Brief Reports

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Energy eigenvalues for Yukawa potentials

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(Received 2 April 1982)

A simple formula is given for the energy levels of a particle bound by a Yukawa potential which is accurate at the 1% level over the entire range of Z for a large range of n and l.

The bound states of the Yukawa, Debye-Hückel, or screened Coulomb potential have been the subject of many studies[1–14] in atomic, nuclear, particle, solid-state, and plasma physics. Recently motivated by an electron-transport problem, Green *et al.*[15] (to be referred to as GRSSG) developed an approximate analytic representation for the phase shifts for elastic scattering by a Yukawa potential. This potential may be cast in the form

$$Y=-\frac{2Z}{r}e^{-r} \tag{1}$$

by using the screening distance d as the unit of length and $\hbar^2/2\mu d^2$ as the corresponding unit of energy.

The GRSSG study provided an accurate formula

$$\nu=(\sqrt{Z}-\sqrt{Z_l})S_l+1 \tag{2}$$

for the number of bound states of a given angular momentum, l, sustainable by a given Z, where

$$Z_l=Z_0(1+\alpha l+\beta l^2)\ ,\quad S_l=S_0(1+\gamma l+\delta l^2)\ , \tag{3}$$

and $Z_0=0.839\,908$, $\alpha=2.7359$, $\beta=1.6242$, $S_0=1.1335$, $\gamma=0.019\,102$, and $\delta=-0.001\,684$.

Figure 1 illustrates this relationship. The points represent 45 data points given in Table III of Rogers, Graboske, and Harwood[12] (to be referred to as RGH). Equation (2) is represented by solid straight lines. The dashed lines represent the loci of points with the same total quantum numbers $n=\nu+l$. Equations (2) and (3) may also be applied to other short-range potentials by the use of appropriate constants.

In GRSSG, Eq. (2) was incorporated into analytic formulas for the phase shift to insure satisfaction of Levinson's theorem. For our present study of bound states we may invert Eq. (2) to solve for the critical values Z_{nl} which just lead to bound states at zero energy ($E_{nl}=0$). These are given to within 0.4% ($Z_{1s}\equiv 0.839\,908$ is exact[2]) by

$$Z_{nl}=\{\sqrt{Z_l}+[(n-l-1)/S_l]\}^2\ . \tag{4}$$

Thus Eq. (4) can serve as a precise boundary condition in formulas relating energy eigenvalues to Z.

Our approach to the representation of nonvanishing eigenvalues largely rests upon an observation that the arrays of E_{nl} given in Tables I and II of GRH take on a simpler behavior when represented by the combination variable

$$Y_{nl}=Z(1+n^2E_{nl})\ . \tag{5}$$

This is illustrated in Fig. 2 where the dots represent

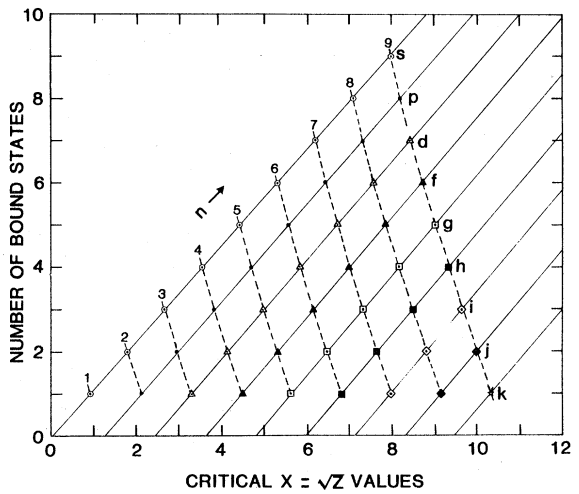

FIG. 1. Number of bound states vs critical $X=\sqrt{Z}$ values for various angular momentum states. The solid curves represent iso-l lines. The dashed curves represent iso-n lines (adapted from Ref. 15).

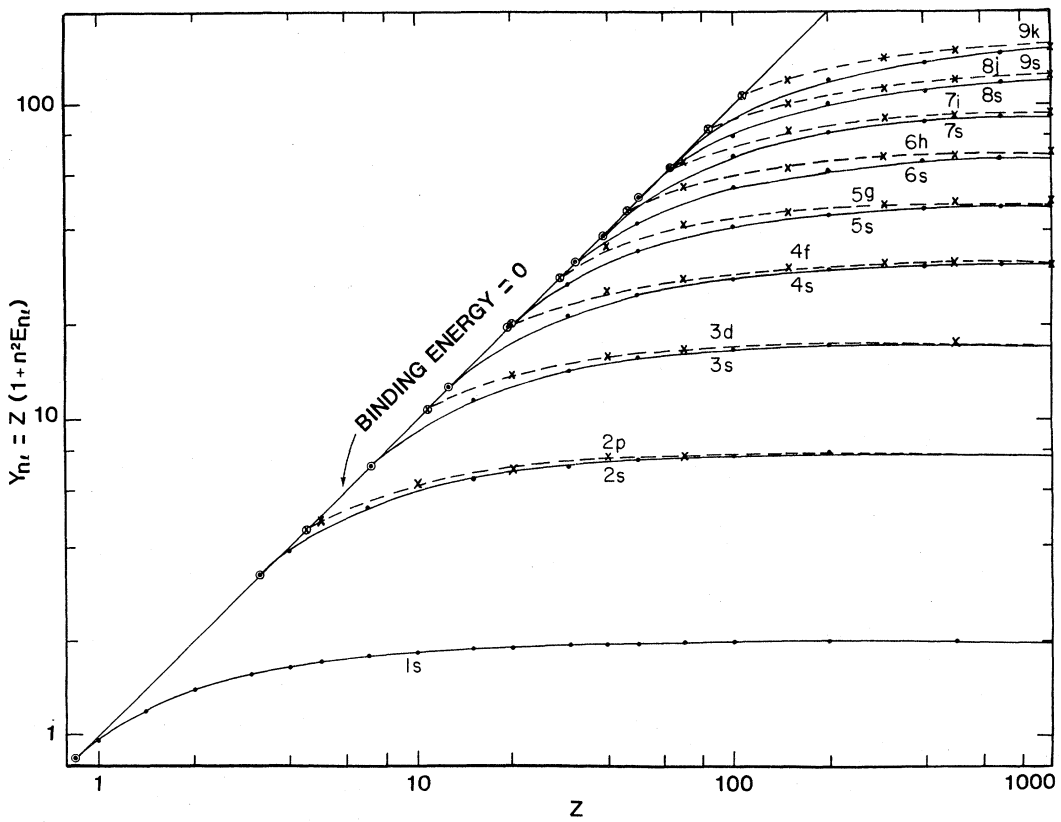

FIG. 2. Contours of $Y_{nl}=Z(1+n^2E_{nl})$ based upon the data of RGH (Ref. 12). The points denote ns data. The ×'s n, $n-1$ data. The solid curves represent Eq. (6) for ns states and the dashed curves the same equation for n, $n-1$ states.

Y_{ns} for $n=1$ to 9 and the ×'s represent $Y_{n,n-1}$. Points for intermediate l values fall in between but are omitted to avoid cluttering the figure. Equation (5) shows that as $Z\to Z_{nl}$, $E_{nl}\to 0$, hence $Y_{nl}\to Z_{nl}$. The data in Fig. 2 suggest that as $Z\to\infty$ all Y_{nl} for a given total quantum number n merge to a single asymptote: $Y_{nl}\to Z_{an}\sim 2n^2$. A simple interpolation formula between these limits is

$$Y_{nl}=\frac{Z_{nl}Bn^2+Z_{an}(Z-Z_{nl})}{Bn^2+(Z-Z_{nl})}\,, \tag{6}$$

where $B=1.2464$ and for greater precision

$$Z_{an}=A(n+\sigma)^2 \tag{7}$$

with $A=1.9875$ and $\sigma=0.003\,951$. The solid lines in Fig. 2 represent Eq. (6) for Y_{ns} and the dashed lines represent Eq. (6) for $Y_{n,n-1}$. Curves for intermediate l values would fall in between and would fit the corresponding RGH Schrödinger eigenvalues equally well. The average percentage departure of Eq. (6) from the corresponding 488 RGH "data" points is 0.58%. Only 48 points deviate by more than 1% with 1.37% representing the largest deviation.

Combining Eq. (5) and (6) and allowing for RGH's unit of energy (Z^2 Ry), we arrive at the final formula for energy levels in a Yukawa potential

$$E_{nl}(Z,d,\mu)=-\frac{\hbar^2}{2\mu d^2}\frac{Z(Z-Z_{nl})}{n^2}\times\left[\frac{Z-A(n+\sigma)^2+Bn^2}{Z-Z_{nl}+Bn^2}\right]. \tag{8}$$

This is good at the 1% level over the entire range of Z for all n and $l\lesssim 10$ and, of course, for all d and μ.

This analytic formula appears simpler and more accurate than other approximate representations of Yukawa eigenvalues[7,13,14] particularly in the physically important Z region above criticality, i.e., immediately to the right of the binding energy equal to 0 line in Fig. 2. It should be useful in atomic, nuclear, particle, solid-state, and plasma physics.

The Yukawa function may be viewed as a special case of the Green-Sellin-Zachor[16] potential

$$V(r)=-\frac{2Z}{r}\frac{1}{H(e^r-l)+1}\,, \tag{9}$$

which reduces to Eq. (1) when $H=1$. Equation (9) has been used to provide accurate independent particle potentials for electrons in negative ions.[17] It would appear rather straightforward to generalize Eq.

(8) to apply to Eq. (9) by determining the dependence of the parameters in Z_{nl}, Z_{an}, and B upon H. Generalizations for neutrals and positive ions should also be straightforward.

When $2Z/r$ in Eq. (9) is replaced by $2Z$ (i.e., r is replaced by 1 or the scale length) Eq. (9) encompasses the Einstein-Bose function ($H \rightarrow \infty$), the Maxwell-Boltzmann function ($H = 1$) and the Fermi-Dirac function ($H << 1$). In the latter case the potential has the flat bottom and diffuse boundary characteristics of nuclear potentials. The resemblance of Fig. 2 to Figs. 3–7 of Green and Lee[18] suggests that Eq. (4) can serve a critical role in the development of eigenvalue formulas for a variety of nuclear potentials including the Woods-Saxon[19] potential. Such formulas and Eq. (8) should greatly facilitate the process of inferring approximate potentials from experimental binding energies.

ACKNOWLEDGMENTS

The writer greatly appreciates the computational support of Mr. J. M. Schwartz which was essential to the completion of this effort. The assistance of Paul Schippnick, Brian Walters, and Linda Green is also acknowledged. This work was supported in part by the U. S. Department of Energy under Contract No. DE-AS-05-76 EV03798.

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