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Eigenvalue formulas for short-range potentials

A. E. S. Green and J. M. Schwartz
Nuclear Engineering Sciences Department, University of Florida, Gainesville, Florida 32611

A. Khosravi
Department of Physics, University of Florida, Gainesville, Florida 32611

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The critical potential parameter $T_c=(Z_c)^{1/2}$ expressed as a biquadratic function of the nodal and orbital quantum numbers is incorporated into two analytic eigenvalue formulas. The first uses an explicit modification of the Morse-potential eigenvalue formula. The second uses an analytic simplification of the zeroth-order approximation of Imbo, Pagnamenta, and Sukhatme. Both procedures are validated with large sets of eigenvalues obtained by numerical solutions of Schrödinger's equation for three related short-range potentials whose shapes differ widely.

I. INTRODUCTION

Previously we observed a simple regularity in the critical potential parameters Z_c of the Yukawa potential associated with bound states at zero energy.[1,2] Essentially $T_c=(Z_c)^{1/2}$ is approximately bilinear in the nodal quantum number v and the orbital quantum number l and very accurately biquadratic. This regularity at the interface between bound and scattering states was useful in developing approximate analytic expressions for eigenvalues[1] and phase shifts of the Yukawa potentials.[2] The present work began in an effort to extend and generalize this earlier work. We used the exponential potential as a simpler representative of short-range potentials since it is well behaved at the origin and at infinity.[3] We adapted a framework provided by the Morse potential eigenvalue formula which we modify further in this work to handle a greater range of potential shapes.

To test our formulas and adjust their parameters we utilize large collections of eigenvalues for a family of short-range potentials of the form $u^{\nu}e^{-u}$. The case $\nu=-1$ is the Yukawa or the Debye potential which is highly attractive at short ranges. The case $\nu=0$ is the exponential potential which is weakly attractive at short ranges. The case $\nu=1$ is a molecularlike potential which is weakly repulsive at short ranges. The three potentials can also be written $Y(\mu,r)$, $(-\partial/\partial\mu)Y(\mu,r)$, and $(-\partial/\partial\mu)^2Y(\mu,r)$, where $Y(\mu,r)=[\exp(-\mu r)]/r$, all evaluated at $\mu=1$. Such short-range potentials are representative of those used in models of nuclear forces, nuclear shell structure, negative atomic ions, superlattices in semiconductors, and quark-antiquark bound states. As test "data" for the Yukawa potential ($\nu=-1$) we use 489 eigenvalues of Rogers, Graboske, and Harwood.[4] For the exponential potential ($\nu=0$) we use 347 eigenvalues generated by Green, Schwartz, and Suh.[3] For the molecularlike potential ($\nu=1$) we use 335 eigenvalues generated in connection with this work.

During the course of the above effort the work of Imbo, Pagnamenta, and Sukhatme[5,6] (IPS) came to our attention and the zeroth-order approximation (0IPS) seemed to provide a more systematic framework for our original purpose. The present work also modifies 0IPS by incorporating the biquadratic behavior of the critical potential parameter T_c, near which the leading IPS approximation breaks down. In addition, we simplify the problem of determining the equilibrium distance by replacing their iterative method by an approximate analytical method. The results are also tested against the same eigenvalue sets.

Formulas which successfully organize the energy levels of a particle in variously shaped potentials can be useful in the following ways: (1) the development of independent particle models,[7] (2) the approximate inversion of experimental binding energy data, (3) inputting eigenvalue guesses for refinement with a Schrödinger code, and (4) communicating large data sets in a compact way.

II. CRITICAL STRENGTH PARAMETERS

We consider potentials of the form

$$V(r)=-2ZE_0f(u)\,,\quad f(u)=u^{\nu}e^{-u}\,,\quad u=r/a\,. \tag{1}$$

Here a is the range, $E_0=\hbar^2/2ma^2$ is the natural unit of energy, and $2Z$ is a dimensionless magnitude parameter. The radial Schrödinger equation then takes on the form

$$d^2G/du^2+[2Zu^{\nu}e^{-u}-l(l+1)u^{-2}]G=(-E_{vl}/E_0)G\,. \tag{2}$$

In this work we utilize our previous observation[1-3] that $T_c=(Z_c)^{1/2}$ is approximately bilinear and very accurately biquadratic in the radial quantum v and the orbital quantum number l. Thus the Z values leading to $E_{vl}=0$ conform to

$$\sqrt{Z_c}=T_c=t_0+t_1l+t_2v+t_3l^2+t_4lv+t_5v^2\,. \tag{3}$$

Figure 1 illustrates this relationship for the three potentials.

III. MODIFIED MORSE POTENTIAL EIGENVALUE FORMULA

Of the many variations and modifications of the Morse potential eigenvalue formula which we have examined the simplest one which does well is

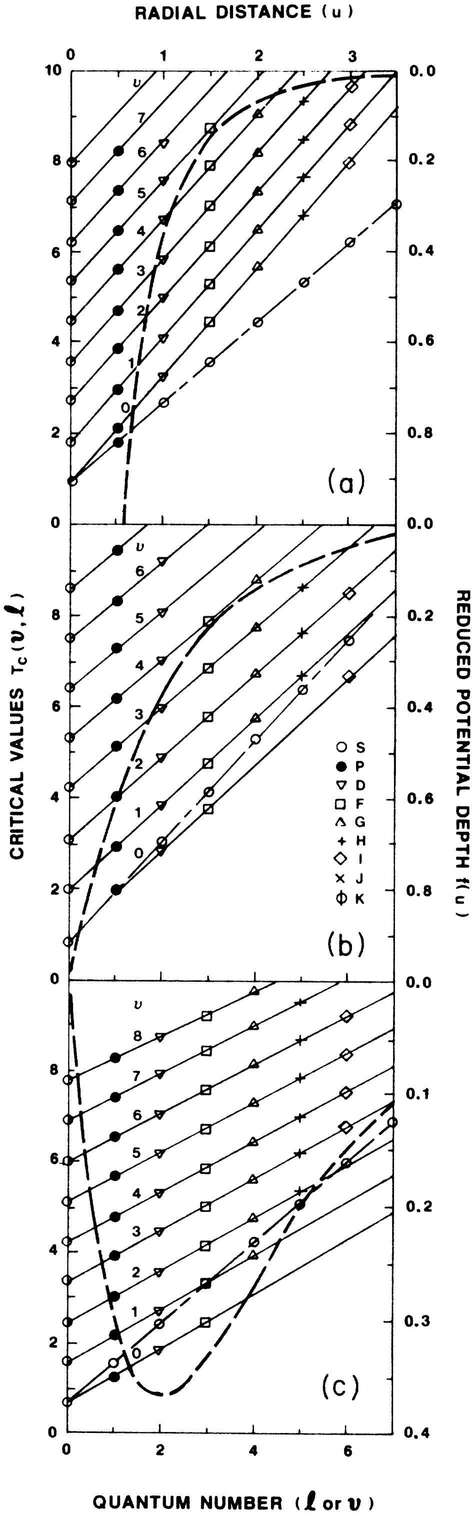

FIG. 1. Critical values $T_c(v,l)=(Z_c)^{1/2}$ vs l for various values of the nodal quantum number v. The points are determined by numerical solutions of the Schrödinger equation. The solid curves represent our biquadratic fit with the parameters in Table I. The long-short dashed curves are $T_c(v,0)$ for comparison with $T_c(0,l)$, the lowest solid curves. The dashed curves are the reduced potentials $f(u)$ relative to the right and upper scales. (a), Yukawa; (b), exponential; (c), molecularlike.

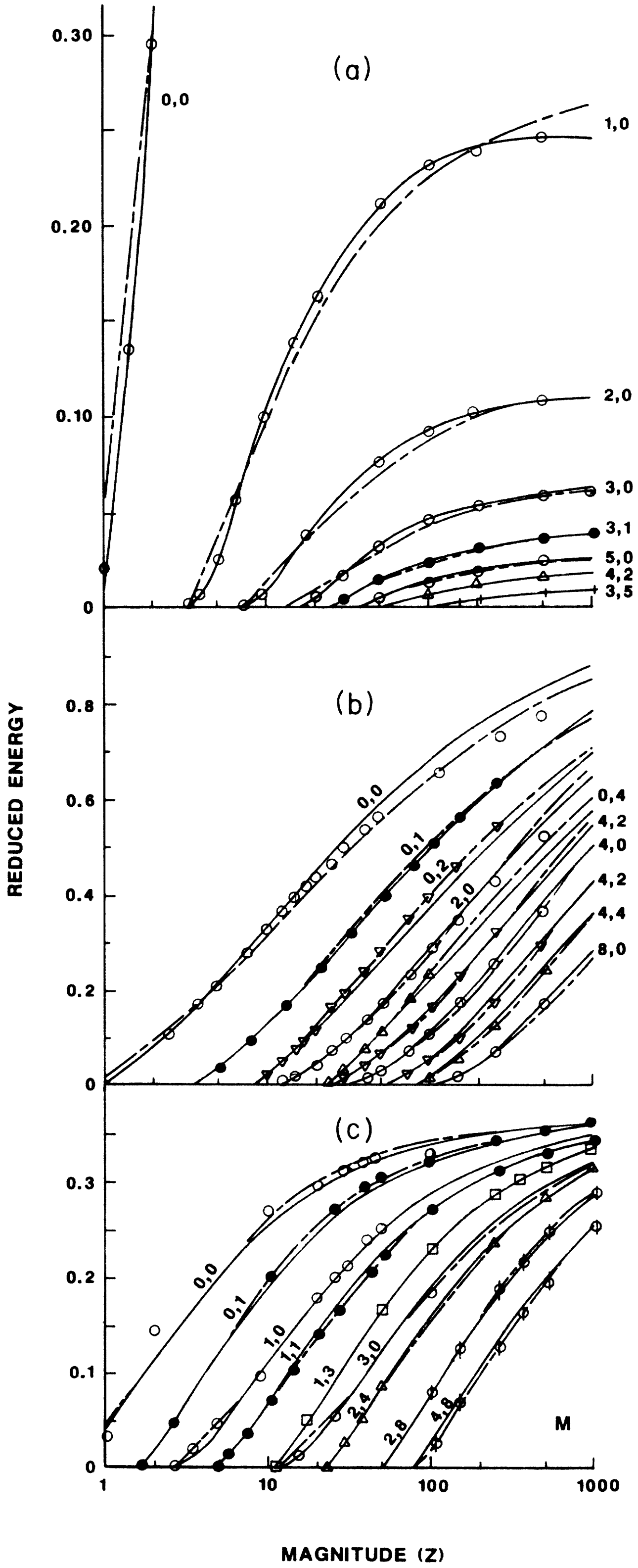

FIG. 2. Illustrative reduced eigenvalues and analytic fits with (solid curves) the modified Morse-potential eigenvalue formula and with (dashed curves) the modified OIPS formulas. (a), Yukawa $(-E_{vl}/Z^2E_0)$; (b), exponential; (c), molecularlike $(-E_{vl}/2Ze_0)$.

TABLE I. Parameters for analytic formulas. Numbers in parentheses denote powers of 10.

		Critical magnitude parameters	
	Yukawa	Exponential	Molecular
t_0	9.242(−1)	8.502(−1)	6.974(−1)
t_1	1.189	1.017	5.499(−1)
t_2	8.730(−1)	1.106	8.755(−1)
t_3	−1.689(−3)	−8.041(−3)	7.135(−3)
t_4	−9.799(−3)	−2.632(−2)	−1.002(−2)
t_5	1.200(−3)	2.416(−4)	1.366(−3)
		Modified Morse parameters	
D_0	$Z/2n^2$	1	e^{-1}
P_1	1.891	1.128	3.651
P_2	−1.072(−1)	4.044	2.665
P_3	1.750(−1)	3.567(−1)	1.962(−1)
		Modified 0IPS parameters	
K	$Z^{1/2}/n$	1	1
ϕ_1	−1.256	−2.214	0
θ_1	−7.683(−1)	1.764	5.781(−1)
τ_1	−8.162(−1)	−2.232	1.320
ϕ_2	1.0	1.570	3.033(−1)
θ_2	1.0	9.064(−1)	8.918(−1)
τ_2	1.0	2.105	3.229(−1)

$$E_{vl}=-2ZE_0D_0\left[\left[1-\frac{T_c}{T}+\frac{P_3 l}{T}\right]^2-\left[\frac{P_3 l}{T}\right]^2\right]\times\frac{T+P_1T_c}{T+P_2T_c}\ , \tag{4}$$

where T_c is given in Eq. (3), D_0, is the limiting reduced eigenvalue as $Z\rightarrow\infty$, and P_1, P_2, and P_3 are adjusted parameters. The solid curves in Fig. 2 show fits obtained to numerically determined eigenvalues for a number of representative states. The values of D_0 and the numerically adjusted parameters are also given in Table I.

IV. THE MODIFIED ZEROTH-ORDER IPS METHOD

The zeroth-order IPS approximation[5,6] (0IPS) works exceedingly well for power-law potentials. However, in application to the Yukawa and exponential potentials, this approximation breaks down near the critical values of the potential magnitude parameter Z. We have attempted to improve the 0IPS approximation phenomenologically: (1) to incorporate Eq. (3), and (2) to be analytically solvable.

The 0IPS eigenvalue equation which follows algebraically using Eq. (1) is

$$E_{vl}=V(r)+\frac{rV'(r)}{2}=-2ZE_0[f(u)+\tfrac{1}{2}uf'(u)]$$
$$=-2ZE_0u^{\nu}e^{-u}[1-(u-\nu)/2]\ , \tag{5}$$

where the dimensionless equilibrium distance (u) must satisfy

$$(l+\tfrac{1}{2})+(v+\tfrac{1}{2})w(u)=Tq(u)\ . \tag{6}$$

Here $T=\sqrt{Z}$,

$$q(u)=(-u^3f')^{1/2}=[u^{\nu+2}e^{-u}(u-\nu)]^{1/2}\ , \tag{7}$$

and

$$w(u)=[3+(uf''/f')]^{1/2}$$
$$=\left[3+\frac{\nu(\nu-1)u^{\nu-1}-2\nu u+u^{\nu+1}}{\nu u^{\nu-1}-u^{\nu}}\right]^{1/2}\ . \tag{8}$$

We next define a critical dimensionless distance parameter u_c as the location of the zero of E_{vl}, which for the class of potentials given by Eq. (1) is $u_c=2+\nu$. The vanishing of $q(u)$ also sets up a restriction on the range of u. When ν is negative $q(0)=0$. When ν is positive q also vanishes at $u_0=\nu$. For uniformity we define a new equilibrium distance parameter

$$z=(u-u_0)/(u_c-u_0)\ ,\quad 0\leq z\leq 1\ . \tag{9}$$

Thus $z=1$ constitutes the maximum (critical) equilibrium distance associated with zero binding and $z=0$ constitutes the minimum equilibrium distance. It is also convenient to transform Eq. (6) by division by q which leads to

$$T=l\phi+v\theta+\tau\ , \tag{10}$$

$$\tau=(\phi+\theta)/2\ , \tag{11}$$

where

$$\phi=1/q(u(z))\ , \tag{12}$$

and

$$\theta=w(u(z))/q(u(z))\ . \tag{13}$$

After considerable experimentation we found accurate analytic representations for ϕ and θ of the form

$$\phi=\phi_0+\phi_1 f+\phi_2 f^2\ , \tag{14}$$

where

$$f=1/z^{1/2}\ . \tag{15}$$

We may now solve the equilibrium f using the usual formula for the roots of a quadratic equation. The result may be cast in the form

$$z(v,l,Z)=\{2T_2/[T_2^2+4T_2(T-T_c+T_1+T_2)]^{1/2}-T_1\}^2\ , \tag{16}$$

where

$$T_c=l\phi_c+v\theta_c+\tau_c\ , \tag{17}$$

$$T_1=l\phi_1+v\theta_1+\tau_1\ , \tag{18}$$

$$T_2=l\phi_2+v\theta_2+\tau_2\ , \tag{19}$$

$$\phi_c=\phi_0+\phi_1+\phi_2\ , \tag{20}$$

$$\theta_c=\theta_0+\theta_1+\theta_2\ , \tag{21}$$

$$\tau_c=\tau_0+\tau_1+\tau_2\ . \tag{22}$$

Inverting Eq. (9) to relate u to z and inserting the result into Eq. (5) we obtain the energy eigenvalue formula

$$E_{vl}=-2ZE_0K[z(u-u_0)^{\nu}] \times\left\{1+\tfrac{1}{2}(\nu-u_0)-\frac{z}{2}(u_c-u_0)\right\}e^{-z(u-u_0)-u_0}\ , \tag{23}$$

where K is a parameter to make up for the trucation of the IPS series.

Rather than fix the parameters if Eqs. (17)—(22) in the above way we fit our large arrays of eigenvalues using the biquadratic formula for T_c [Eq.(3)], Eqs. (18) and (19) for T_1 and T_2 together with Eqs. (16) and (23). For $\nu=1$ and 0 we adjusted six parameters; ϕ_1, θ_1, τ_1 ϕ_2, θ_2, and τ_2. For the Yukawa potential we know the strong Z limit $E_{vl}=Z^2/n^2$, where $n=l+v+1$. We can obtain this limit by letting $K=Z^{1/2}/n$ and $\phi_2=\theta_2=\tau_2=1$. Thus we only adjust ϕ_1, θ_1, and τ_1 parameters to the eigenvalue data. Table I lists all the parameters for the three cases. The dashed curves in Fig. 2 shows the fits to representative eigenvalue data obtained by these modified 0IPS formulas.

V. CONCLUSIONS

As Figs. 1 and 2 indicate, the formulas presented in this work do quite well in representing the quantum-mechanical data. These formulas might be extended into the positive energy domain to encompass size resonances. While intended for short-range potentials they might be adapted to potentials with Coulomb tails by referring eigenvalues to the hydrogen levels ($-1/n^2$). By making the adjusted parameters dependent upon spin-orbit coupling, nonlocality, spheroidal deformation, etc., these formulas might be used to encompass other physical effects as well.[8]

We have examined several alternatives to the factor $(T+P_1T_c)/(T+P_2T_c)$ in Eq. (4) which interpolates between the large Z and small Z limits. Several of these lead to better eigenvalue fitting but at the cost of additional parameters. Finally, it should be noted that the accuracy of representation of T_c [Eq. (3)] is of primary importance to the success of the modified Morse and 0IPS approaches.

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