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Energy levels of screened Coulomb and Hulthén potentials

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Abstract. We have investigated the structure of the energy levels of the screened Coulomb and Hulthén potentials near the critical coupling strengths. Incorporating this structure and using the strong-coupling series for the energy levels, we obtain expressions which give satisfactory values for the energy levels of all the states.

1. Introduction

The screened Coulomb potential is of importance in several contexts. It may be used as a rough approximation to the potential experienced by electrons in an atom where the remaining electrons screen the nuclear charge. It describes the shielding effect in plasmas where it is called the Debye–Hückel potential. It is also present in nuclear interactions as the dominant Yukawa potential arising from the exchange of particles with non-zero mass. In all these cases, a knowledge of the various bound-state energies is essential for understanding and correlating the properties of the different systems. Another potential of some interest is the Hulthén potential which is closely related to the screened Coulomb potential. Its behaviour for small r is similar to that of the screened Coulomb potential, but it goes to zero a little more slowly for large r . The main advantage of the Hulthén potential is that it yields closed, analytic solutions for the s waves, and therefore is often used as an approximation for the screened Coulomb potential. However, one does not have such nice solutions for higher partial waves. The usefulness of the Hulthén potential would be enhanced if one obtained accurate energies for the non-zero angular momentum states as well.

There have been a large number of varied attempts to deduce the bound-state energies of the screened Coulomb and Hulthén potentials. They may be classified into the following broad groups.

(1) Some attempts are based on approximating the given potential by a suitable potential for which solutions are known (Ecker and Weizel 1956, Lam and Varshni 1976, Ray and Ray 1980, Dutt *et al* 1981, Dutt and Mukherji 1982). The correction due to the small difference may be evaluated perturbatively (Smith 1964).

(2) Variational approaches based on different forms of the trial wavefunctions have been used to estimate the bound-state energies. While earlier efforts (Harris 1962) were not particularly successful, more recent calculations (Greene and Aldrich 1976, Roussel and O'Connell 1974) have provided very accurate values for the energies.

(3) Several calculations are based on the fact that both screened Coulomb and Hulthén potentials allow a strong-coupling expansion. This allows one (Iafrate and Mendelsohn 1969, Müller-Kirsten and Vahedi-Faridi 1973, McEnnan *et al* 1976) to

obtain quite satisfactory bound-state energies for large coupling constants. However, the rate of convergence of the strong-coupling series is a serious problem for smaller values of the coupling constant. Fortunately, it appears (Lai and Lin 1980, Lai 1981) that the use of Padé approximants greatly aids the convergence of the series.

(4) Finally one has the very accurate numerical calculations of Rogers *et al* (1970) who have obtained the bound-state energies of all the states with $n \leq 9$, n being the principal quantum number for a large range of coupling strengths. It may also be noted that Green (1982) has recently given a quite accurate semi-empirical expression for the energy eigenvalues of the Yukawa potential.

One of the characteristics of the screened Coulomb and Hulthén potentials is that their bound-state energies are functions of essentially only one variable which may be taken to be the charge Z . A difficulty in the use of the strong-coupling expansion in powers of $1/Z$ is the nature of the series. While the series is convergent for the Hulthén potential, it is only asymptotic (Mehta and Patil 1978) for the screened Coulomb potential. It would be useful to clarify the structure of this asymptotic series. Another important property of these potentials is that for any finite Z , the potentials support only a finite number of bound states. For every bound state there is a critical strength Z_c of the coupling constant at which the binding energy is zero and the bound state disappears for $Z < Z_c$. A really satisfactory analytic description of the bound-state energies must incorporate the correct behaviour of the energies near $Z = Z_c$.

Here we try to analyse the nature of the strong-coupling series for the bound-state energies. With the use of the wkb approximation and the Bender–Wu (1969, 1973) formalism, it is shown that the series is asymptotic for the screened Coulomb potential. As such, the series is useful only for large values of Z . Our main effort is directed towards understanding the behaviour of the energies near $Z = Z_c$. We first deduce the general behaviour in terms of the properties of the poles of the T matrix near the critical value Z_c . This behaviour is different for s, p and higher partial waves, and is controlled by the value of Z_c , the residue and the value of $\partial E/\partial Z$ at $Z = Z_c$. The values of Z_c correspond (Schey and Schwartz 1965) to changes in the signs of the phase shifts, and can be deduced from the perturbation series (Patil 1981) for the scattering length and its generalisations to higher partial waves. We develop sum rules which allow us to obtain quite accurate values for scattering lengths and the residues. One can also obtain satisfactory estimates for $\partial E/\partial Z$ by using the Hellmann–Feynman theorem and the wkb wavefunctions. Finally we propose an interpolation for the bound-state energies which incorporates the required behaviour near the critical strength Z_c and also has a strong-coupling expansion in conformity with the first few known terms of the strong-coupling expansion. We have applied these results to the screened Coulomb and Hulthén potentials. The predictions of their energies, governed by the above constraints are in very good agreement with the numerical (Rogers *et al* 1979), variational (Roussel and O’Connell 1974) results and those based on Padé approximants (Lai and Lin 1980), over the entire range of n , l and Z values. What is more, we are now in a position to give the energy of almost any state for any value of the coupling strength Z .

In § 2 we develop the formalism which can be used to obtain the energy levels of a class of one-parameter potentials. These potentials have a strong-coupling expansion and support a finite number of bound states. The formalism is utilised to obtain the bound-state energies of (1) the screened Coulomb potential in § 3 and (2) the Hulthén potential in § 4. In § 5, the significance of these results is discussed.

2. The general approach

We are interested in solutions to the radial Schrödinger equation (in atomic units)

$$-\frac{1}{2}[\mathrm{d}^2/\mathrm{d}r^2 - l(l+1)/r^2]R(r) + ZV(r)R(r) = ER(r) \quad (2.1)$$

where $V(r)$ is of the form

$$V(r) = -(1/r)f(\lambda r). \quad (2.2)$$

Two particular realisations of special interest are the screened Coulomb potential

$$V_I(r) = -(1/r)e^{-\lambda r}, \quad (2.3)$$

and the Hulthén potential

$$V_{II}(r) = -(1/r)\lambda r e^{-\lambda r}/(1 - e^{-\lambda r}). \quad (2.4)$$

The energy eigenvalues of (2.1) are known to be functions of essentially only one variable.

2.1. Scaling

Let E be characterised by Z and λ . Now consider a scale transformation

$$r \rightarrow r/Z \quad (2.5)$$

which takes (2.1) into

$$-\frac{1}{2}[\mathrm{d}^2/\mathrm{d}r^2 - l(l+1)/r^2]R - (1/r)f(\lambda r/Z)R = Z^{-2}E(Z, \lambda)R. \quad (2.6)$$

This leads to the relation

$$Z^{-2}E(Z, \lambda) = E(1, \lambda/Z). \quad (2.7)$$

Thus, apart from the factor of Z^2 , one may regard the energy levels as being functions of only one variable

$$\varepsilon = \lambda/Z. \quad (2.8)$$

In particular one may take $\lambda = 1$ without any loss of generality. An expansion in powers of ε then allows us to obtain a strong-coupling series for the energy levels.

2.2. Strong-coupling expansion

If $f(r\lambda)$ has an expansion

$$f(r\lambda) = 1 + \sum_{i=1}^{\infty} B_i(\lambda r)^i, \quad (2.9)$$

one can obtain the solution to (2.1), as a perturbation series in powers of ε . For example, it has been shown (Iafate and Mendelsohn 1969, Müller-Kirsten and Vahedi-Faridi 1973, McEannan *et al* 1976) that

$$-2E/Z^2 = n^{-2} + 2B_1\varepsilon + B_2(3n^2 - x)\varepsilon^2 + B_3n^2(1 + 5n^2 - 3x)\varepsilon^3 + \dots \quad (2.10)$$

where n is the principal quantum number and $x = l(l+1)$. The utility of this strong-coupling expansion depends on the nature of convergence of the series. The nature of the series is governed by the asymptotic behaviour of $V(r)$ For $\varepsilon \rightarrow 0_{\pm}$. For example, in the case of the Hulthén potential, the potential vanishes in the limit $r \rightarrow \infty$ for $\varepsilon \rightarrow 0_{+}$ as well as for $\varepsilon \rightarrow 0_{-}$, and the strong-coupling series converges for $Z > Z_c$. However, in the case of the screened Coulomb potential, while the potential vanishes in the limit $r \rightarrow \infty$ for $\varepsilon \rightarrow 0_{+}$, it diverges exponentially for $\varepsilon \rightarrow 0_{-}$. As a consequence, the series in (2.10) is only asymptotic. Of course, even this series is quite useful for small ε .

In all these cases, the series either diverges as $Z \rightarrow Z_c$ or converges very slowly. Therefore, to obtain an accurate representation of the energy levels, one must understand the behaviour of E near $Z = Z_c$.

2.3. Bound states as poles

The behaviour of the energy levels near the critical coupling strength Z_c can be effectively analysed in terms of bound states regarded as poles of the T matrix.

At the critical value Z_c , the bound state energy is zero. Therefore, expanding T_l^{-1} near $Z = Z_c$, one gets for small q^2 (q is the momentum)

$$(e^{i\delta_l} \sin \delta_l) / q^{2l+1} \approx [d(Z - Z_c) + aq^2 - iq^{2l+1}]^{-1}. \quad (2.11)$$

Since the bound state corresponds to the pole, this leads to the following relations for the energy levels near $Z = Z_c$:

$$2E = -d^2(Z - Z_c)^2 + O[(Z - Z_c)^3] \quad \text{for } l = 0, \quad (2.12)$$

$$2E = -(d/a)(Z - Z_c) + (i/a)[-(d/a)(Z - Z_c)]^{3/2} + O[(Z - Z_c)^2] \quad \text{for } l = 1, \quad (2.13)$$

$$2E = -(d/a)(Z - Z_c) + O[(Z - Z_c)^2] \quad \text{for } l \geq 2. \quad (2.14)$$

It may be noted that for attractive potentials, $d < 0$ and $a < 0$. Furthermore, for $Z > Z_c$, the bound state corresponds to a positive imaginary value for q so that the second term in (2.13) is also negative. Equations (2.12)–(2.14) are our basic relations governing the behaviour of the energy levels near $Z = Z_c$. It is interesting to note that for the Hulthén potential, one has the exact solution for the s waves

$$2E_n = -n^{-2}(Z - n^2/2)^2 \quad (2.15)$$

in conformity with (2.12).

The parameters which determine the behaviour of the energy levels near Z_c are:

- (1) the critical coupling strength Z_c ,
- (2) the residue of the pole, $1/d$,
- (3) the derivative $\partial E / \partial Z$ which is equal to $-d/2a$ for $l \neq 0$.

These parameters for low-lying states are closely related to the perturbation series for the T_l matrix for small q^2 .

2.4. Perturbation series for T_l

The partial-wave projection of the T matrix may be written as

$$T_l(q) = -(2\pi e^{i\delta_l} \sin \delta_l) / q = \int_0^\infty F(q, r) dr \quad (2.16)$$

where

$$F(q, r) = u(q, r) + u(q, r) \int G(q, r, r') F(q, r') dr' \tag{2.17}$$

with

$$u(q, r) = 4\pi Z V(r) j_l^2(qr) r^2, \tag{2.18}$$

$$G(q, r, r') = (q/2\pi) [n_l(qr_>)/j_l(qr_>) - i] \tag{2.19}$$

where j_l and n_l are spherical Bessel functions of the first and second kind. For small q^2 , we expand the various terms in powers of q^2 , and retain the first two terms. Defining

$$D(q, r) = \{[(2l+1)!!]^2/4\pi q^{2l}\} F(q, r) = A(r) + q^2 B(r) + O(q^4), \tag{2.20}$$

one obtains

$$A(r) = ZV(r)r^{2l+2} - \frac{2Z}{(2l+1)} V(r)r^{2l+2} \int_0^\infty \frac{1}{r'^{2l+1}} A(r') dr', \tag{2.21}$$

$$B(r) = -\frac{Z}{(2l+3)} V(r)r^{2l+4} - \frac{2Z}{(2l+1)(2l+3)} V(r)r^{2l+2} \times \int_0^\infty \frac{1}{r'^{2l+1}} \left[\left(\frac{2l+1}{2l-1} r'^2 - r^2 \right) A(r') + (2l+3)B(r') \right] dr'.$$

These equations are very convenient for iteration and lead to the perturbation series for $T_l(q)$ for small q :

$$t_l(q) = \sum_{i=1}^\infty Z^i (a_i + b_i q^2) + O(q^4) \tag{2.22}$$

where

$$t_l(q) = -[(2l+1)!!]^2 (e^{i\delta_l} \sin \delta_l) / 2q^{2l+1}, \tag{2.23}$$

$$a_i = \int_0^\infty A_i(r) dr, \tag{2.24}$$

$$b_i = \int_0^\infty B_i(r) dr, \tag{2.25}$$

$$A(r) = \sum_{i=1}^\infty Z^i A_i(r), \tag{2.26}$$

$$B(r) = \sum_{i=1}^\infty Z^i B_i(r). \tag{2.27}$$

It is known that the high-order coefficients of a power series are dominated by the nearest singularity. Assuming that the nearest singularity corresponds to the pole in (2.11), we get on expanding (2.11) in powers of Z and using (2.22),

$$a_i \xrightarrow{i \rightarrow \infty} (2dZ_c^{i+1})^{-1} \quad \text{for } l=0 \tag{2.28}$$

$$a_i + b_i q^2 \xrightarrow{i \rightarrow \infty} [(2l+1)!!]^2 / [Z_c - (a/d)q^2]^{i+1} \quad \text{for } l \neq 0. \tag{2.29}$$

In particular, taking the ratio of two successive terms, one obtains

$$a_i/a_{i+1} \xrightarrow{i \rightarrow \infty} Z_c \quad \text{for all } l, \quad (2.30)$$

$$Z_c(b_{i+1}/a_{i+1} - b_i/a_i) \xrightarrow{i \rightarrow \infty} a/d \quad \text{for } l \neq 0. \quad (2.31)$$

These two relations together allow us to determine two of the parameters which determine the behaviour of the lowest energy level for a given l , near $Z = Z_c$. In principle, one could subtract the pole corresponding to (2.11) from the series in (2.22) and repeat the procedure (Patil 1981) for the next level. However, this requires very accurate values for the coefficients a_i and b_i , and we will use relations (2.30) and (2.31) only for the lowest-lying levels. For levels with large quantum numbers, it is convenient to use wKB relations to deduce the parameters.

2.5. wKB relation for Z_c

Within the framework of wKB approximation, it has been shown (Trubnikov and Yavlinskii 1965) that for the screened Coulomb potential, one has the relation

$$Z_c \rightarrow \frac{1}{4} \pi n^2 \quad \text{for } n \rightarrow \infty. \quad (2.32)$$

This relation has been generalised by Chadan (1968) using the Jost function description, to the form

$$Z_c \rightarrow \pi^2 n^2 / 2 \left[\int_0^\infty (-V(r))^{1/2} dr \right]^2 \quad \text{for } n \rightarrow \infty. \quad (2.33)$$

It is worthwhile rederiving this relation using the wKB approach since it provides us with an insight into its domain of validity. We start with the first-order wKB relation

$$\int_{r_1}^{r_2} p dr = \pi(n_r + \frac{1}{2}) \quad (2.34)$$

where

$$p = [2(E - ZV) - (l + \frac{1}{2})^2/r^2]^{1/2}, \quad (2.35)$$

r_1, r_2 are turning points and n_r is the radial quantum number. For $Z = Z_c$ one has $E = 0$. Taking the derivative of the two sides of (2.34) with respect to Z_c , we get

$$\pi \frac{\partial n_r}{\partial Z_c} = - \frac{1}{(2Z_c)^{1/2}} \int_{r_1}^{r_2} \frac{V(r) dr}{[-V(r) - (l + \frac{1}{2})^2/2Z_c r^2]^{1/2}}. \quad (2.36)$$

For $Z_c \gg (l + \frac{1}{2})^2$, and for the short-range potentials, this relation leads to

$$\pi \partial n_r / \partial Z_c = (2Z_c)^{-1/2} \int_0^\infty [-V(r)]^{1/2} dr. \quad (2.37)$$

On integration with respect to Z_c , and noting that for fixed l , $n_r \rightarrow n$ for $n_r \rightarrow \infty$, one gets (2.33). This derivation is useful since it also points out that (2.33) may be used for finite Z_c , provided $Z_c \gg (l + \frac{1}{2})^2$. Therefore it is suggestive that we use for extension to finite n

$$Z_c = (c_0 n + c_1 + c_2/n)^2 \quad (2.38)$$

where

$$c_0 = \pi/2^{1/2} \int_0^\infty (-V(r))^{1/2} dr, \tag{2.39}$$

$$c_1 = \delta_0 + \delta_1 l, \tag{2.40}$$

$$c_2 = \alpha_0 + \alpha_1 l + \alpha_2 l^2. \tag{2.41}$$

Higher powers of l in c_1 and c_2 than those involved would invalidate (2.37) even for $Z_c \gg (l + \frac{1}{2})^2$.

Our procedure to determine Z_c will be to use (2.38) which is essentially an expansion in inverse powers of n , and determine the parameters $\delta_0, \delta_1, \alpha_0, \alpha_1, \alpha_2$ so as to give the correct values of Z_c for the low-lying states as determined by (2.30) or the Schey-Schwartz (1965) approach. In practice, the expression in (2.38) is found to give a fairly accurate representation of Z_c .

2.6. WKB expression for $\partial E/\partial Z$

For obtaining $\partial E/\partial Z$, we start with the Hellmann-Feynman theorem:

$$\partial E/\partial Z = \langle \psi | V(r) | \psi \rangle / \langle \psi | \psi \rangle. \tag{2.42}$$

We evaluate this expression at $Z = Z_c$, using WKB wavefunctions:

$$\chi(r) = p^{-1/2} \sin \left(\int_{r_1}^r p(r') dr' + \frac{1}{4}\pi \right) \tag{2.43}$$

where $\chi(r) = r\psi(r)$, and

$$p = [-2Z_c V(r) - (l + \frac{1}{2})^2/r^2]^{1/2}. \tag{2.44}$$

However, since $\psi(r) \rightarrow r^{-l-1}$ for $r \rightarrow \infty$, the denominator in (2.42) diverges for $l \leq \frac{1}{2}$. Therefore the contribution to the denominator from the region $r > r_2$ is quite important for l near $\frac{1}{2}$, especially for $l = 1$. The WKB wavefunction for $r > r_2$ is

$$\chi = \frac{1}{2p^{1/2}} \exp \left[- \int_{r_2}^r \left(\frac{(l + \frac{1}{2})^2}{r'^2} + 2Z_c V(r') \right)^{1/2} dr' \right]. \tag{2.45}$$

We substitute these wavefunctions in (2.42), replace the square of the sine function by its average value, and retain only the leading contribution from the region $r > r_2$ to obtain

$$\left. \frac{\partial E}{\partial Z} \right|_{Z=Z_c} = \frac{-(2Z_c)^{-1/2} \int_{r_1}^{r_2} [-V(r)]^{1/2} dr}{\int_{r_1}^{r_2} dr/p(r) + r_2^2/(2l+1)(2l-1)} \quad \text{for } l \geq 1, \tag{2.46}$$

where the numerator has been evaluated by assuming $Z_c \gg (l + \frac{1}{2})^2$. Since this relation is obtained by assuming that the wavefunction has a large number of oscillations, it is valid for large n_r . We may regard it as the leading term in the expansion in inverse powers of $\pi(n_r + \frac{1}{2})$ which is a measure of the largeness of the variable of the sine function (see (2.34)). For using the expression in (2.46) for smaller n_r , we introduce

a multiplicative factor $[1 + \Delta / (n_r + \frac{1}{2})]$ and determine Δ so as to give the correct value of $\partial E / \partial Z$ as determined from (2.31) for $n_r = 0$ (recollect that $\partial E / \partial Z = -d / 2a$ at $Z = Z_c$). Finally we get

$$\frac{d}{a} = \frac{(2 / Z_c)^{1/2} \int_{r_1}^{r_2} [-V(r)]^{1/2} dr}{\int_{r_1}^{r_2} dr / p(r) + r_2^2 / (2l + 1)(2l - 1)} \left(1 + \frac{\Delta}{n_r + \frac{1}{2}} \right) \quad \text{for } l \geq 1, \tag{2.47}$$

where Δ is to be chosen so as to yield the value of d/a obtained from (2.31) for $n_r = 0$ (say for $n = 2, l = 1$).

2.7. Sum rules for $1/d$

It is found that as Z increases, the scattering length goes through a series of poles at the critical values Z_c . We may generalise the behaviour of the scattering length to higher partial waves by defining

$$x_l = \lim_{q \rightarrow 0} [-(e^{i\delta_l} \sin \delta_l) / q^{2l+1}] \tag{2.48}$$

which according to (2.11), has the behaviour

$$x_l \approx (-1/d) / (Z - Z_c), \quad Z \approx Z_c. \tag{2.49}$$

We now consider the possibility that x_l may be represented by a sum of such poles. This idea has been found to be quite useful (Patil 1981) for $l = 0$. Designating the successive critical strengths for a given l by $Z_n(l)$ and the corresponding residues by $R_n(l)$ we get

$$x_l = Z \sum_{n>l} R_n(l) / Z_n(l)(Z - Z_n(l)) \tag{2.50}$$

where we have introduced a factor of $Z / Z_n(l)$ which does not alter the residue, so as to ensure that x_l vanishes at $Z = 0$. for the residue we use the form

$$R_n = Z_n(f_0 + f_1/n + f_2/n^2 + \dots). \tag{2.51}$$

Here we have suppressed the dependence of R_n and Z_n on l . Expanding x_l in powers of Z and using the series expansion in (2.22) one gets a set of sum rules:

$$a_i = \frac{[(2l+1)!!]^2}{2} \left(-f_0 \sum_n \frac{1}{Z_n^i} - f_1 \sum_n \frac{1}{nZ_n^i} - f_2 \sum_n \frac{1}{n^2Z_n^i} + \dots \right), \quad i = 1, 2, \dots, \tag{2.52}$$

where we use Z_n given in (2.38), and the summation is over $n > l$. It is usually quite satisfactory to retain only the first two or three terms in R_n and determine the parameters f_0, f_1, \dots from the relations in (2.52). This will allow us to obtain R_n and hence the parameters $d_n = -1/R_n$. Actually we will be using sum rules of the type in (2.52) only for s and p waves. In particular, the determination of R_n for the s wave will give us a very useful representation for the scattering length:

$$x_0 = Z \sum_{n=1}^{\infty} \frac{R_n(0)}{Z_n(0)(Z - Z_n(0))}. \tag{2.53}$$

One is now in a position to deduce all the parameters which determine the behaviour of the energy levels near $Z = Z_c$: the critical coupling strengths are determined from (2.38), $\partial E/\partial Z$ from (2.47), the residue $R_n = -1/d_n$ from (2.51) and the sum rules in (2.52).

2.8. General expression for $E_n(l)$

We supplement the information about the small- ϵ behaviour in terms of the strong-coupling expansion with that near the critical coupling strength. One can now try a simple interpolation between these two regions. Since the behaviour near $Z = Z_c$ is different for different partial waves, their interpolation also will be different.

For the s wave, we use

$$-\frac{2E_n}{Z^2} = (1 - Z_n\epsilon)^2 c_6 + \frac{c_2(1 - Z_n\epsilon)^3}{1 + c_3\epsilon + c_4\epsilon^2 + c_5\epsilon^3} \quad \text{for } l = 0 \tag{2.54}$$

where $c_6 = d_n^2$, and determine the parameters c_2, c_3, c_4 and c_5 so that this expression agrees with the small- ϵ expansion in (2.10) up to ϵ^3 terms. The expressions for the parameters in terms of the expansion coefficients in (2.9) are

$$\begin{aligned} c_6 &= d_n^2, & c_2 &= 1/n^2 - c_6, & c_3 &= -3Z_n - (2/c_2)(c_6 Z_n + B_1), \\ c_4 &= c_3^2 + 3c_3 Z_n + 3Z_n^2 + (1/c_2)(Z_n^2 c_6 - 3n^2 B_2), \\ c_5 &= 2c_3 c_4 - c_3^3 + 3Z_n(c_4 - c_3^2) - 3Z_n^2 c_3 - Z_n^3 - n^2(1 + 5n^2)B_3/c_2, \end{aligned} \tag{2.55}$$

where $d_n = -1/R_n$ with R_n given in (2.51).

For the higher partial waves we use an interpolation (the dependence of Z_n, d_n and a_n on l will not be indicated explicitly)

$$-\frac{2E_n}{Z^2} = c_6(1 - Z_n\epsilon) + c_7(1 - Z_n\epsilon)^{3/2} + \frac{c_2(1 - Z_n\epsilon)^2}{1 + c_3\epsilon + c_4\epsilon^2 + c_5\epsilon^3} \quad \text{for } l \neq 0 \tag{2.56}$$

where $c_6 = d_n/a_n Z_n, c_7 = -(d_n/a_n)^{3/2}(1/a_n Z_n^{1/2})$ for $l = 1$ but $c_7 = 0$ for $l > 1$. As before, we determine the parameters c_2, c_3, c_4 and c_5 so that the expression agrees with the small- ϵ expansion in (2.10) up to ϵ^3 terms. The expressions for the parameters in terms of the expansion coefficients in (2.9) are

$$\begin{aligned} c_6 &= d_n/a_n Z_n, \\ c_7 &= -c_6^{3/2}(Z_n/a_n) \quad \text{for } l = 1, & c_7 &= 0 \quad \text{for } l > 1, \\ c_2 &= 1/n^2 - c_6 - c_7, & c_3 &= -2Z_n + (1/c_2)(-2B_1 - c_6 Z_n - \frac{3}{2}c_7 Z_n), \\ c_4 &= c_3^2 + 2Z_n c_3 + Z_n^2 + (1/c_2)[\frac{3}{8}c_7 Z_n^2 - B_2(3n^2 - x)], \\ c_5 &= 2c_3 c_4 - c_3^3 + 2Z_n c_4 - 2Z_n c_3^2 - Z_n^2 c_3 + (1/c_2)[\frac{1}{16}Z_n^3 c_7 - B_3 n^2(1 + 5n^2 - 3x)], \end{aligned} \tag{2.57}$$

where d_n/a_n is given by (2.47) and $d_n = -1/R_n$ is obtained from (2.51).

Thus (2.54) and (2.56) provide us with closed expressions which allow us to calculate the energy levels of any state for any short-range potential with an expansion of the form given in (2.9). In the following we apply these results to the screened Coulomb and Hulthén potentials.

3. The screened Coulomb potential

For the screened Coulomb potential given in (2.3), one has the expansion coefficients $B_1 = -1, B_2 = \frac{1}{2}, B_3 = -\frac{1}{6}$ etc so that

$$-2E/Z^2 = 1/n^2 - 2\epsilon + \frac{1}{2}(3n^2 - x)\epsilon^2 - \frac{1}{6}n^2(1 + 5n^2 - 3x)\epsilon^3 + \dots \tag{3.1}$$

where $x = l(l + 1)$. It is found that the coefficients of the series increase rather rapidly. We first show by using the Bender–Wu (1969, 1973) method that the series is asymptotic.

3.1. Asymptotic series

Consider the solution to (2.6) for small negative ϵ . For large r , the potential tends to large negative values:

$$V(r) = -r^{-1} e^{\epsilon r} \rightarrow -\infty \quad \text{for } r \rightarrow \infty. \tag{3.2}$$

As a result, a bound particle can now escape. The escape probability P is given by (Bender and Wu 1969, 1973)

$$P = 2\text{Im } E_n = 4\pi |R(r)|^2 v_r \tag{3.3}$$

where $R(r)$ is to be evaluated at a large value of r , in particular at r greater than r_t ,

$$r_t = |\epsilon|^{-1} [\ln(1/|\epsilon|) + O(\ln \ln \epsilon)]. \tag{3.4}$$

This is the classically allowed escape region.

We use the wkb approximation (Bender and Wu 1969, 1973) for $R(r)$,

$$R(r) \sim [p(r)]^{-1/2} \exp\left(-\int_{r_0}^r |p(r')| dr'\right), \tag{3.5}$$

for

$$1 \ll r_0 \ll r_t, \quad r_0 < r < r_t, \tag{3.6}$$

where

$$p(r) = [-1/n^2 + (2/r) e^{\epsilon r} - (l + \frac{1}{2})^2/r^2]^{1/2}. \tag{3.7}$$

For $\epsilon \rightarrow 0_-$ and $r \rightarrow r_t$, the leading term in the integral is r_t/n , so that

$$\text{Im } E_n(1, \epsilon) \sim \exp\{-(2/n|\epsilon|)[\ln(1/|\epsilon|) + O(\ln \ln \epsilon)]\} \quad \text{for } \epsilon \rightarrow 0_-. \tag{3.8}$$

Writing once-subtracted dispersion relations (Bender and Wu 1969, 1973) for $E_n(1, \epsilon)$, but not including possible contributions from singularities away from the origin, we get

$$E_n(1, \epsilon) = -\frac{1}{2n^2} + \frac{\epsilon}{\pi} \int_{-\infty}^0 \frac{\text{Im } E_n(1, \epsilon')}{\epsilon'(\epsilon' - \epsilon)} d\epsilon'. \tag{3.9}$$

One can expand the second term in powers of ϵ and obtain

$$E_n(1, \epsilon) = \sum_{i=0}^N g_i \epsilon^i + \frac{\epsilon^{N+1}}{\pi} \int_{-\infty}^0 \frac{\text{Im } E_n(1, \epsilon')}{\epsilon'^{N+1}(\epsilon' - \epsilon)} d\epsilon', \tag{3.10}$$

where

$$g_i \rightarrow \frac{1}{\pi} \int_{-\infty}^0 \frac{\text{Im } E_n(1, \epsilon')}{\epsilon'^{i+1}} d\epsilon' \quad \text{for } i \rightarrow \infty. \tag{3.11}$$

Substituting for $\text{Im } E_n(1, \epsilon)$ from (3.8), we can deduce the leading behaviour for g_i :

$$\dot{g}_i \rightarrow -\frac{(i-1)!}{\pi} \left(\frac{-n/2}{\ln[(i+1)/4n] + O(\ln \ln i)} \right)^i \quad \text{for } i \rightarrow \infty. \tag{3.12}$$

Clearly, the series is asymptotic. In particular we note that

$$a_{i+1}/a_i \rightarrow -(in/2)/[\ln i + O(\ln \ln i)] \quad \text{for } i \rightarrow \infty. \tag{3.13}$$

For $n = 1, i = 8$, this has a value of about 1.92 whereas the correct value (Iafate and Mendelsohn 1969) is about 3.28. This means that for $i = 8$, one cannot as yet neglect $\ln(\ln i)$ terms.

3.2. Perturbation series

The perturbation series in (2.22) for small q^2 determines the relevant parameters for the energy levels near $Z = Z_c$. The coefficients in (2.22) are determined by iterating (2.21) and using (2.24)–(2.27). The coefficients for the first few partial waves are given in table 1. From (2.30) and (2.31), it then follows that

$$Z_1(l = 0) = 0.8386, \tag{3.14}$$

$$Z_2(l = 1) = 4.524, \tag{3.15}$$

$$Z_3(l = 2) = 10.893, \tag{3.16}$$

$$a/d = 3.888 \quad \text{for } l = 1, n = 2. \tag{3.17}$$

The critical strengths are in reasonable agreement (within 0.5% with the accurate numerical values (Rogers *et al* 1970, Greene and Aldrich 1976). The predictions for other partial waves are accurate to about the same extent. In principle, one could now subtract the series corresponding to these poles from the perturbation series and look for the critical strengths for higher levels. But the results of such a sequential analysis (Patil 1981) are less accurate.

Table 1. The expansion coefficients $a_i(l)$ and $b_i(l)$ of t_i in (2.22) for the screened Coulomb potential.

i	$a_i(0)$	$a_i(1)$	$b_i(1)$	$a_i(2)$
1	-1.000	-6.000	2.400 (1)	-1.200 (2)
2	-1.000	-5.000 (-1)	-1.700	-1.500
3	-1.151	-7.945 (-2)	-4.138 (-1)	-6.233 (-2)
4	-1.364	-1.530 (-2)	-9.678 (-2)	-3.878 (-3)
5	-1.623	-3.177 (-3)	-2.311 (-2)	-2.895 (-4)
6	-1.934	-6.820 (-4)	-5.571 (-3)	-2.374 (-5)
7	-2.306	-1.487 (-4)	-1.345 (-3)	-2.051 (-6)
8	-2.750	-3.269 (-5)	-3.238 (-4)	-1.827 (-7)
9	-3.279	-7.212 (-6)	-7.764 (-5)	-1.659 (-8)
10	-3.910	-1.594 (-6)	-1.853 (-5)	-1.523 (-9)

3.3. Critical strengths

We now use (2.38) to obtain a general expression for $Z_n(l)$. The integral in (2.39) gives for the screened Coulomb potential,

$$c_0 = (\pi/4)^{1/2}. \quad (3.18)$$

The coefficients δ_1 , δ_2 , α_0 , α_1 and α_2 are determined so as to give the correct critical strengths for the first five low-lying states (e.g. three of them are given in (3.14)–(3.16), slightly more accurate values are given by Schey and Schwartz (1965) or Rogers *et al* (1970)). This gives us

$$Z_n(l) = [(\pi/4)^{1/2}n + 0.015\,4014 + 0.227\,31l \\ + (0.014\,8326 + 0.162\,86l + 0.053\,914l^2)n^{-1}]^2 \quad (3.19)$$

which predicts the critical strengths of all the states with $n \leq 9$ to an accuracy of about 1%.

It is interesting to compare our expression for the critical strengths with that of Green (1982),

$$Z_n(l) = [S_l^{-1}n + Z_l^{1/2} - S_l^{-1}(l+1)]^2, \quad (3.20)$$

$S_l = 1.1335(1 + \gamma_l + \delta_l^2)$, $Z_l = 0.8399(1 + \alpha l + \beta l^2)$. Green's expression is a good overall fit to the critical strengths of the states with $n \leq 9$, and its values are within 0.4% of the exact values (Rogers *et al* 1970). On the other hand, our expression is a fit to the low-lying states and an extension to the higher states based on the expansion in (2.38). As such, the accuracies of the two expressions in terms of average errors are comparable. It may be noted that in Green's expression, $Z_n(l)^{1/2}$ is strictly linear in n whereas our expression has an additional $1/n$ term. It should also be observed the coefficient of n in Green's expression has a slight l dependence (γ and δ are quite small). For $l=0$ it has the value $1/S_0 = 0.8822$ which is quite close to the exact value of $(\pi/4)^{1/2} \approx 0.8862$ in the limit of large n .

3.4. Expression for $\partial E/\partial Z$

The integrals in (2.47) can be evaluated in the limit of large Z . The turning points satisfy the condition

$$Z_c e^{-r}/r = (l + \frac{1}{2})^2/2r^2 \quad (3.21)$$

which for large Z_c gives

$$r_1 \approx (l + \frac{1}{2})^2/2Z_c, \quad (3.22)$$

$$r_2 \approx \ln[2Z_c/(l + \frac{1}{2})^2] + O(\ln \ln Z_c). \quad (3.23)$$

For large Z_c , the integral in the numerator tends to $(2\pi)^{1/2}$. For the integral in the denominator, the main contributions come from the regions near the turning points. We divide the region of integration into two parts, one from r_1 to r_0 ,

$$r_0 = 1 - (2Z_c)^{-1}(l + \frac{1}{2})^2, \quad (3.24)$$

and the other from r_0 to r_2 . Retaining the leading terms for large Z_c in the integrations, one obtains

$$\frac{d}{a} = 2(\pi/Z_c)^{1/2} [1 + \Delta/(n_r + \frac{1}{2})] \times \left(\frac{1}{4}\pi(2/Z_c)^{1/2} + \frac{6.3166}{(2l+1)}(r_2 - r_0) + \frac{r_2^2}{(2l+1)(2l-1)} \right)^{-1} \quad \text{for } l \geq 1. \tag{3.25}$$

The numerical factor 6.3166 in the denominator comes from the summation of the series

$$\sum_{n=0}^{\infty} \frac{(2n+1)!!}{2^{n-2}n!(2n+1)^2} \approx 6.3166 \tag{3.26}$$

which results from the integration. Though these integrations are evaluated for large Z_c , they are found in general to be quite close (within a few percent) to the values which follow from numerical integrations.

Finally, the value of Δ is determined by requiring that $d/a \approx 0.26$ for $l = 1, n = 2$, which follows from (3.17). Thus the parameters for d/a in (3.25) are

$$\Delta \approx -0.1033, \tag{3.27}$$

$$r_0 = 1 - (2Z_n)^{-1}(l + \frac{1}{2})^2, \tag{3.28}$$

and r_2 is determined from

$$r_2 = \ln[2Z_n/(l + \frac{1}{2})^2] + \ln r_2 \tag{3.29}$$

by iteration. It may again be recollected that $\partial E/\partial Z$ at $Z = Z_c$ is equal to $-\frac{1}{2}(d/a)$ for $l \neq 0$.

3.5. Sum rules for residues

We need to know the residues $R_n \approx -1/d_n$ for $l = 0$ and $l = 1$ states (see (2.55) and (2.57)). For this we use the sum rules in (2.52).

For $l = 0$, we retain only the f_1 and f_2 terms. Using a_i in table 1, and the values of Z_n in (3.19) for $l = 0$, the sum rules for $i = 1$ and 2 give

$$-2 = -1.442\ 89f_1 - 1.293\ 13f_2, \quad -2 = -1.474\ 68f_1 - 1.444\ 35f_2. \tag{3.30}$$

The solutions yield for the residues

$$R_n(0) = Z_n(0)(1.707\ 84/n - 0.358\ 99/n^2) \tag{3.31}$$

in terms of which one can get $d_n = -1/R_n$. The justification for not considering f_0, f_3 and higher terms, is that the above residue satisfies the higher-order sum rules quite accurately. For example, the sum rule in (2.52) for $i = 3$ reads

$$-2.302 = -1.703\ 78f_1 - 1.695\ 59f_2. \tag{3.32}$$

The above values of f_1 and f_2 give a value of -2.301 for the right-hand side.

The determination of $R_n(0)$ and $Z_n(0)$ provides a closed expression for the scattering length in (2.53):

$$x_0 = \sum_{n=1}^{\infty} \left(\frac{1.70784}{n} - \frac{0.35899}{n^2} \right) \left(\frac{Z}{Z - Z_n(0)} \right), \tag{3.33}$$

$$Z_n(0) = [(\pi/4)^{1/2}n + 0.0154014 + (0.0148326)(1/n)]^2.$$

The prediction for the scattering length for several values of Z are given in table 2, and are seen to be in good agreement with the numerical solutions (Patil 1981).

Table 2. Predictions for the scattering length for the screened Coulomb potential, based on (2.53), compared with the numerical solutions of the Schrödinger equation.

Z	Predicted scattering length x_0	Numerical values of x_0
0.5	-2.207	-2.207
1.5	2.125	2.128
2.5	-1.13	-1.11
3.5	10.57	10.47
4.5	2.97	2.95
5.5	1.04	1.04
6.5	-2.91	-2.91
7.5	13.8	13.7
9.5	2.87	2.84
12.0	-4.36	-4.38
15.0	4.21	4.19
20.0	30.3	29.7

For $l=1$, the f_0 and f_1 terms are adequate. Using a_i in table 1 for $l=1$, and the values of $Z_n(1)$ in (3.19) for $l=1$, one gets for the $i=1$ and 2 sum rules in (2.52),

$$-\frac{4}{3} = -0.6644f_0 - 0.19298f_1, \quad -\frac{1}{5} = -0.07050f_0 - 0.03039f_1. \tag{3.34}$$

The residues which follow from the solutions to these equations are

$$R_n(1) = Z_n(1)(2.8978 - 3.0644/n). \tag{3.35}$$

These solutions for f_0 and f_1 satisfy the $i=3$ sum rule to within a few percent accuracy.

3.6. Expressions for $E_n(l)$

The interpolating expressions for the energy levels $E_n(l)$ which incorporate the behaviour for small ϵ and for Z near the critical strength are given by (2.54)–(2.57), with $B_1 = -1$, $B_2 = \frac{1}{2}$ and $B_3 = -1/6$. For the s wave, one uses (2.54) and (2.55), and

$$1/d_n = -Z_n(0)(1.70784/n - 0.35899/n^2). \tag{3.36}$$

For higher partial waves, we use (2.56) and (2.57), with

$$1/d_n = -Z_n(1)(2.8978 - 3.0684/n) \quad \text{for } l=1 \tag{3.37}$$

and d_n/a_n given by (3.24). The critical strengths $Z_n(l)$ are taken from (3.19).

The values of the energy levels calculated are in quite good agreement with the numerical values of Rogers *et al* (1970) (some of them are given in tables 3, 4 and 5). Following Green (1982), we state the accuracy of our results in terms of the

Table 3. Predicted values of $-2E/Z^2$ for some states with $n \leq 4$, along with the numerical values of Rogers *et al* (1970) given in brackets.

State \ Z	500	100	50	30	20	10	5	1
1s	0.9960 (0.9960)	0.9801 (0.9801)	0.9606 (0.9606)	0.9350 (0.9350)	0.9036 (0.9036)	0.8141 (0.8141)	0.6535 (0.6536)	0.020 48 (0.020 57)
2p	0.2460 (0.2460)	0.2305 (0.2305)	0.2119 (0.2119)	0.1886 (0.1886)	0.1615 (0.1615)	0.093 23 (0.093 07)	0.008 49 (0.008 20)	
3s	0.1072 (0.1072)	0.092 40 (0.092 40)	0.076 03 (0.076 04)	0.057 41 (0.057 44)	0.038 63 (0.038 70)	0.006 35 (0.006 42)		
3d	0.1072 (0.1072)	0.092 12 (0.092 12)	0.075 01 (0.075 03)	0.054 85 (0.054 94)	0.033 57 (0.033 83)			
4p	0.058 59 (0.058 59)	0.044 62 (0.044 63)	0.030 45 (0.030 47)	0.016 35 (0.016 38)	0.005 20 (0.005 20)			
4f	0.058 57 (0.058 57)	0.044 19 (0.044 20)	0.028 93 (0.028 98)	0.012 83 (0.013 02)				

Table 4. Predicted values of $-2E/Z^2$ for some states with $n = 5, 6, 7$, along with the numerical values of Rogers *et al* (1970) in brackets.

State \ Z	500	300	200	100	70	50	40	30
5s	0.036 15 (0.036 15)	0.033 73 (0.033 73)	0.030 88 (0.030 88)	0.023 32 (0.023 32)	0.017 90 (0.017 92)	0.012 03 (0.012 06)	0.008 02 (0.008 05)	0.003 35 (0.003 37)
5g	0.036 11 (0.036 11)	0.033 63 (0.033 63)	0.030 66 (0.030 66)	0.022 52 (0.022 53)	0.016 42 (0.016 46)	0.009 48 (0.009 57)	0.004 55 (0.004 65)	
6p	0.023 98 (0.023 98)	0.021 66 (0.021 67)	0.018 99 (0.018 99)	0.012 27 (0.012 28)	0.007 884 (0.007 90)	0.003 71 (0.003 73)	0.001 42 (0.001 43)	
6h	0.023 93 (0.023 93)	0.021 53 (0.021 53)	0.018 69 (0.018 70)	0.011 26 (0.011 28)	0.006 09 (0.006 14)	0.000 98 (0.001 01)		
7s	0.016 69 (0.016 68)	0.014 49 (0.014 49)	0.012 04 (0.012 04)	0.006 33 (0.006 34)	0.003 10 (0.003 11)	0.000 71 (0.000 71)	0.000 01 (0.000 01)	
7g	0.016 65 (0.016 65)	0.014 40 (0.014 40)	0.011 84 (0.011 84)	0.005 70 (0.005 73)	0.002 11 (0.002 15)			

Table 5. Predicted values of $-2E/Z^2$ for some states with $n = 8, 9$, along with the numerical values of Rogers *et al* (1970) in brackets.

State \ Z	500	400	300	200	100	70
8p	0.011 98 (0.011 98)	0.011 17 (0.011 17)	0.009 91 (0.009 91)	0.007 67 (0.007 67)	0.002 92 (0.002 94)	0.000 77 (0.000 78)
8h	0.011 93 (0.011 93)	0.011 10 (0.011 10)	0.009 78 (0.009 78)	0.007 41 (0.007 42)	0.002 18 (0.002 21)	
9s	0.008 79 (0.008 79)	0.008 03 (0.008 03)	0.006 86 (0.006 87)	0.004 87 (0.004 88)	0.001 17 (0.001 17)	0.000 06 (0.000 06)
9g	0.008 76 (0.008 76)	0.007 98 (0.007 98)	0.006 78 (0.006 78)	0.004 70 (0.004 71)	0.000 76 (0.000 78)	
9l	0.008 67 (0.008 67)	0.007 85 (0.007 85)	0.006 55 (0.006 55)	0.004 26 (0.004 26)	0.002 33 (0.002 33)	

expression

$$Y_{nl} = Z[1 + (2/Z^2)n^2 E_n(l)]. \quad (3.38)$$

The average absolute percentage departure of our values for Y_{nl} from the exact values given by Rogers *et al* (1970) is about 0.06%, with the largest deviation being about 0.38%. Of course, for Z near the critical values $Z_n(l)$, $E_n(l)$ is close to zero and small deviations in Y_{nl} are reflected as relatively large percentage errors in $E_n(l)$.

We note that the simple behaviour of Y_{nl} for large Z noted by Green (1982) is related to the strong coupling expansion in (3.1). Using the first two terms in (3.1) one gets for Y_{nl}

$$Y_{nl} \xrightarrow{Z \rightarrow \infty} 2n^2. \quad (3.39)$$

It is also interesting to observe that Green's expression (1982) for the energy of $l=0$ states has only a first-order zero at the critical strength $Z_n(0)$, whereas our general result in (2.12) indicates a second-order zero. However, Green's expression has another factor $Z - 1.9875(n + 0.003951)^2 + 1.2464n^2$ which has a zero fairly close to the critical strength.

4. Hulthén potential

For the Hulthén potential given in (2.4), the expansion coefficients are

$$B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{12}, \quad B_3 = 0. \quad (4.1)$$

In this case one has closed solutions for the s waves, with the energies given in (2.15). We will therefore concentrate on the higher partial waves, i.e. waves with $l \geq 1$.

4.1. Perturbation series

Iterating (2.21), we can get the coefficients in (2.22). They are given in table 6, for the $l=1$ and 2 partial waves. From these we obtain by using (2.30) and (2.31),

$$Z_2(l=1) \approx 2.65, \quad (4.2)$$

$$Z_3(l=2) \approx 6.33, \quad (4.3)$$

$$a/d \approx 5.17 \quad \text{for } l=1, n=2. \quad (4.4)$$

For the $n=3, l=2$ case, the ratio of the coefficients a_i is still decreasing slowly and the value of $Z_3(l=2)$ given in (4.3) is the ratio extrapolated to larger i values.

4.2. Critical strength

For extrapolating the critical strengths to other values of n and l , we use (2.38). The integral in (2.39) is carried out to give

$$c_0 = 1/2^{1/2}. \quad (4.5)$$

It is interesting to notice that this is in conformity with (2.15) for $l=0$. Since the s -wave critical strengths are given by

$$Z_n(0) = n^2/2, \quad (4.6)$$

Table 6. Expansion coefficients $a_i(1)$, $b_i(1)$ and $a_i(2)$ of t_i in (2.22) for the Hulthén potential.

i	$a_i(1)$	$b_i(1)$	$a_i(2)$
1	-2.4886 (1)	1.4520 (2)	-7.2598 (2)
2	-4.1737	-2.3368 (1)	-2.1730 (1)
3	-1.2063	-1.1198 (1)	-1.8031
4	-4.0869 (-1)	-4.8170	-2.0906 (-1)
5	-1.4714 (-1)	-2.0532	-2.8076 (-2)
6	-5.4384 (-2)	-8.6999 (-1)	-4.0592 (-3)
7	-2.0341 (-2)	-3.6590 (-1)	-6.1078 (-4)
8	-7.6514 (-3)	-1.5268 (-1)	-9.4020 (-5)
9	-2.8862 (-3)	-6.3235 (-2)	-1.4667 (-5)
10	-1.0901 (-3)	-2.6009 (-2)	-2.3064 (-6)

one has $\delta_0 = \alpha_0 = 0$ in (2.40) and (2.41). For simplicity we neglect the α_2 term in (2.41). The fits to the Z_c values in (4.2) and (4.3) then give

$$Z_n(l) = [2^{-1/2}n + 0.1645l + 0.0983l/n]^2. \tag{4.7}$$

4.3. Expression for d/a

For evaluating the integrals in (2.47), we note that the turning points satisfy the condition

$$e^{-r}/(1 - e^{-r}) = (l + \frac{1}{2})^2 / 2Z_c r^2. \tag{4.8}$$

An analysis similar to that carried out for the screened Coulomb potential leads to

$$\frac{d_n}{a_n} = \{ \pi(2/Z_n)^{1/2} [1 + \Delta/(n_r + 1/2)] \} \times \left\{ \pi(1/Z_n)^{1/2} + \frac{6.3166}{(2l+1)}(r_2 - r_0) + \frac{r_2^2}{(2l+1)(2l-1)} \right\}^{-1} \quad \text{for } l \geq 1, \tag{4.9}$$

where

$$r_0 = 2 - (1/2Z_n)(l + \frac{1}{2})^2$$

and r_2 is determined by iterating the equation

$$r_2 = \ln[2Z_n/(l + \frac{1}{2})^2] + \ln[r_2^2/(1 - e^{-r_2})]. \tag{4.10}$$

The quantity Δ is chosen so as to give $d/a \approx 0.19$ for $l = 1, n = 2$, corresponding to the value given in (4.4) and comes out to be

$$\Delta \approx -0.188. \tag{4.11}$$

4.4 Sum rules for residues

We are interested in the residues for the $l = 1$ states (see (2.57)). For this we use the sum rules in (2.52) with $i = 1$ and 2, and retain only the f_0 and f_1 terms. With the $Z_n(l = 1)$ values given in (4.7), one gets

$$-5.53 = -1.096f_0 - 0.3238f_1, \quad -0.927 = -0.2012f_0 - 0.08772f_1. \quad (4.12)$$

The residues which follow from these equations are

$$R_n(1) = Z_n(1)(5.978 - 3.155/n), \quad (4.13)$$

and $d_n = -1/R_n$. It may again be mentioned that these solutions for f_0 and f_1 satisfy the $i = 3$ sum rule as well, within an accuracy of a few percent.

4.5. Expressions for $E_n(l)$

The energy levels are obtained from (2.56) and (2.57), with $B_1 = -\frac{1}{2}$, $B_2 = \frac{1}{12}$, $B_3 = 0$. One has

$$1/d_n = -Z_n(1)(5.978 - 3.155/n) \quad \text{for } l = 1, \quad (4.14)$$

and d_n/a_n is given by (4.9). The critical strengths $Z_n(l)$ are taken from (4.7).

The predictions for a few low-lying states are given in table 7, and compared with the values calculated by Lai and Lin (1980). The agreement between the two sets of values is generally good, the maximum disagreement being about 6%. One may now use (2.56) to obtain the energy levels of almost any bound state with $l \neq 0$ ($l = 0$ levels being trivially given by (2.15)), of the Hulthén potential.

Table 7. Predicted values of $-2E/Z^2$ for $n \leq 4$ states with $l \neq 0$, along with the results of Lai and Lin (1980) given in brackets.

State \ 1/Z	0.025	0.05	0.075	0.10	0.15	0.20	0.35
2p	0.225 52	0.202 08 (0.202 09)	0.179 70	0.158 36 (0.158 36)	0.118 89	0.083 79 (0.083 77)	0.007 675 (0.007 558)
3p	0.087 417 (0.087 414)	0.066 37 (0.066 33)	0.0480 33	0.032 44 (0.032 11)	0.009 399 (0.008 932)		
3d	0.087 205 (0.087 206)	0.065 49 (0.065 51)	0.045 98	0.028 78 (0.028 97)	0.002 751 (0.002 782)		
4p	0.039 90 (0.039 90)	0.022 15 (0.022 12)	0.009 317 (0.009 244)	0.001 504 (0.001 508)			
4d	0.039 69 (0.039 69)	0.021 36 (0.021 33)	0.007 750 (0.007 668)				
4f	0.039 38 (0.039 38)	0.020 09 (0.020 12)	0.005 114 (0.005 112)				

5. Discussion

It is clear that the structure of the energy levels near the critical strengths is a significant input towards our understanding of the energy levels of the screened Coulomb and Hulthén potentials. The perturbation series for the t -matrix (2.23) and the w_{KB}

analysis of the relevant parameters allow us to make quite accurate predictions not only for all the energy levels, but also for the scattering length.

We conclude by making two observations.

(1) It may be noted that the approach outlined is applicable to a general class of potentials which are essentially functions of only one parameter and which have a strong-coupling expansion for the energy levels. In addition to the energy levels, our knowledge of the d and a parameters allows us to determine the phase shifts for small q^2 from (2.11).

(2) There is some similarity between our analysis and the analysis of the hydrogen atom in a strong magnetic field. In the case of the magnetic field, it is found (Galindo and Pascual 1976, Patil 1982) that incorporating the asymptotic behaviour of the energy levels greatly enlarges the utility of the asymptotic series. In our case, it is the inclusion of the behaviour near the critical strength of the coupling which allows us to give an accurate representation of the energy levels.

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