PHYSICAL REVIEW VOLUME 139, NUMBER 5B 6 SEPTEMBER 1965

Counting the Bound States in Short-Range Central Potentials*

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(Received 23 April 1965)

For the case of a short-range central potential, the quantity α_l, defined as the zero-energy limit of $k^{2l+1}\cot\delta_l$, vanishes whenever the range and depth of the potential are such that there is a state of zero binding energy. By solving the zero-energy scattering problem we obtain α_l as a function of range and depth and thus determine the number of bound states supportable by a given central potential as a function of the potential parameters without having to solve the associated and more difficult eigenvalue problem. The method is applied to the Debye-Hückel (Yukawa) and Woods-Saxon potentials.

Several attempts have been made and reported in the literature[1–3] to determine the number of bound states in the Debye-Hückel (Yukawa) potential as a function of range and depth. These attempts usually involve considerable numerical work even though they yield solutions which are only approximate, and one may justifiably inquire why no effort is made to find an exact, though numerical, solution. We believe the answer lies, at least in part, in the cumbersome and time-consuming procedure required by the straightforward approach to this problem. This involves replacing the radial-wave equation by an appropriate difference equation, guessing an eigenvalue and integrating the equation step by step from the origin to large values of the radial variable r, and then determining whether the resulting solution exhibits the proper asymptotic behavior. If it does not, the trial eigenvalue is changed and the process repeated until it does. This must be done for every negative energy state in the spectrum and for many sets of potential parameters in the desired range. In addition to being a lengthy process, this technique never provides complete assurance that all bound states have been found; one or more levels, especially loosely bound ones at the top of the spectrum, can easily be overlooked.

If one desires to know only the number of states bound for each set of potential parameters rather than the eigenvalues themselves, there is another method for doing this which is both simple in concept and easy to carry out. To begin with, an appropriate scaling of the wave equation makes it possible to characterize some potentials by a single parameter. To make this discussion specific let us deal with the Debye-Hückel potential as an example. Thus we write

$$V(r)=-ge^2r^{-1}\exp(-r/\lambda)\,,$$

where e is the electronic charge, λ a range parameter, and g a dimensionless coupling constant. The reduced radial-wave equation is thus

$$d^2u_l/dr^2+[2mE/\hbar^2+(2g/a_0)e^{-r/\lambda}/r-l(l+1)/r^2]u_l=0\,,$$

where u_l is the reduced radial-wave function, m and E are the mass and energy of the particle bound in the potential, and $a_0=\hbar^2/me^2$. Introducing the variable $x=r/\lambda$ and defining $k^2=-2m\lambda^2E/\hbar^2$ and $\omega=2g\lambda/a_0$, we find

$$d^2u_l/dx^2-[k^2-\omega e^{-x}/x+l(l+1)/x^2]u_l=0. \qquad (1)$$

With the equation in this form the Debye-Hückel potential is characterized by the single parameter ω. Clearly there are many potentials which, by some scaling procedure, can be characterized in terms of a single parameter. For the present we assume that the potentials with which we deal are of this kind; later we shall generalize our methods to include potentials which must be characterized by more than one parameter.

By assumption, the potentials we work with are short range and so, at large values of the radial variable x, the reduced radial-wave function at zero energy is

$$u_l(x)=(1/x^l)+b_l(\omega)x^{l+1}\,, \qquad (2)$$

with arbitrary choice of normalization. The quantity b_l, as indicated, depends upon the potential parameter ω. Let us now suppose that for $\omega=\omega_c$ there is a zero-energy bound state of angular momentum l. For this value of ω, the function u_l must then be normalizable and the second term in Eq. (2) cannot be present. We conclude that

$$b_l(\omega_c)=0\,, \qquad (3)$$

if there is a zero-energy bound state of angular momentum l for $\omega=\omega_c$. Since all the bound-state levels enter the spectrum at zero energy for some value of ω and, to quote Schwinger,[4] ". . . a decrease of the potential in some region must lower the energies of the bound states and therefore cannot lessen their number," the procedure for counting the number of bound states is thus the following: We solve the reduced radial-wave equation at zero energy at a series of values of ω. The function $b_l(\omega)$ is determined by joining the solution smoothly at each ω to the asymptotic form given in Eq. (2). The number of bound states of angular mo-

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* Work done under the auspices of the U. S. Atomic Energy Commission.

[1] G. M. Harris, Phys. Rev. **125**, 1131 (1962).

[2] D. Kelley and H. Margenau, Progress Report, 1956 (unpublished), as reviewed by H. Margenau and M. Lewis, Rev. Mod. Phys. **31**, 569 (1959).

[3] G. Ecker and W. Weizel, Ann. Physik **17**, 126 (1956).

[4] J. Schwinger, Proc. Natl. Acad. Sci. U. S. **47**, 122 (1961).

mentum l at any $\omega=\omega_0$ is then the number of zeros of $b_l(\omega)$ for values of ω less than or equal to ω_0. We shall call $b_l(\omega)$ the counting function, which is inversely proportional to the lth partial-wave scattering length.

The above line of reasoning is not applicable to s states because binding in attractive short-range central potentials results from the centrifugal barrier which, of course, is absent when $l=0$. Thus, rather than a true bound state at zero energy, for s waves we have a "zero-energy resonance" which, when the well is deepened by an arbitrarily small amount, becomes a true bound state with a small negative eigenvalue. However, the criterion for a zero-energy resonance and, therefore, for counting s states is $b_0(\omega)=0$, the s-wave version of the general statement (Eq. 3). This can be made evident from the following alternative derivation of the criterion.

For energies different from zero the *scattering* (i.e., $k^2>0$) wave function outside the range of the potential is

$$u_l(x)=-k^{l+1}x[n_l(kx)-j_l(kx)\cot\delta_l],$$

where δ_l is the lth wave phase shift, j_l and n_l are the regular and irregular spherical Bessel functions, and the normalization has been chosen for convenience. We now take the limit of this expression as k approaches zero. To do this we use the forms of the two Bessel functions at small argument[5] as well as the generalized finite range expansion,[6]

$$k^{2l+1}\cot\delta_l=\alpha_l(\omega)+\beta_l(\omega)k^2+\cdots, \tag{4}$$

where the constants α_l, β_l, etc. depend upon the potential parameter ω. Thus in the zero-energy limit we find

$$u_l(x)=(2l-1)!!/x^l+\alpha_l(\omega)x^{l+1}/(2l+1)!!.$$

By comparing this form with the one given in Eq. (2) we see that

$$b_l(\omega)=[(2l+1)!!(2l-1)!!]^{-1}\alpha_l(\omega). \tag{5}$$

This way of looking at the problem relates the function $b_l(\omega)$ to the leading term of the finite-range expansion, $\alpha_l(\omega)$, and shows that our method of counting bound states actually involves solving the associated zero-energy scattering problem, and this is generally far easier than attempting an eigenvalue problem, especially if the latter must be carried out many times.

Now for the s-wave case. Levinson's theorem[7] tells us that if there is a zero-energy resonance then, provided the phase shift is normalized to zero at infinite energy,

$$\delta_0(0)=(n+1/2)\pi,$$

where n is an integer (the number of bound s states, as a matter of fact) and $\delta_0(0)$ is the s-wave phase shift at zero energy. Clearly, then, $\cot\delta_0(0)=0$ under these circumstances. But from the finite-range expansion, Eq. (4),

$$\lim_{k\to0}\cot\delta_0(k)=\lim_{k\to0}[\alpha_0(\omega)/k].$$

If these two results are to be compatible, it is clear that $\alpha_0(\omega)$ must be zero for any value of ω for which there is a zero-energy resonance. Our expression relating b_l and α_l [Eq. (5)] thus establishes that the counting procedure for s states is the same as in states of higher angular momentum.

It may have occurred to the reader that Levinson's theorem might be applied directly to count the number of bound states. This theorem asserts that the difference between the phase shift at zero and infinite energies is equal to $n\pi$ where n is the number of bound states. (For s states this statement must be modified in a way inessential to the following discussion.) Thus it appears that we need only solve the scattering problem at zero energy and at some large ("infinite") energy, take the difference of the two resulting phase shifts, and divide by π. Unfortunately, the solution of a scattering problem does not provide the phase shift itself but some function of it, such as the tangent, from which the phase shift can be determined only to within an additive integral multiple of π. But this multiple of π is clearly crucial in this context. For a direct application of Levinson's theorem it is necessary to solve the scattering problem over the entire range of energy for each value of ω so as to obtain the entire history of $\tan\delta_l$ (or whatever equivalent function is determined) and from it reconstruct the phase shift without any ambiguity. The method of counting bound states put forth in this paper is clearly preferable, since it requires only the solution to the zero-energy scattering problem at each value of the parameter ω which varies over a finite range.

To apply our counting procedure to the Debye-Hückel potential, we require solutions of

$$d^2u_l/dx^2+[\omega e^{-x}/x-l(l+1)/x^2]u_l=0$$

which is Eq. (1) now written for zero energy. This equation, which must be solved numerically, is replaced by an equivalent difference equation by standard means[8] and then integrated once and only once at each ω in the desired range from the origin to large values of x. At large x the function u_l is joined smoothly to the zero-energy asymptotic form given by Eq. (2) and $b_l(\omega)$ is thus determined.

The counting functions $b_l(\omega)$ for the Debye-Hückel potential are plotted in Fig. 1. Since only the positions of the zeros of these functions are relevant to us here, we have not calibrated the vertical scale. It will also be noticed that, except for s waves, no counting function is

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[5] See, for example, L. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), 1st ed., p. 78.

[6] See, for example, M. Goldberger and K. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964), p. 289.

[7] Reference 6, p. 284.

[8] See, for example, B. J. Scarborough, *Numerical Mathematical Analysis* (Johns Hopkins Press, Baltimore, Maryland, 1955), 3rd ed., pp. 265 ff.

TABLE I. Critical values of ω as a function of principal quantum number (n) and angular momentum (l) as given (a) by present calculation and (b) by Harris' variational calculation.

$n \backslash l$	0		1		2		3		4	
	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
1	1.68	1.74								
2	6.45	5.00	9.08	9.52						
3	14.3	6.78	17.7	18.2	21.8	22.2				
4	25.4	9.09	29.5	25.0	34.4	40.0	40.2	40.0		
5	39.5	11.3	44.3	33.3	50.0	50.0	56.5	57.1	63.8	66.6
6	56.8	13.8	62.2	38.5	68.5	58.8	75.9	74.1	84.0	87.0
7	77.3	15.9	83.2	43.5	90.2	69.0	98.2	95.2	107	111
8	101	18.5	107	50.0	115	80.0	124	111	134	125

plotted for values of ω less than a minimum value below which no binding is possible. This minimum ω is determined by observing that the effective potential in a state of angular momentum l,

$$V_l(x) = -\omega e^{-x}/x + l(l+1)/x^2,$$

cannot give rise to binding unless its minimum is negative. The limiting value of ω in any angular-momentum state l is that value for which $V_l(x)$ and its first derivative $V_l'(x)$ are zero at the same value of x. Carrying out the algebra we find that $\omega_{\min}{}^l = l(l+1)e = 2.718l(l+1)$. No counting function need be computed for any value of ω less than this minimum value.

The critical values of ω for the Debye-Hückel potential (that is, the values for which states are just bound at zero energy) are presented in Table I. To the best of our knowledge the only entry listed in the table which has been at all accurately determined earlier is the value $\omega = 1.68$ at which the ground (1s) state is first bound.[9] The remaining values are to be compared with those obtained by Harris[1] using a variational method; these also are presented in Table I. We see that (1) for fixed angular momentum, agreement between the two sets of numbers deteriorates as the principal quantum number increases; while (2) for fixed principal quantum number, it improves as angular momentum increases. The first of these observations is to be understood from the fact that for the most tightly bound state of a given l, and for that state only, the variational method yields a lower bound on the energy. In the remaining cases the variational method leads to uncontrolled and apparently unreliable approximations. The second observation is to be understood by noting that Harris' trial wave functions are chosen to be eigenstates of angular momentum. As the angular momentum increases, the centrifugal barrier becomes the increasingly dominant contribution to the effective potential. Therefore, as long as the trial function is the appropriate angular-momentum eigenstate, its specific form becomes less important as l increases.

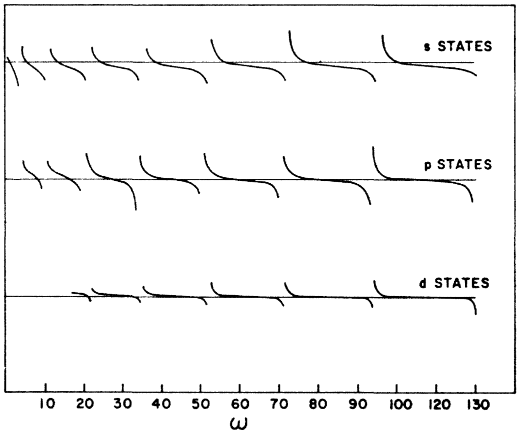

FIG. 1. The counting function $b_l(\omega)$ versus ω for s, p, and d waves in the Debye-Hückel potential.

Another aspect of our results concerns the order in which levels appear as a function of ω compared with the order of the levels in a Coulomb potential. We find (see Table I) that the levels enter as ω increases in the same order in which they appear in the Coulomb well for all states up to and including the 4d. This is in accord with one's intuition as to how these levels should be ordered, since a low-lying state has a large overlap with the region of small x where the Debye-Hückel potential has a Coulomb-like behavior. Harris' results deviate from the Coulomb order at an earlier stage, the 3s state making its appearance before the 2p.

Before discussing potentials of a somewhat different type, we mention two difficulties encountered in applying our counting method to the Debye-Hückel potential. The first of these occurs because for large l the term $b_l(\omega)x^{l+1}$ in Eq. (2) very strongly dominates the term $1/x^l$. Thus as one goes to larger l values it becomes increasingly difficult to extract the counting function from the reduced radial-wave function. It might be suggested that one could overcome this problem by taking advantage of it and writing for x and l large

$$u_l(x) \cong b_l(\omega) x^{l+1},$$

whence

$$b_l(\omega) \cong x^{-l-1} u_l(x).$$

The objection (not necessarily insuperable) to this is

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[9] R. G. Sachs and M. Goeppert-Mayer, Phys. Rev. **53**, 991 (1938); C. Lovelace and D. Masson, Nuovo Cimento **26**, 472 (1962).

that it will yield a counting function which is arbitrarily normalized (since u_l is arbitrarily normalized) and, worse, normalized differently at each ω, making it impossible to construct a continuous curve of b_l versus ω. Perhaps a better way out of this problem is to note that near any critical value of ω, b_l is small so that in this range $b_l(\omega)x^{l+1}$ will, in fact, not dominate $1/x^l$. This requires knowing in advance at least the approximate location of the critical ω and leads directly to the second of the two difficulties. This is the observed fact that as l increases each branch of b_l consists of two very steep sections separated by a very flat section. The critical value of ω always appears near the beginning or the end of the flat section. Thus the "neighborhood of the critical ω" is a region containing steep sections of two adjacent branches of b_l and the precise position of the critical value is as a consequence hard to locate. For $l>4$, we found, however, that the location of this range can be determined by taking finite differences $\omega_{ns}-\omega_{np}$, $\omega_{np}-\omega_{nd}$, etc., and using the resulting succession of numbers to locate the approximate position of the critical ω. Construction of the counting function in this region with a sufficiently fine mesh in ω enabled us in every case to locate the critical ω accurately.

One fact already alluded to makes the two difficulties discussed in the preceding paragraph less important than they might otherwise be: Both occur for large values of angular momentum where the variational method of Harris works quite well. Hence, even if our scheme became irremediably defective for states of high angular momentum, an accurate approximate scheme is available as a substitute.

We turn our attention next to potentials which, unlike the Debye-Hückel well discussed above, cannot be characterized by a single parameter. We take as an example the Woods-Saxon potential which we write in the form

$$V(r)=-V_0[1+\exp(r-r_0)/a]^{-1},$$

in which V_0, r_0, and a are all constants. The reduced radial-wave equation at zero energy is now

$$\frac{d^2u_l}{dr^2}+\left[\frac{(2mV_0/\hbar^2)}{1+e^{(r-r_0)/a}}-\frac{l(l+1)}{r^2}\right]u_l=0. \qquad (6)$$

Defining a new variable $x=r/a$ and two constants, $x_0=r_0/a$ and $\omega=2mV_0a^2/\hbar^2$, we find that Eq. (6) can now be rewritten in the form

$$\frac{d^2u_l}{dx^2}+\left[\frac{\omega}{1+e^{x-x_0}}-\frac{l(l+1)}{x^2}\right]u_l=0$$

and we see that the potential is characterized by *two* parameters, ω and x_0. All statements made earlier in the one-parameter case are valid here, except that functions of ω become functions of ω and x_0. In particular, then, our counting criterion still rests upon determining the zeros of the counting function, the precise statement now being that there is a bound state of zero energy and angular momentum l (or a zero-energy resonance in the s-wave case) for all pairs of ω and x_0 which satisfy the equation

$$b_l(\omega,x_0)=0.$$

If we take ω and x_0 as defining a pair of orthogonal axes in a "parameter plane," then this equation defines a family of curves $\omega=\omega(x_0)$ any one of which is a locus of points for which the counting function is zero. In Fig. 2 we plot these curves for a Woods-Saxon potential, confining our attention to s states. The number of bound states supportable by this potential for any pair of values (ω,x_0) is equal to the number of curves to the left of (or below) the point (ω,x_0) on the parameter plane.

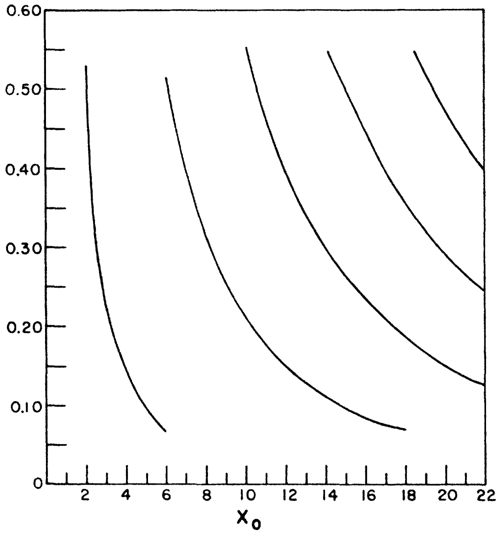

FIG. 2. Curves of zero counting function (parameter plane) for the Woods-Saxon potential.

The actual process of counting bound states in a two-parameter potential like the Woods-Saxon well does not require a knowledge of the family of curves $\omega=\omega(x_0)$ such as those shown in Fig. 2. If, for example, we wish to know the number of states in the Woods-Saxon well for $\omega=\bar{\omega}$, $x_0=\bar{x}_0$, we could simply fix the value of ω at $\bar{\omega}$ and determine the zeros of $b_l(\bar{\omega},x_0)$ as x_0 varies from zero to $\bar{x}_0$. Alternatively, we might determine the zeros of $b_l(\omega,\bar{x}_0)$ as ω varies from zero to $\bar{\omega}$. In fact, there are obviously infinitely many paths ending at $(\bar{\omega},\bar{x}_0)$ any one of which could be used, the only restriction being that the path be traversed in the direction of increasing parameter values. For this procedure to yield a unique result for the number of bound states requires that the curves in the parameter plane be monotonic and single valued, and that two such curves never intersect. To establish that the curves are, in fact, monotonic and single valued we observe that if the contrary were true we would be dealing with a situation in which a state moves in and out of the discrete spectrum as the

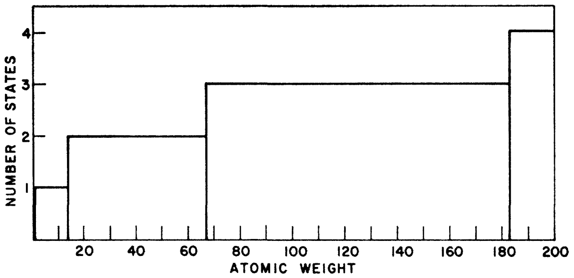

FIG. 3. Number of bound single-neutron s states as a function of atomic weight using a Woods-Saxon potential with the parameters of Ross *et al.* (Ref. 10).

potential is made more attractive (say by steadily increasing the range at a fixed well depth). But Schwinger's statement[4] quoted earlier precludes this possibility. To show that two curves in the parameter plane do not intersect, we observe that if such an intersection were to occur, then two linearly independent states of the same angular momentum would be degenerate at zero energy:

$$u''+\left[V(r)-\frac{l(l+1)}{r^2}\right]u(r)=0$$

and

$$v''+\left[V(r)-\frac{l(l+1)}{r^2}\right]v(r)=0.$$

Since $u(0)=v(0)=0$, we have at once that $u(r)v'(r)-u'(r)v(r)=0$ whence $u(r)=cv(r)$, contradicting the assumption of linear independence.

Although we have performed our calculations merely to illustrate the counting method, we can attach some physical significance to the results for the Woods-Saxon potential, since this is the central nuclear part of the average field assumed in many shell-model calculations. Thus the results plotted in Fig. 2 can be used to determine the number of neutron s states as a function of the atomic weight A. According to Ross *et al.*,[10] single-particle neutron states are described by the parameters $\omega=0.468$, $x_0=2.73A^{1/3}$ (i.e., $V_0=42.8$ MeV, $r_0=1.3A^{1/3}\times10^{-13}$ cm, and $a=0.4766\times10^{-13}$ cm). Thus, fixing ω at the value 0.468 and letting x_0 vary from zero, we can determine the values of x_0 at which the $1s$, $2s$, $\cdots$ states become bound. Then with $A=(x_0/2.73)^3$, we can calculate the corresponding atomic weight. Our results are shown in Fig. 3.

To count neutron states of angular momentum greater than zero would require two generalizations of our method, for we would need, in addition to the central Woods-Saxon well, a spin-orbit term in the potential. Thus, first of all, we would require an analysis of a potential characterized by more than two parameters, but this could be accomplished by a straightforward extension of the methods we have been discussing. Second, because of the spin-orbit force, we could no longer label eigenstates of the system by l alone, but would require $j=|l\pm\frac{1}{2}|$ as well. However, in each such state there is an effective radial potential, and the entire method described here is directly applicable. We shall not consider these matters in detail here, however, since our purpose is merely to describe a method and illustrate it in a few cases.

ACKNOWLEDGMENT

All computations involved in this paper were made on the Livermore CDC-3600 computer by Raymond L. Tarp whose expert work the authors take pleasure in acknowledging.

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[10] A. A. Ross, H. Mark, and R. D. Lawson, Phys. Rev. **102**, 1613 (1956).