule

$$\rho_1=1+\delta+0.1 \quad (31)$$

was chosen as the simplest result which goes over to Eq. (30) for $\delta=0$. This simple rule is admittedly somewhat arbitrary; however, since only a small correction is involved here, it is difficult to see how Eq. (31) can lead to appreciable errors. Most certainly this procedure represents an improvement over the usual approximation of replacing ρ^{-2} by 1 which is equivalent to making the second point of agreement at infinity. Inserting Eq. (31) into Eq. (26) leads immediately to the function $\alpha^2(\delta)$. Values of this function are given in Table I.

5. RESULTS AND DISCUSSION

The ϵ'^2 *vs* ν and l, and k^2 *vs* ν and l relationships arrived at by the procedure described in Sec. 3 may now be translated into ϵ'^2 *vs* ϵ_0^2 relationships for comparison with Fig. 3. These are shown in Figs. 4, 5, 6, and 7 for $\delta=0.1$, 0.2, 0.3 and 0.4, respectively. For case $\delta=0$, the eigenvalues arrived at by the approximate method rarely deviate by more than a line width from

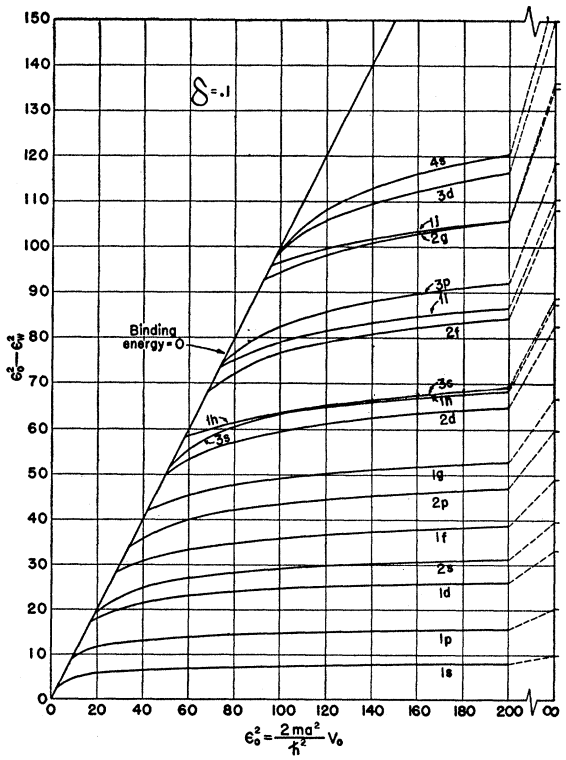

FIG. 4. Eigenvalues for $\delta=0.1$.

the curves shown in Fig. 3 It must be remembered that the results for $\delta \neq 0$ are exact for s states but are approximate for $p, d, \ldots f$. By first-order perturbation theory the error of the energy eigenvalue in natural units may be estimated to be

$$\Delta\epsilon_w^2 = l(l+1)\frac{\int_1^\infty G_e^2[\rho^{-2}-\alpha^2-(1-\alpha^2)\exp(1-\rho/\delta)]d\rho}{\int_0^1 G_i^2 d\rho + \int_1^\infty G_e^2 d\rho}. \tag{32}$$

By virtue of the vanishing of the perturbation at $\rho=1$ and $\rho=1+\delta+0.1$, the factor in the bracket is less than 0.05 in the intermediate region, which is the region within which the external wave function is significantly large. Accordingly the error is expected to be less than $0.05l(l+1)f$, where f is the probability for the particle being found beyond $\rho=1$. Since f is expected to be considerably less than 1, the error in ϵ_w^2 due to the method of approximation is expected to be considerably less than unity. Quantitative estimates using numerical integration substantiate this statement. At the present stage of our knowledge of the nucleus the approximate eigenvalues given in Figs. 3–7 should be sufficiently accurate so that their further refinement at this time is unnecessary. If these approximate eigenvalues and the corresponding analytical eigenfunctions prove helpful in resolving nuclear problems, further efforts toward refining them would certainly be warranted. In many instances refinements may be accomplished by the direct use of available tables of Bessel functions.[8,9] As an illustration of such a calculation it can be shown that the critical ϵ_0 values at which various s states of binding set in, satisfy

$$j_1(\epsilon_0)/j_0(\epsilon_0) = \epsilon_0^{-1} - J_1(2\delta\epsilon_0)/J_0(2\delta\epsilon_0), \tag{33}$$

where j_1 and j_0 are spherical Bessel functions and J_1 and J_0 are ordinary Bessel functions. Using the graphical results to locate the approximate ϵ_0 values, it is relatively simple to refine them to four or even five significant figures by interpolation. The results of this particular calculation are given in Table II. These ϵ_0 values are listed because of their possible usefulness in connection with the interpretation of the low velocity maxima in the Barschall neutron cross section surface.[10] On the "diffuse-cloudy crystal ball" model of neutron scattering the observed low velocity maxima at $A=11$, 55 and 150 would be expected to correspond to the $2s$, $3s$, and $4s$ critical ϵ_0 values for the appropriate diffuseness parameters, hence the "well strengths" in

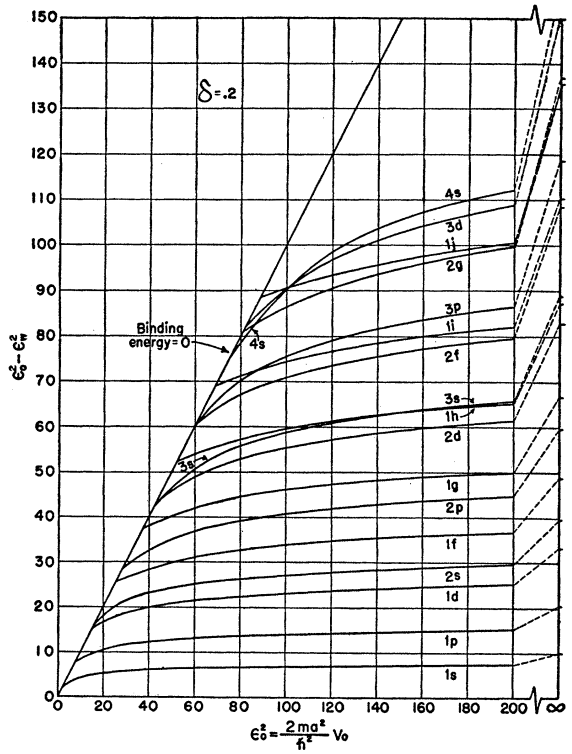

FIG. 5. Eigenvalues for $\delta=0.2$.

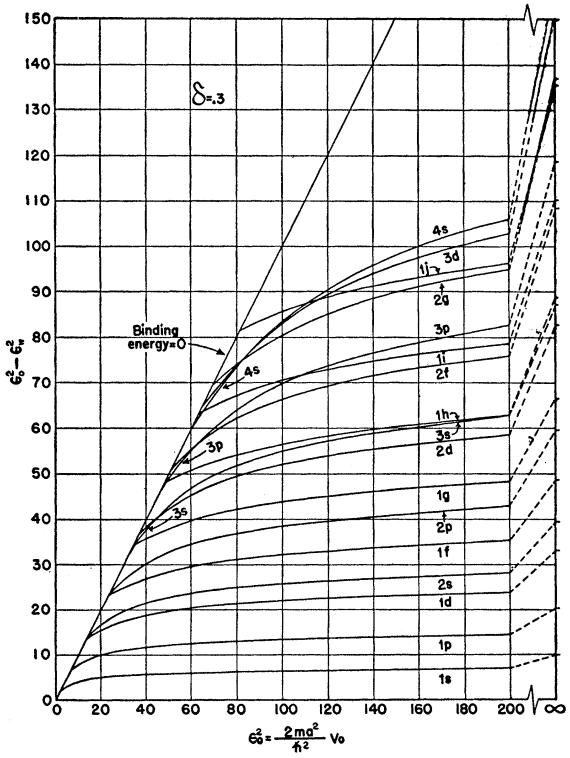

FIG. 6. Eigenvalues for $\delta=0.3$.

[8] *Tables of Spherical Bessel Functions* (Columbia University Press, New York, 1947), Vols. 1 and 2.

[9] E. Cambi, *Bessel Functions* (Dover Publications, Inc., New York, 1948).

[10] H. H. Barschall, Phys. Rev. **86**, 431 (1952).

TABLE II. The critical ϵ_0 values for the s states.

δ	$\epsilon_0(1s)$	$\epsilon_0(2s)$	$\epsilon_0(3s)$	$\epsilon_0(4s)$
0	1.571	4.712	7.854	10.996
0.1	1.428	4.272	7.084	9.825
0.2	1.307	3.855	6.204	8.370
0.3	1.202	3.454	5.371	7.324
0.4	1.111	3.081	4.747	6.554
0.5	1.031	2.761	4.280	5.896

any one column are effectively equivalent from the standpoint of these observations.

In a number of other instances, it is possible to arrange the calculations to take advantage of existing tables of Bessel functions for the refinement of the approximate eigenvalues presented in Figs. 3–7. However, with the advent of high-speed digital computers, the best way of refining the eigenvalues would probably be to solve the exact radial wave equation directly by numerical methods. Here again, the eigenvalues shown in Figs. 3–7 should be helpful by providing starting points which will greatly speed up the calculations.[11] Indeed one might expect that this family of eigenvalues and their analytical eigenfunctions might provide good initial approximations for the investigation of any other potential functions similar in general shape to the exponentially diffuse spherical well cases treated here.

In conclusion, it is important to note that the infinite spherical well eigenvalues provide a poor representation of the finite spherical well eigenvalues in the range of ϵ_0^2 values of interest in nuclear physics (certainly less than 200). When the boundary is made diffuse to a moderate degree the infinite spherical well eigenvalues are hopelessly inaccurate. Thus the numerous theoretical results in the nuclear literature which are based upon the infinite spherical or cubic well approximations must clearly be treated with great care. Even the finite square spherical well eigenvalues differ considerably from the diffuse boundary eigenvalues, particularly in the region of small energies, which is the region of greatest interest in nuclear physics.[12] Accordingly, one might

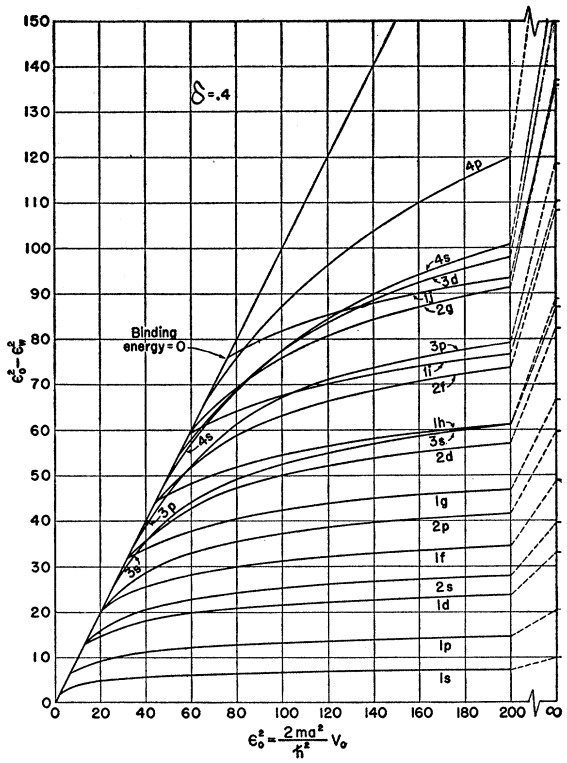

FIG. 7. Eigenvalues for $\delta=0.4$.

hope that some of the well-known difficulties of the independent-particle model based upon square well eigenvalues and eigenfunctions might be removed by the use of the diffuse boundary eigenvalues and eigenfunctions.

ACKNOWLEDGMENTS

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[11] The writer is indebted to Dr. Ward C. Sangren of the Oak Ridge National Laboratory Mathematics Panel for an illuminating discussion relative to this point.

[12] In examining the influence of an increase in the diffuseness parameter δ one must, of course, reduce the radius parameter a (hence increase the natural energy unit E_0) and the well strength parameter ϵ_0 in order to preserve an effective radius and an effective well strength defined by a particular set of experimental observations. Similar considerations are applied in the so-called shape-independent treatment of two-nucleon systems in which the critical $1s$ well strengths of various types of potentials are placed in correspondence. In the study of complex nuclei, the best prescriptions for $a(\delta)$ and $\epsilon_0(\delta)$ will depend upon the intended application.