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Critical Values of the Coupling Constant of Short Range Potentials*

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In order to determine the critical values of the coupling constant of a given potential, i.e., the values at which there exists a zero energy bound state, the perturbative expansion of the Jost function at zero energy is analyzed. This expansion is carried out with the help of the defining integral equation, giving rise to a very accurate and stable procedure. Some numerical examples are presented, with a particular emphasis on Yukawa potential. © 1985 Academic Press, Inc.

1. INTRODUCTION

The determination of the critical values of the coupling constant, i.e., those values at which there exist only a few bound states, one of them at zero energy, has been traditionally considered as a cumbersome problem in numerical analysis. The usual and straightforward method consists in solving the Schrödinger equation for different values of the coupling constant so as to find a bound state with energy close to zero, and then determining the critical coupling constant after some interpolation mechanism. This is a costly approach. First, given that one is involved with very low energies, the numerical integration must be extended to very large values of the distance. Second, it is necessary to carry out two iterative procedures, one to determine the eigenvalue closest to zero, and the other to determine the coupling constant.

With this procedure the critical values of the coupling constant of the Yukawa potential (sometimes referred to as the screened Coulomb potential) have been determined with a high degree of precision [1, 2]. The calculations of Ref. [2] following this method are, in our opinion, the most precise determination of the critical values corresponding to the Yukawa potential.

There is a simple modification of this procedure which simplifies the computation: it consists in a change of variables in the Schrödinger equation which adds a classical turning point to the right [3], so that the zero-energy bound state is converted into a *normal* bound state with a prescribed, non-zero energy. This

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avoids the need of a great deal of numerical integration. However, the critical values must be determined again by means of an interpolation mechanism.

A different approach is based on the study of the low-energy scattering parameters, and particularly the behaviour of the scattering length (or its inverse) in terms of the coupling constant [4, 5]. The behaviour of the scattering length with the coupling constant is simple to describe [6]. For a null coupling constant, i.e., in the absence of interaction, the scattering length is zero, and when the coupling constant increases there appears a critical value at which the scattering length has a pole. This is the critical value for having only one bound state at zero energy. Afterwards there follows a sequence of zeros and poles, showing a shape analogous to that of the function $\tan(x)$, each pole corresponding to a new bound state at zero energy.

From the numerical point of view, this procedure has been implemented in two ways. Schey and Schwarz [4] determined the values of the inverse scattering length at several values of the coupling constant, and after a polynomial interpolation, the corresponding zeros. On the other hand, Patil [5] determined the expansion of the scattering length in powers of the coupling constant. From this expansion the poles were determined by constructing the appropriate Padé approximants.

The advantage of the study based on properties of the scattering length over the usual shooting method described at the beginning is that in the former case one is not faced with an eigenvalue problem. Actually, the zero energy Schrödinger equation is solved starting at the origin with the value $u(0)=0$ with an arbitrary slope, and looking to the asymptotic behaviour at large distances. This method is both simple and accurate.

We should finally mention other specialized methods for the Yukawa potential which have also provided values for the critical values of the coupling constant. Hulten and Laurikainen [7] used a variational method. Iafrate and Mendelsohn [8] and Galindo and Pascual [9] used a perturbation expansion in terms of the inverse coupling constant. This expansion is extended to low values of the coupling constant by means of Padé approximants [9] and then solved for the coupling constant at zero energy. Nauemberg [10] converts the Schrödinger equation into a pair of coupled integral equations, obtaining an implicit equation relating the bound state energy with the coupling constant.

The method followed in this paper borrows some basic ideas from the work of Schey and Schwarz [4] and Patil [5]. The main idea is to determine the expansion of the Jost function at zero energy in terms of the coupling constant of the potential. This expansion is known to convergent for all values of the coupling constant under very general and not too restrictive conditions on the potential. The coefficients of the expansion are determined by iteratively computing one-dimensional integrals. Finally, the critical values of the coupling constant correspond to the zeros of the Jost function. The general theory is briefly described in Section 2, and the numerical method is described in Section 3. Section 4 includes some results corresponding to Yukawa and exponential potentials. Finally, Section 5 contains the conclusions and main results of this work.

2. THEORETICAL DEVELOPMENT

In this section we will use some results from the theory of potential scattering. We will follow the notation of Taylor [11].

As is well known, the bound states of angular momentum l correspond to the zeros of the Jost function $f_l(p) = 0$ in the upper half plane. The Jost function may be determined from the regular solution by means of the integral

$$f_l(p) = 1 + \frac{\lambda}{p} \int_0^{\infty} dr\, \hat{h}_l^{(+)}(pr)\, U(r)\, \phi_{l,p}(r) \tag{1}$$

where the regular solution satisfies the integral equation

$$\phi_{lp}(r) = \hat{j}_l(pr) + \lambda \int_0^r dr'\, g_{lp}(r, r')\, U(r')\, \phi_{lp}(r') \tag{2}$$

and

$$g_{lp}(r, r') = \frac{1}{p}\{\hat{j}_l(pr)\, \hat{n}_l(pr') - \hat{n}_l(pr)\, \hat{j}_l(pr')\} \tag{3}$$

is the free hamiltonian Green function determined in such a way that ϕ_{lp} behaves at small r as $\hat{j}_l(pr)$. The roof symbol on j_l, n_l and h_l indicates that these spherical Bessel functions have been multiplied by pr, i.e., $\hat{j}_l(z) = zj_l(z)$.

For our purposes we need the above equations in the $p \to 0$ limit. According to the behaviour at the origin of the Bessel functions it is convenient to redefine the regular solution by removing the dominant dependence at $r \to 0$; i.e., we will introduce the function

$$\varphi_l(r) = \lim_{p \to 0} \frac{(2l+1)!!}{(pr)^{l+1}}\, \phi_{lp}(r)$$

and the corresponding equations are now

$$\varphi_l(r) = 1 + \frac{\lambda}{(2+1)} \int_0^r dr'\, r' \left\{1 - \left(\frac{r'}{r}\right)^{2l+1}\right\} U(r')\, \varphi_l(r') \tag{4}$$

and

$$f_l(0) = 1 + \frac{\lambda}{2l+1} \int_0^R r\, dr\, \varphi_l(r)\, U(r). \tag{5}$$

Note that in the equation determining $f_l(0)$ we have introduced an upper limit R to the integral instead of ∞. This step is certainly necessary in any numerical approach and it takes into account that the potential goes sufficiently fast to zero at long distances. Moreover, it permits the substitution of $\hat{h}_l(pr)$ by its limit at $pr \to 0$.

Equations (4) and (5) are the basis of a simple expansion in terms of the coupling constant of the potential. If we write

$$\varphi_l(r) = \sum_{k=0} \lambda^k \varphi_l^{(k)}(r) \tag{6}$$

$$f_l(0) = \sum_{k=0} \lambda^k f_l^{(k)} \tag{7}$$

then the recurrence relations

$$\varphi_l^{(k)}(r) = \frac{1}{2l+1} \int_0^r dr'\, r' \left\{1 - \left(\frac{r'}{r}\right)^{2l+1}\right\} U(r')\, \varphi_l^{(k-1)}(r') \tag{8}$$

$$f_l^{(k)} = \frac{1}{2l+1} \int_0^R dr\, r\varphi_l^{(k-1)}(r)\, U(r) \tag{9}$$

emerge, with the starting values

$$\varphi_l^{(0)}(r) = 1$$

$$f_l^{(0)} = 1.$$

Once the coefficients $f_l^{(k)}$ are determined, the threshold values of the coupling constant λ for having zero-energy bound states are the zeros of the polynomial $\sum_0^N \lambda^k f_l^{(k)}$. The value of the upper limit N must be carefully chosen, particularly for large values of λ.

It is interesting to determine the behaviour of the regular solution φ_l at short distances and we have to distinguish the cases of potentials regular at the origin and potentials having a singularity. In all cases $\varphi_l^0(r) = 1$.

For non-singular poentials we may use the recurrence relation (8) to obtain

$$\varphi_l^{(k)} \xrightarrow[r \to 0]{} C_l^{(k)} r^{2k} \tag{10}$$

where

$$C_l^{(1)} = \frac{1}{2(2l+3)} U(0) \tag{11}$$

and

$$C_l^{(k)} = C_l^{(k-1)} \frac{1}{2k(2l+2k+1)} U(0). \tag{12}$$

Equation (10) will be used later to increase the accuracy of the quadratures needed to evaluate the integrals (8) and (9).

The case of singular potentials of the type $1/r$ near the origin can also be worked out. If we define $V = \lim_{r \to 0} rU(r)$, the recurrence relation (8) gives the result

$$\varphi_l^{(k)} \xrightarrow[r \to 0]{} B_l^{(k)} r^k \tag{13}$$

with

$$B_l^{(1)} = \frac{V}{2l+2} \tag{14}$$

and

$$B_l^{(k)} = B_l^{(k-1)} \frac{1}{k(2l+k+1)}. \tag{15}$$

3. Numerical Method

The objective is to integrate the chain of Eqs. (8) and (9) up to some value of $k = N$.

Let us consider first Eq. (8) for non-singular potentials (i.e., $U(0)$ is a constant). The corresponding integral is converted into a sum by means of the trapezoidal rule, and using the notation

$$\begin{aligned} U(n) &= U(nh) \\ \varphi_l^{(k)}(n) &= \varphi_l^{(k)}(nh) \\ r &= nh \end{aligned} \tag{16}$$

there results

$$\varphi_l^{(k)}(n) = \frac{h^2}{2l+1} \sum_{p=1}^{n-1} p \left\{ 1 - \left(\frac{p}{n}\right)^{2l+1} \right\} U(p)\, \varphi_l^{(k-1)}(p). \tag{17}$$

For practical calculations it is convenient to define the sums

$$S_{n-1} = \sum_{p=1}^{n-1} p U(p)\, \varphi_l^{(k-1)}(p)$$

$$T_{n-1} = \sum_{p=1}^{n-1} p^{2l+2} U(p)\, \varphi_l^{(k-1)}(p)$$

which satisfy the trivial recurrence relations

$$\begin{aligned} S_n &= S_{n-1} + nU(n)\, \varphi_l^{(k-1)}(n) \\ T_n &= T_{n-1} + n^{2l+2} U(n)\, \varphi_l^{(k-1)}(n) \end{aligned} \tag{18}$$

and construct $\varphi_l^{(k)}(n)$ from those quantities. In this form, all integrals required in (8) (one for each value of r) are evaluated recurrently with little effort. In the same iteration loop we may include also the evaluation of Jost function after transforming Eq. (9) into a sum

$$f_l^{(k)} = \frac{h^2}{2l+1} \sum_{p=1}^{(R/h)} p\varphi_l^{(k-1)}(p)\, U(p). \tag{19}$$

This is a very quick method producing results in order h^2, the error of the trapezoidal rule.

When the potential is singular at the origin in such a form that $\lim_{r\to 0} rU(r) = V$, it is necessary to include into the above sums the contribution at $p=0$ (the point of the origin). Taking into account the characteristic behaviour of the regular solution $\varphi_l^{(k)}(r)$ at the origin, Eq. (13), this correction only applies in the case where we are computing $\varphi_l^{(1)}(r)$ and $f_l^{(1)}$.

To improve the precision of the numerical method we have used the Euler–Maclaurin expansion [12] at the lowest order. This expansion relates the trapezoidal rule with the exact value of an integral in the form

$$\int_0^{nh} F(r')\, dr' = h\{\tfrac{1}{2}F(0) + F(h) + F(2h) + \cdots + \tfrac{1}{2}F(nh)\}$$
$$-\frac{h^2}{12}\{F'(nh) - F'(0)\} + O(h^4). \tag{20}$$

In the case of the computation of $\varphi_l^{(k)}(r)$ the argument of the integral is given by

$$F(r') = r'\left\{1 - \left(\frac{r'}{r}\right)^{2l+1}\right\} U(r')\, \varphi_l^{(k-1)}(r')$$

and the derivatives involved in Eq. (20) may be easily computed with the results

(a) Non-singular potentials

$$\begin{aligned} F(0) &= 0 \\ F(nh) &= 0 \\ F'(0) &= U(0)\, \delta_{k,1} \\ F'(nh) &= -(2l+1)\, U(nh)\, \varphi_l^{(k-1)}(nh). \end{aligned} \tag{21}$$

(b) Singular potentials ($1/r$ behaviour)

$$\begin{aligned} F(0) &= V\delta_{k,1} \\ F(nh) &= 0 \\ F'(0) &= \frac{1}{2l+1}\left\{\delta_{k,1} V' - \delta_{k,1}\delta_{l,0}\frac{V}{r} + \delta_{k,2}\frac{V^2}{2l+2}\right\} \\ F'(nh) &= -(2l+1)\, U(nh)\, \varphi_l^{(k-1)}(nh) \end{aligned} \tag{22}$$

where $V = \lim_{r\to 0} rU(r)$ and $V' = (d/dr)(rU(r))$ at $r=0$.

To obtain the results given in Eqs. (21) and (22) we simply derive the function $F(r')$ and consider the behaviour of the functions $\varphi_l^{(k-1)}$ stated in the previous section near the origin.

An analogous correction must be considered in the calculation of the Jost function. In this case the function to be integrated is $F(r) = rU(r)\, \varphi_l^{(k-1)}(r)$. At the upper limit R, both $F(R)$ and $F'(R)$ can be considered null (actually, we must go far enough so as to have these properties). The corrections related with the origin are given by

(a) Non-singular potentials

$$\begin{aligned} F(0) &= 0 \\ F'(0) &= U(0)\, \delta_{k,1}. \end{aligned} \tag{23}$$

(b) Singular potentials ($1/r$ behaviour)

$$\begin{aligned} F(0) &= V\delta_{k,1} \\ F'(0) &= V'\delta_{k,1} + \frac{V^2}{2l+2}\, \delta_{k,2} \end{aligned} \tag{24}$$

with the same values of V and V' as above.

4. Some Numerical Calculations

The first case we have considered is the exponential potential $V(r) = -\lambda \exp(-r)$. The s-wave bound states of this potential are determined by solving the transcendental equation ($\hbar^2/2m = 1$)

$$J_{2\sqrt{E}}(2\sqrt{\lambda}) = 0 \tag{25}$$

so that the critical values of the coupling constant are related in a very simple way to the zeros of the Bessel function J_0.

TABLE I

Critical Values for the Coupling Constant of the Exponential Potential for s-Wave States

	Trapezoidal		Euler–Maclaurin Corr.		
nl	250 points	1000 points	250 points	1000 points	Exact
1s	1.4454	1.44577	1.445793	1.44579649	1.44579649
2s	7.60	7.616	7.6172	7.6178149	7.61781559
3s	18.6	18.71	18.71	18.72174	18.72175169
4s	34.4	34.74	34.70	34.76000	34.76007105

TABLE II

Expansion Coefficients of the Zero Energy Jost Function in Terms of the Coupling Constant for the Exponential Potential

$f^{(k)}$	Exact	Numerical	Percentage error
$f^{(1)}$	1	1.000000001	10^{-7}
$f^{(2)}$	0.25	0.249999941	2×10^{-5}
$f^{(3)}\times 10^{2}$	2.77777777	2.777771825	2×10^{-4}
$f^{(4)}\times 10^{3}$	1.73611111	1.736096510	8×10^{-4}
$f^{(5)}\times 10^{5}$	6.94444444	6.944286301	2×10^{-3}
$f^{(6)}\times 10^{6}$	1.92901234	1.928916237	5×10^{-3}
$f^{(7)}\times 10^{8}$	3.93675989	3.936386594	9×10^{-3}
$f^{(8)}\times 10^{10}$	6.15118732	6.150181362	2×10^{-2}
$f^{(9)}\times 10^{12}$	7.59405843	7.592068168	3×10^{-2}
$f^{(10)}\times 10^{14}$	7.59405843	7.591045501	4×10^{-2}

In Table I we present our numerical calculations corresponding to 250 and 1000 mesh points, with $R=25$ and with and without the first order Euler–Maclaurin correction. In all cases presented we have computed up to $N=20$, i.e., the first 20 terms of the perturbative expansion of the Jost function.

Comparison between the exact results and the numerical calculations shows that our method deteriorates when the critical value increases. There are two ways this may happen. First, at large values of the coupling constant it is necessary to increase the degree N of the perturbative expansion. A second way is the propagation and accumulation of numerical errors along the successive iterations. Both alternatives are easily checked in the case of the exponential potential, because the s-wave Jost function at zero energy is given by

$$f_0(E=0,\lambda)={}_0F_1(-;\,1;\,-\lambda)=\sum_{n=0}\frac{(-1)^k\,\lambda^k}{(k!)^2} \tag{26}$$

and in our case, i.e., up to the fourth bound state, it is sufficient to consider for the above sum (26) an upper limit of 20. Consequently, this means that the increase in error with the critical value of the coupling constant must be due to propagation errors. In Table II we compare the exact values of the perturbative expansion of the Jost function, Eq. (26), with the numerical ones, showing clearly the effect of error propagation. Nevertheless, the relative errors are still very small. These results correspond to a mesh of 1000 points only.

The second case we have studied corresponds to Yukawa potential $U(r)=-\lambda\exp(-r)/r$. In that case we have taken into account the appropriate corrections to deal properly with the singularity at the origin, as was described in Section 3. Table III collects a series of results regarding this potential obtained by means of a wide variety of methods.

TABLE III

Critical Coupling Constants Corresponding to Several *nl* Levels of the Yukawa Potential, Computed by Different Techniques

nl	1*s*	2*s*	3*s*	2*p*	3*p*	3*d*
This work	1.6798077	6.4472586	14.342011	9.07971	17.7254	21.8825
Direct int. [2]	1.6798077	6.4472603	14.342027	9.081959	17.74457	21.89498
Direct int. [1]	1.679816	—	—	—	—	—
Direct int. [3]	1.6798076	6.44726	14.342028	9.081958	17.74457	21.89495
Scatt. length [4]	1.68	6.45	14.3	9.08	17.7	21.8
Scatt. length [5]	1.680	6.42	—	—	—	—
Perturbative [9]	1.6798474	6.449072	14.35332	9.191516	18.01449	22.28410
Variational [7]	1.6798194	6.44772	14.372	—	—	—
Analytic [10]	1.67974	—	—	—	—	—

Notes. See the text for further details. The numbers in brackets in the first column are the references to the original works.

The first row contains our estimates for the critical coupling constants corresponding to the 1*s*, 2*s*, 3*s*, 2*p*, 3*p*, and 3*d* levels, computed with a mesh of 1000 points and step 0.025. The second row contains the estimates of Singh and Varshni [2], and the third the results of Rogers, Graboske, and Harwood [1], both obtained by direct numerical integration by searching for a zero energy bound state. The fourth row contains the results of Oset and Salcedo [3], which follow an analogous mechanism after transforming the Schrödinger equation so as to move the bound state from zero. The number of mesh points used in Ref. [1] is 20,000, up to $R = 40$. The calculations of Oset and Salcedo use an unpredictable number of mesh points.

Rows 5 and 6 include the calculations of Schey and Schwarz [4] and Patil [5], respectively. Both methods are based on the determination of the poles of the scattering length as a function of the coupling constant. Schey and Schwarz [4] compute the inverse of the scattering length for several values of the coupling constant by ditectly integrating the zero energy Schrödinger equation. Patil [5] carries out a perturbative expansion of the scattering length by means of numerical methods.

Finally, the table also includes other results based on analytical methods: perturbation in terms of the inverse coupling constant [9] variational calculations [7] and a direct iterative method due to Nauemberg [10].

Again our results are very good, and in addition the calculations require a short computing time. As in the previous case, our results deteriorate at higher values of the coupling constant.

5. FINAL COMMENTS

We have developed an iterative perturbation expansion scheme for the determination of the Jost function at zero energy. By solving a polynomial equation in the coupling constant the values of the coupling constant are determined at a high degree of precision with quite low number of points for the needed quadratures. In contrast with other numerical methods, our approach is both a simple and a stable algorithm, and is easily extended to deal with a class of singular potentials at the origin.

For the sake of determining the critical values of the coupling constant we have found our method much more stable than the analysis of the equivalent expansion of the scattering length. The expansion of the scattering length in powers of the coupling constant can also be carried out in a way analogous to that used to expand the Jost function. The first step is to construct the integral equation equivalent to the Schrödinger equation (s-waves)

$$\varphi'' = \lambda U(r)\, \varphi$$

$$\varphi(0) = 0$$

$$\varphi'(\infty) = 1;$$

i.e., we look for a regular solution with the behaviour $\varphi(r) \to_{r \to \infty} r - a$, which turns out to be

$$\varphi(r) = r - \lambda \int_0^\infty dr'\, U(r')\, \varphi(r')(r'\theta(r-r') + r\theta(r'-r))$$

so that $a = \lim_{r \to \infty} (\varphi(r) - r)$ is given by

$$a = -\lambda \int_0^\infty dr'\, r' V(r')\, \varphi(r').$$

The perturbative expansion of this integral equation may be solved numerically in just the same form as described in Section 3, and the corresponding expansion of a in powers of λ turns out to be again very stable. However, the very rich structure of a (λ), alternating zeros and poles at real values of λ, makes numerically unstable the determination of all but the first pole.

In conclusion we would like to stress the great simplicity of the whole procedure that results from the use of integral equations perturbatively expanded instead of the corresponding expansion of the differential equation. Similarly, we consider the improvement of the quadrature rule by means of the Euler–Maclaurin correction as a very effective way of increasing the precision of the numerical calculations.

REFERENCES

1. F. ROGERS, H. C. GRABOSKE, JR., AND D. J. HARWOOD, *Phys. Rev. A* 1 (1970), 1577.
2. D. SINGH AND Y. P. VARSHNI, *Phys. Rev. A* **29** (1984), 2895; *A* **28** (1983), 2606.
3. E. OSET AND L. L. SALCEDO, *Anal. Fis. Madrid A* **80** (1984), 109.
4. H. M. SCHEY AND J. L. SCHWARZ, *Phys. Rev. B* **139** (1965), 1428.

5. S. H. PATIL, *Phys. Rev. A* **24** (1981), 3038; *J. Phys. A* **17** (1984), 575.
6. R. G. NEWTON, "Scattering Theory of Waves and Particles," McGraw–Hill, New York, 1966.
7. L. HULTHEN AND K. V. LAURIKAINEN, *Rev. Mod. Phys.* **23** (1951), 1.
8. G. J. IAFRATE AND L. B. MENDELSOHN, *Phys. Rev.* **182** (1969), 244.
9. A. GALINDO AND P. PASCUAL, *Nuovo Cimento Soc. Ital. Fis. A* **30** (1975), 111.
10. M. NAUEMBERG, *Phys. Rev. A* **8** (1973), 2217.
11. J. R. TAYLOR, "Scattering Theory," Wiley, New York, 1972. [See particularly Chap. 11.]
12. E. T. WHITTAKER AND G. N. WATSON, "A Course of Modern Analysis," Cambridge Univ. Press, Cambridge, 1965.