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Simple wavefunctions for Yukawa- and Hulthén-type potentials

S H Patil

Max-Planck-Institut für Strömungsforschung, Bunsenstrasse 10, D-37073, Göttingen, Germany,
and Department of Physics, Indian Institute of Technology, Bombay 400 076, India

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Abstract

Based on the general properties of the Yukawa and Hulthén potentials, that they have Coulombic behaviour for small r and are exponentially damped for large r , we have deduced the threshold and asymptotic properties of their energy eigenfunctions. We have then developed simple wavefunctions incorporating these properties for the lowest and the first excited states for all l values, which give quite accurate energies for a wide range of the screening parameters and which give a clear, physical insight into their structure. The quality of these wavefunctions is analysed in terms of a virial relation, a threshold relation and a local energy test.

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1. Introduction

The screened Coulomb potential is of importance in the description of many physical systems. It can be used as an approximation to the potential experienced by an electron in an atom where the other electrons screen the nuclear charge. It describes the shielding effects in plasmas where it is called the Debye–Hückel potential. It is also used in the form of Yukawa potential for the description of the nuclear interaction. The Yukawa potential and the Hulthén potential are two simple representations of the screened Coulomb potential. They have Coulombic behaviour for small r but go down exponentially for large r . The Hulthén potential has the special property that it has closed, analytic solutions for s waves, but not for higher l partial waves.

There have been a large number of attempts at deducing the energy levels of the Yukawa and Hulthén potentials. They may be grouped into the following classes.

1. Some attempts are based on approximating [1–6] the given potential by a potential for which one has closed solutions. The corrections to the small differences may be evaluated perturbatively [2, 7].
2. There have been many variational calculations [8–14] using different basis wavefunctions. They have provided quite accurate values for the energy eigenvalues.

3. Several calculations [15–17] are based on the strong coupling or weak damping expansion. They give quite satisfactory energies for large coupling constants. However, the rate of convergence is a serious problem for smaller values of the coupling constant since the series may be asymptotic [18]. It has been indicated [19–21] that the use of Padé approximants greatly aids the convergence of the series.
4. The energy levels have been obtained from some other techniques such as $1/N$ expansion [22], where N is the dimension of the space, from an iterative procedure in the momentum space [23], and from a linear combination of atomic orbitals [24].
5. Then there are numerical calculations [25–27] of the bound state energies. The calculations of Rogers *et al* [26] and of Nunez [27] are of high accuracy.

While the various attempts have provided satisfactory bound state energies, adequate attention has not been given to the structural properties of the potentials and their implications for the energy eigenfunctions. An emphasis and understanding of these properties will provide a deeper appreciation of the physical properties of the wavefunctions and the energies. Here we carefully analyse the structural, local properties of the energy eigenfunctions, based on the general properties of the potential. We also point out the virial relation between the kinetic and potential energies. Based on these properties, we develop simple wavefunctions for the Yukawa and Hulthén potentials, which are relevant to a whole class of screened Coulomb potentials. These wavefunctions also provide fairly accurate values for the energies. The good quality of these wavefunctions based on the local properties is confirmed by the virial relation, and by the local energy test. Apart from providing reliable values for energy eigenvalues, these wavefunctions provide a clear understanding of the physical properties of the system. We will be using atomic units throughout, $m = \hbar = e = 1$.

2. Some general properties of energy eigenfunctions

Here we analyse some general properties of energy eigenfunctions of a class of screened Coulomb potentials. The potentials will be required to have two properties:

1. For small r they tend to a Coulombic form,

$$V(r) \rightarrow -\frac{Z}{r} \quad \text{for } r \rightarrow 0. \quad (2.1)$$

We expect them to have a small- r expansion

$$rV(r) \rightarrow -Z + V_0 r + \dots \quad \text{for } r \rightarrow 0. \quad (2.2)$$

2. They will be exponentially damped in the asymptotic region,

$$V(r) \rightarrow O(e^{-\mu r}) \quad \text{for } r \rightarrow \infty \quad (2.3)$$

apart from a possible power factor.

Both Yukawa and Hulthén potentials are in this class of screened Coulomb potentials.

2.1. Threshold conditions

The radial part of the l partial-wave, energy eigenfunction satisfies the equation

$$-\frac{1}{2} \left[\frac{1}{r} \frac{d^2}{dr^2} r - \frac{l(l+1)}{r^2} \right] R_l(r) + V(r) R_l(r) = E R_l(r). \quad (2.4)$$

Taking out the threshold behaviour, we substitute

$$R_l(r) = r^l [a_0 + a_1 r + a_2 r^2 \dots] \quad (2.5)$$

in equation (2.4) and obtain

$$-\frac{1}{2} \sum i(2l + i + 1) a_i r^{l+i-2} + \left(-\frac{Z}{r} + V_0 + \dots \right) \sum a_i r^{l+i} = E \sum a_i r^{l+i}. \quad (2.6)$$

Taking the coefficients of r^{l-1} and r^l , we obtain

$$a_1 = -\frac{Z}{l+1} a_0 \quad (2.7)$$

$$(2l+3)a_2 = -Za_1 - (E - V_0)a_0. \quad (2.8)$$

The relation in equation (2.7) is of course effectively the Kato condition [28]. Substituting this relation in equation (2.8) we obtain

$$a_2 = \frac{1}{(2l+3)} \left(|E| + V_0 + \frac{Z^2}{l+1} \right) a_0. \quad (2.9)$$

The two relations can be written in the form

$$\frac{f'(0)}{f(0)} = -\frac{Z}{l+1} \quad (2.10)$$

$$\frac{f''(0)}{f(0)} = \frac{2}{(2l+3)} \left(|E| + V_0 + \frac{Z^2}{l+1} \right) \quad (2.11)$$

with

$$f(r) = r^{-l} R_l(r). \quad (2.12)$$

Though the relation in equation (2.11) depends on the energy, it can be used as a test for the quality of the model wavefunction.

2.2. Asymptotic behaviour

For large r , since the potential is exponentially small, the wavefunction has the asymptotic behaviour

$$R_l(r) \rightarrow h_l(i\alpha r) (1 + O(e^{-\mu r})) \quad \text{for } r \rightarrow \infty \quad (2.13)$$

where

$$\alpha = (-2E)^{1/2} \quad (2.14)$$

and $h_l(z)$ are the spherical Hankel functions [29]. The leading term in the asymptotic behaviour is therefore given by

$$R_l(r) \rightarrow \frac{1}{r} e^{-\alpha r}. \quad (2.15)$$

Indeed, the successive power terms can also be deduced from the expression for the spherical Hankel function

$$h_l(z) = -iz^l \left(-\frac{1}{z} \frac{d}{dz} \right)^l \frac{1}{z} e^{iz} \quad (2.16)$$

but for simplicity we will confine our attention mainly to the leading term in equation (2.15).

2.3. Virial relation and the local energy

From the general property of eigenstates of energy

$$\langle \psi | [H, \vec{r} \cdot \vec{p}] | \psi \rangle = 0 \quad (2.17)$$

one has the virial relation

$$\langle \psi | \frac{1}{2} p^2 | \psi \rangle = \frac{1}{2} \langle \psi | \vec{r} \cdot \vec{\nabla} V | \psi \rangle. \quad (2.18)$$

For the model energy eigenfunctions, we can use this relation as a test of the quality of the eigenfunction. Specifically, we will consider the virial ratio

$$T_v = \frac{\langle \psi | \frac{1}{2} p^2 | \psi \rangle}{\frac{1}{2} \langle \psi | \vec{r} \cdot \vec{\nabla} V | \psi \rangle} \quad (2.19)$$

which is equal to 1 for the exact eigenstates.

Another useful test for the quality of an energy eigenfunction is provided by the local energy [30]

$$E = \frac{1}{\psi(\vec{r})} H \psi(\vec{r}) \quad (2.20)$$

where H is the Hamiltonian. For an exact eigenfunction, this should be a constant independent of \vec{r} , or equivalently,

$$L = \frac{H \psi(\vec{r})}{\langle \psi | H | \psi \rangle \psi(\vec{r})} \quad (2.21)$$

should be equal to 1. For an approximate wavefunction, the deviation of L from 1 can be taken to be a test of the quality of the wavefunction in the local region.

We now use these structural properties to develop simple, reliable wavefunctions for the class of potentials which satisfy the conditions in equations (2.1) and (2.3).

3. Eigenfunctions for the Yukawa potential

For the Yukawa potential

$$V(r) = -\frac{Z}{r} e^{-\mu r} \quad (3.1)$$

a scale transformation leads to the relations

$$E(Z, \mu) = Z^2 E\left(1, \frac{\mu}{Z}\right) \quad (3.2)$$

$$\psi(Z, \mu, r) = Z^{3/2} \psi\left(1, \frac{\mu}{Z}, Zr\right). \quad (3.3)$$

Therefore, we will consider only the case of $Z = 1$, and develop energy eigenfunctions as a function of the screening parameter μ .

3.1. Lowest-energy l states

For the lowest-energy eigenstate with a given l , we propose a wavefunction

$$\psi(\vec{r}) = A \frac{1}{r} e^{-\alpha r} (1 - e^{-\lambda r})^{l+1} P_l(\cos \theta). \quad (3.4)$$

Incorporating the asymptotic behaviour in equation (2.15) requires that

$$\alpha = (-2E)^{1/2}. \quad (3.5)$$

Incorporating the cusp condition in equation (2.7) or (2.10) implies that

$$\lambda = \frac{2}{l+1} \left(\frac{1}{l+1} - \alpha \right). \quad (3.6)$$

Thus we have a wavefunction for the lowest-energy l states, which has no free parameters, but which incorporates the correct asymptotic and cusp structures. The quantities α and λ do depend on the energy E which is determined iteratively, with

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (3.7)$$

It needs only two or three iterations for the input and output energies to be equal to an accuracy of first five digits.

To emphasize the simplicity of the wavefunction and the calculations, we provide the expressions for the various expectation values. The wavefunction is

$$\begin{aligned} \psi(\vec{r}) &= \frac{1}{r} \sum_{j=0}^{l+1} C_j e^{-a_j r} P_l(\cos \theta) \\ a_j &= \alpha + j\lambda \\ C_j &= A(-1)^j \frac{(l+1)!}{j!(l+1-j)!} \end{aligned} \quad (3.8)$$

for which one has

$$\langle \psi | \psi \rangle = \frac{4\pi}{2l+1} \sum C_i C_j \frac{1}{a_i + a_j} \quad (3.9)$$

$$\langle \psi | \frac{p^2}{2} | \psi \rangle = -\frac{2\pi}{2l+1} \sum C_i C_j \left[\frac{a_j^2}{a_i + a_j} - 2l(l+1)a_i \ln(a_i + a_j) \right] \quad (3.10)$$

$$\langle \psi | V | \psi \rangle = \frac{4\pi}{2l+1} \sum C_i C_j \ln(a_i + a_j + \mu). \quad (3.11)$$

The calculated values of the energies for 1s, 2p, 3d, 4f states are given in tables 1 and 2. They compare well with the accurate results from other calculations. The tables also give the normalization constant A . The values of the parameters α and λ are easily deduced from equations (3.5) and (3.6).

To test the quality of the wavefunction, we first note that for the Yukawa potential, the virial relation in equation (2.18) reduces to

$$\langle \psi | \frac{1}{2} p^2 | \psi \rangle = -\frac{1}{2} \langle \psi | V | \psi \rangle + \frac{1}{2} \mu \langle \psi | e^{-\mu r} | \psi \rangle. \quad (3.12)$$

For the second term one has

$$\langle \psi | e^{-\mu r} | \psi \rangle = \frac{4\pi}{2l+1} \sum C_i C_j \frac{1}{a_i + a_j + \mu}. \quad (3.13)$$

Table 1. Eigenstate energies for the 1s and 2p states in the Yukawa potential for some values of the screening parameter μ , along with normalization constant A and the virial ratio T_v of the left and right-hand terms in equation (3.12). The energies in the brackets are the accurate values from: ^a [26], ^b [27] and ^c [21].

μ	1s state			2p state		
	A	$-E$	T_v	A	$-E$	T_v
0.01	28.3	0.490 08 (0.490 05) ^a	1.00	2.52×10^2	0.115 25 (0.115 25) ^c	1.00
0.02	14.2	0.480 30 (0.480 30) ^b	1.00	63.2	0.105 96 (0.105 96) ^c	1.00
0.03	9.47	0.470 66	1.00	28.2	0.097 13 (0.097 13) ^c	1.00
0.05	5.70	0.451 82 (0.451 80) ^a	1.00	10.1	0.080 74 (0.080 74) ^c	1.01
0.07	4.09	0.433 52	1.00	5.07	0.065 94 (0.065 94) ^c	1.01
0.10	2.87	0.407 06 (0.407 06) ^b	1.00	2.37	0.046 52 (0.046 54) ^c	1.01
0.15	1.92	0.365 45	1.00	0.887	0.021 09 (0.021 10) ^c	1.01
0.20	1.45	0.326 79 (0.326 81) ^b	1.01	0.309	0.004 04 (0.004 10) ^c	0.99
0.30	0.959	0.257 58	1.01			
0.50	0.551	0.147 95 (0.148 12) ^b	1.02			
0.70	0.355	0.071 58	1.02			
1.00	0.169	0.010 11 (0.010 29) ^a	1.02			
1.15	0.069	0.000 41 (0.000 46) ^c	1.02			

In the tables we have also given the virial ratio T_v defined in equation (2.19), which corresponds to the ratio of the left-hand side term to the right-hand side term in equation (3.12). This is generally close to 1, emphasizing the good quality of the wavefunction. We also test the quality of the wavefunction in terms of the second threshold relation in equation (2.11). For our wavefunction, the left-hand side is given by

$$\frac{f''(0)}{f(0)} = \frac{2}{(l+2)(l+3)} \frac{\sum C_i a_i^{l+3}}{\sum C_i a_i^{l+1}} \quad (3.14)$$

and V_0 defined in equation (2.2) is equal to μ for the Yukawa potential. We calculate the ratio of this quantity to the quantity on the right-hand side in equation (2.11). We find it generally close to 1. For the 1s state it varies from 1.00 at $\mu = 0.01$ to 0.93 at $\mu = 1.0$, and for the 2p state, from 1.00 at $\mu = 0.005$ to 0.99 at $\mu = 0.20$. We finally subject our wavefunction to the local energy test in equation (2.21). We find that L in equation (2.21) for the 1s state is close to 1 for all values of r , for μ up to about 0.5, with some variation for larger μ . For the 2p state, it is close to 1 for all values of r for μ up to 0.1.

It must be noted that while the wavefunction in equation (3.4) provides quite a good description of the eigenstates over a large range of the screening parameter μ , there are some reservations for μ near its critical value. Since the asymptotic exponent α in equation (3.5) depends directly on the binding energy E which is very small near the critical value, even a

Table 2. Eigenstate energies for the 3d and 4f states in Yukawa potential for some values of the screening parameter μ , along with normalization constant A and the virial ratio T_v of the left-hand and right-hand terms in equation (3.12). The energies in the brackets are the accurate values from: ^a [26] and ^b [13].

μ	3d state			4f state		
	A	$-E$	T_v	A	$-E$	T_v
0.005	5.72×10^3	0.050 68 (0.050 70) ^a	1.00	1.64×10^4	0.026 45 (0.026 47) ^a	1.00
0.01	7.20×10^2	0.046 06 (0.046 06) ^a	1.00	1.03×10^3	0.022 10 (0.022 10) ^b	1.00
0.02	89.2	0.037 51 (0.037 52) ^a	1.00	58.8	0.014 49 (0.014 49) ^b	1.01
0.03	25.7	0.029 84	1.01	9.51	0.008 28 (0.008 28) ^b	1.01
0.04	10.3	0.022 98	1.01	1.99	0.003 41	1.00
0.045	—	—	—	0.808	0.001 46	0.98
0.05	4.85	0.016 91 (0.016 92) ^b	1.01	0.478	0.000 74	0.96
0.06	2.49	0.011 60	1.01			
0.07	1.31	0.007 04	1.01			
0.08	0.644	0.003 23 (0.003 25) ^b	0.99			

small difference in the energy will make a substantial difference in the value of α . Therefore, when one is very close to the critical strength of the screening parameter, it is better to determine the parameter α by some other means, such as the satisfaction of the virial relation in equation (3.12).

3.2. First excited l states

For the first excited state with a given l , we first observe that it has a node. Therefore, we propose a wavefunction

$$\psi(\vec{r}) = A \frac{1}{r} e^{-\alpha r} (1 - e^{-\lambda r})^{l+1} (1 - b e^{-\lambda r}) P_l(\cos \theta). \quad (3.15)$$

Incorporating the asymptotic behaviour in equation (2.15) leads to

$$\alpha = (-2E)^{1/2}. \quad (3.16)$$

Incorporating the cusp condition in equation (2.7) or (2.10) requires that

$$\lambda = \frac{[1/(l+1) - \alpha]}{[(l+1)/2 - b/(1-b)]}. \quad (3.17)$$

The parameter b is determined so as to satisfy the virial relation in equation (3.12). Thus, the parameters α , λ and b are determined by the asymptotic condition, the cusp condition and the virial relation. The asymptotic condition in equation (3.16) depends on the energy E which is determined iteratively so that the input energy is equal to the output energy in equation (3.7). The calculations are again simplified by writing

$$\psi = \frac{1}{r} \sum_{j=0}^{l+2} C_j e^{-a_j r} P_l(\cos \theta) \quad (3.18)$$

Table 3. Eigenstate energies for the 2s and 3p states in Yukawa potential for some values of the screening parameter μ , along with the values of the parameter b and the normalization constant A . The energies in the brackets are the accurate values from: ^a [26], ^b [21] and ^c [13].

μ	2s state			3p state		
	b	A	$-E$	b	A	$-E$
0.005	1.020	1.01×10^3	0.120 07 (0.120 05) ^a	1.061	9.92×10^3	0.050 71 (0.050 70) ^a
0.01	1.040	2.54×10^2	0.115 29 (0.115 29) ^b	1.125	1.22×10^3	0.046 15 (0.046 16) ^a
0.02	1.081	62.9	0.106 15 (0.106 15) ^b	1.261	1.49×10^2	0.037 85 (0.037 85) ^a
0.03	1.123	27.7	0.097 53 (0.097 53) ^b	1.411	42.0	0.030 54
0.05	1.208	9.87	0.081 77 (0.081 77) ^b	1.766	7.80	0.018 57 (0.018 56) ^c
0.07	1.297	4.91	0.067 82 (0.067 82) ^b	2.233	2.24	0.009 71
0.10	1.438	2.28	0.049 94 (0.049 93) ^b	3.483	0.373	0.001 59 (0.001 59) ^c
0.11	—	—	—	4.621	0.124	0.000 174
0.15	1.698	0.884	0.027 24 (0.027 22) ^b			
0.20	2.001	0.404	0.012 13 (0.012 11) ^b			
0.25	2.367	0.184	0.003 40 (0.003 40) ^b			
0.30	2.837	0.0491	0.000 09 (0.000 09) ^b			

with

$$a_j = \alpha + j\lambda \quad (3.19)$$

and

$$C_j = (-1)^j \left[\frac{l!}{j!(l-j)!} + b \frac{l!}{(j-1)!(l-j+1)!} \right]. \quad (3.20)$$

Then the expressions for the norm of the state, the average values for the kinetic and potential energies are given by the expressions in equations (3.9)–(3.11). The virial relation is given in equation (3.12) with the average value of $e^{-\mu r}$ given in equation (3.13). The predicted values for the energies of the first excited states with $l = 0, 1$, i.e. 2s and 3p states, are given in table 3, along with the values of the parameter b , and the normalization constant A . They are generally quite close to the accurate results from other calculations. The values of the parameters α and λ are easily deduced from equations (3.16) and (3.17).

We test the accuracy of our wavefunction in terms of the second threshold relation in equation (2.11) with $V_0 = \mu$ and the left-hand side given by equation (3.14). We calculate the ratio of the quantity on the left-hand side to the quantity on the right-hand side in equation (2.11) and find it to be generally close to 1. For the 2s state, it varies from the value 1.00 at $\mu = 0.01$ to 0.95 at $\mu = 0.30$, and for the 3p state it varies from 1.00 at $\mu = 0.005$ to 0.99 at $\mu = 0.11$. For the local energy test in equation (2.21), we find that the L value is close to 1.00 except near the node points where as expected, there are sharp variations.

4. Eigenfunctions for $l \neq 0$ states of the Hulthén potential

For the Hulthén potential

$$V(r) = -Z\mu \frac{e^{-\mu r}}{1 - e^{-\mu r}} \quad (4.1)$$

a scale transformation leads to the relations

$$E(Z, \mu) = Z^2 E\left(1, \frac{\mu}{Z}\right) \quad (4.2)$$

$$\psi(Z, \mu, r) = Z^{3/2} \psi\left(1, \frac{\mu}{Z}, Zr\right). \quad (4.3)$$

Therefore, we will consider only the case of $Z = 1$, and develop energy eigenfunctions as a function of the screening parameter μ .

4.1. Lowest-energy l states

For the lowest-energy eigenstates with a given l , we propose a wavefunction

$$\psi(\vec{r}) = A \frac{1}{r} e^{-\alpha r} (1 - e^{-\mu r}) (1 - e^{-\lambda r})^l P_l(\cos \theta). \quad (4.4)$$

Incorporating the asymptotic behaviour in equation (2.15) implies that α is once again given by

$$\alpha = (-2E)^{1/2}. \quad (4.5)$$

Incorporating the cusp condition in equation (2.7) or (2.10) requires that

$$\lambda = \frac{2}{l} \left(\frac{1}{l+1} - \alpha - \frac{1}{2}\mu \right). \quad (4.6)$$

Thus our wavefunction incorporating the cusp and the asymptotic conditions has no free parameters. The quantities α and λ do depend on the energy E which is determined iteratively so that the input energy is equal to the output energy in equation (3.7).

For simplifying the calculations we write the wavefunction in the form

$$\begin{aligned} \psi &= \frac{1}{r} (1 - e^{-\mu r}) \sum_{j=0}^l C_j e^{-a_j r} P_l(\cos \theta) \\ a_j &= \alpha + j\lambda \\ C_j &= A (-1)^j \frac{l!}{j!(l-j)!} \end{aligned} \quad (4.7)$$

for which one finds

$$\langle \psi | \psi \rangle = \frac{4\pi}{2l+1} \sum C_i C_j \frac{2\mu^2}{(a_i + a_j)(a_i + a_j + \mu)(a_i + a_j + 2\mu)} \quad (4.8)$$

$$\begin{aligned} \langle \psi | \frac{1}{2} p^2 | \psi \rangle &= -\frac{2\pi}{2l+1} \sum C_i C_j \left[\frac{\mu a_j^2}{(a_i + a_j)(a_i + a_j + \mu)} - \frac{\mu(a_j + \mu)^2}{(a_i + a_j + \mu)(a_i + a_j + 2\mu)} \right. \\ &\quad \left. + 2l(l+1) \left\{ a_j \ln \left(\frac{a_i + a_j + \mu}{a_i + a_j} \right) - (a_j + \mu) \ln \left(\frac{a_i + a_j + 2\mu}{a_i + a_j + \mu} \right) \right\} \right] \end{aligned} \quad (4.9)$$

Table 4. Eigenstate energies for the 2p and 3d states in the Hulthén potential for some values of the screening parameter μ , along with normalization constant A and the virial ratio T_v of the left-hand side and right-hand side terms in equation (4.11). The energies in the brackets are the accurate values from: ^a [13].

μ	2p state			3d state		
	A	$-E$	T_v	A	$-E$	T_v
0.01	1.163×10^3	0.120 04	1.00	5.59×10^3	0.050 64	1.00
0.02	2.47×10^2	0.115 17	1.00	6.83×10^2	0.045 91	1.00
0.03	1.09×10^2	0.110 38	1.00	1.92×10^2	0.041 34	1.00
0.05	38.9	0.101 04	1.00	39.7	0.032 75	1.00
		(0.101 04) ^a			(0.032 75) ^a	
0.10	9.33	0.079 18	1.00	3.61	0.014 48	0.99
		(0.079 18) ^a			(0.014 48) ^a	
0.20	2.00	0.041 88	0.99			
		(0.041 89) ^a				
0.30	0.629	0.013 70	0.98			
		(0.013 79) ^a				
0.35	0.284	0.003 27	0.95			
		(0.003 79) ^a				

Table 5. Eigenstate energies for the 4f and 3p states in Hulthén potential for some values of the screening parameter μ , along with normalization constant A , the virial ratio T_v of the left-hand side and right-hand side terms in equation (4.11) for the 4f state, and the variational parameter b for the 3p state. The energies in the brackets are the accurate values from: ^a [13].

μ	4f state			3p state		
	A	$-E$	T_v	b	A	$-E$
0.01	1.56×10^4	0.026 40	1.00	1.062	9.50×10^3	0.050 66
0.02	9.11×10^2	0.021 85	1.00	1.128	1.14×10^3	0.045 97
0.03	1.33×10^2	0.017 61	1.00	1.200	3.22×10^2	0.041 49
0.04	45.9	0.013 67	1.00	1.277	1.29×10^2	0.037 22
0.05	16.0	0.010 06	1.00	1.360	62.8	0.033 17
		(0.010 06) ^a				(0.033 16) ^a
0.07	2.36	0.003 83	0.97	1.549	20.2	0.025 68
0.10	—	—	—	1.911	5.48	0.016 05
						(0.016 05) ^a
0.15	—	—	—	2.950	0.860	0.004 47
						(0.004 47) ^a

and

$$\langle \psi | V | \psi \rangle = -\frac{4\pi\mu}{(2l+1)} \sum C_i C_j \frac{\mu}{(a_i + a_j + \mu)(a_i + a_j + 2\mu)}. \quad (4.10)$$

Of course the wavefunction gives the exact energies for the 1s state. We have given the energies for the 2p, 3d and 4f states in tables 4 and 5, along with the normalization constant A . The energies compare quite well with the results from other calculations [13]. The values of parameters α and λ are easily deduced from equations (4.5) and (4.6).

To test the quality of our wavefunction, we note that for the Hulthén potential, the virial relation in equation (2.18) reduces to

$$\langle \psi | \frac{1}{2} p^2 | \psi \rangle = \frac{1}{2} \mu^2 \langle \psi | \frac{r e^{-\mu r}}{(1 - e^{-\mu r})^2} | \psi \rangle. \quad (4.11)$$

For the quantity on the right-hand side, we have

$$\langle \psi | \frac{r e^{-\mu r}}{(1 - e^{-\mu r})^2} | \psi \rangle = \frac{4\pi}{2l+1} \sum C_i C_j \frac{1}{(a_i + a_j + \mu)^2}. \quad (4.12)$$

In the tables we have also given the virial ratio T_v which is the ratio of the quantities on the left- and right-hand sides of equation (4.11). It is generally very close to 1 emphasizing the good quality of the wavefunctions. We also test the quality of our wavefunction in terms of the second threshold relation in equation (2.11). For the Hulthén potential, V_0 defined in equation (2.2) is equal to $\frac{1}{2}\mu$, and

$$\frac{f''(0)}{f(0)} = \frac{2}{(l+2)(l+3)} \frac{\sum C_i [a_i^{l+3} - (a_i + \mu)^{l+3}]}{\sum C_i [a_i^{l+1} - (a_i + \mu)^{l+1}]}. \quad (4.13)$$

We calculate the ratio of this quantity to the quantity on the right-hand side in equation (2.11). We find that it is generally close to 1. For the 2p state it varies from a value of 1.00 at $\mu = 0.01$ to a value of 1.03 at $\mu = 0.35$. For the 3d state it is 1.00 for the range of $\mu = 0.01$ to 0.10. We finally subject our wavefunctions to the local energy test in equation (2.21). We find that the value of L in equation (2.21) is generally close to 1 for all values of r , except near the critical values of μ where there is some variation.

4.2. First excited l states

For the first excited states with a given l , we propose a wavefunction

$$\psi(\vec{r}) = A \frac{1}{r} e^{-\alpha r} (1 - e^{-\mu r}) (1 - e^{-\lambda r})^l (1 - b e^{-\lambda r}) P_l(\cos \theta). \quad (4.14)$$

Incorporating the asymptotic behaviour in equation (2.15) implies that

$$\alpha = (-2E)^{1/2} \quad (4.15)$$

and the cusp condition in equation (2.7) or (2.10) requires that

$$\lambda = \frac{[1/(l+1) - \alpha - \frac{1}{2}\mu]}{[l/2 - b/(1-b)]}. \quad (4.16)$$

The parameter b is determined so as to satisfy the virial relation in equation (4.11). Thus the parameters α , λ and b are determined by the asymptotic condition, the cusp condition and the virial relation. The asymptotic condition in equation (4.15) depends on the energy E which is determined iteratively so that the input energy E is equal to the output energy in equation (3.7). The calculations are again simplified by writing

$$\begin{aligned} \psi &= \frac{1}{r} (1 - e^{-\mu r}) \sum_{j=0}^{l+1} C_j e^{-a_j r} P_l(\cos \theta) \\ a_j &= \alpha + j\lambda \\ C_j &= (-1)^j \left[\frac{l!}{j!(l-j)!} + b \frac{l!}{(j-1)!(l-j+1)!} \right]. \end{aligned} \quad (4.17)$$

Then the expressions for the norm of the state, the average values of the kinetic and potential energies are given by the expressions in equations (4.8)–(4.10). The virial relation is given in equations (4.11) and (4.12). The predicted values for the 3p state are given in table 5, along with the values of the parameter b , and the normalization constant A . They are generally close

to the accurate results from other calculations. The values of the parameters α and λ are easily deduced from equations (4.15) and (4.16).

We test the accuracy of our wavefunction in terms of the second threshold relation in equation (2.11) with $V_0 = \frac{1}{2}\mu$ and the left-hand side given by equation (3.14). We calculate the ratio of the quantity on the left-hand side to the quantity on the right-hand side in equation (2.11) and find that it varies from the value 1.00 at $\mu = 0.01$ to 1.01 at $\mu = 0.15$.

5. Eigenfunctions for other potentials

It should be emphasized that our approach is quite general and applies to a whole class of potentials which have Coulombic behaviour for small r and are exponentially damped for large r . For example, one may consider a superposition of the Yukawa potentials

$$V(r) = -\frac{1}{r} \sum_i Z_i e^{-\mu_i r} \quad (5.1)$$

for which we can use the wavefunctions in equations (3.4) and (3.15). One may also consider a superposition of the Hulthén-type potentials

$$V(r) = -\sum_i Z_i \mu \frac{e^{-\mu_i r}}{1 - e^{-\mu r}} \quad (5.2)$$

with different exponents, for which we can use the wavefunctions in equations (4.4) and (4.14). To illustrate the point, we consider a special case

$$V(r) = -\frac{Z}{r} (e^{-\mu r} + e^{-2\mu r}) \quad (5.3)$$

which is a superposition of just two Yukawa potentials with a ratio of 2 for the two exponents. The scaling relation leads to

$$E(Z, \mu) = Z^2 E\left(1, \frac{\mu}{Z}\right) \quad (5.4)$$

so that we will consider only the case of $Z = 1$:

$$V(r) = -\frac{1}{r} (e^{-\mu r} + e^{-2\mu r}). \quad (5.5)$$

This potential may be a reasonable simulation of the potential in a helium atom.

5.1. Lowest-energy l states

We use the same form for the wavefunction as in equation (3.4). The asymptotic condition in equation (2.15) again leads to

$$\alpha = (-2E)^{1/2}. \quad (5.6)$$

The cusp condition in equation (2.7) or (2.10) leads to

$$\lambda = \frac{2}{l+1} \left(\frac{2}{l+1} - \alpha \right). \quad (5.7)$$

The energy E is determined iteratively. The calculations are carried out by writing the wavefunction in the form in equation (3.8). The norm and the kinetic energy are given by equations (3.9) and (3.10). The expectation value of the potential is

$$\langle \psi | V | \psi \rangle = \frac{4\pi}{2l+1} \sum C_i C_j \ln[(a_i + a_j + \mu)(a_i + a_j + 2\mu)]. \quad (5.8)$$

Table 6. Eigenstate energies for the 1s and 2p states for the potential in equation (5.5) for some values of the screening parameter μ , along with normalization constant A and the virial ratio T_v of the left- and right-hand terms in equation (5.9).

μ	1s state			2p state		
	A	$-E$	T_v	A	$-E$	T_v
0.01	53.3	1.970 19	1.00	6.34×10^2	0.470 61	1.00
0.02	26.7	1.940 74	1.00	1.60×10^2	0.442 42	1.00
0.05	10.8	1.854 55	1.00	26.0	0.364 42	1.00
0.10	5.43	1.717 7	1.00	6.48	0.254 02	1.01
0.20	2.75	1.467 5	1.01	1.41	0.095 17	1.03
0.30	1.85	1.245 2	1.01	0.323	0.007 94	1.00
0.50	1.11	0.872 85	1.02			
1.00	0.492	0.274 17	1.04			
1.50	0.209	0.026 09	1.04			
1.70	0.0805	0.000 78	1.03			

Table 7. Eigenstate energies for the 2s and 3p states for the potential in equation (5.5) for some values of the screening parameter μ , along with the values of the parameter b and the normalization constant A .

μ	2s state			3p state		
	b	A	$-E$	b	A	$-E$
0.01	1.030	6.35×10^2	0.470 74	1.093	4.10×10^3	0.193 72
0.02	1.060	1.61×10^2	0.442 88	1.189	5.24×10^2	0.168 00
0.03	1.091	70.8	0.416 36	1.291	1.54×10^2	0.144 79
0.05	1.152	25.8	0.367 06	1.514	31.7	0.105 03
0.07	1.214	13.2	0.322 34	1.768	10.7	0.073 07
0.10	1.309	6.37	0.263 01	2.234	3.02	0.037 46
0.15	1.472	2.72	0.182 14	3.570	0.436	0.004 69
0.20	1.643	1.43	0.120 329			
0.30	2.02	0.509	0.041 34			
0.40	2.47	0.183	0.006 20			

The calculated values of the energies for the 1s and 2p states are given in table 6. The virial relation in equation (2.18) now reduces to

$$\langle \psi | \frac{1}{2} p^2 | \psi \rangle = -\frac{1}{2} \langle \psi | V | \psi \rangle + \frac{1}{2} \mu \langle \psi | e^{-\mu r} | \psi \rangle + \mu \langle \psi | e^{-2\mu r} | \psi \rangle. \quad (5.9)$$

The expectation values of the exponential quantities are obtained by using the result in equation (3.13). In the table we have given the virial ratio T_v which is the ratio of the left- and right-hand terms in equation (5.9). It being generally close to 1 again illustrates the good quality of the energy eigenfunctions.

5.2. First excited l states

For the first excited states with a given l , we use the same wavefunction as in equation (3.15). The asymptotic condition again leads to

$$\alpha = (-2E)^{1/2}. \quad (5.10)$$

The cusp condition in equation (2.7) or (2.10) leads to

$$\lambda = \frac{[2/(l+1) - \alpha]}{[(l+1)/2 - b/(1-b)]}. \quad (5.11)$$

The parameter b is determined so as to satisfy the virial relation in equation (5.9). Since the asymptotic exponent α depends on the energy, the energy E is determined iteratively so that the input energy is equal to the output energy in equation (3.7). The calculations are simplified by writing the wavefunction in the form given in equations (3.18)–(3.20). The norm and the kinetic energy are given by equations (3.9) and (3.10), and the expectation value of the potential is given in equation (5.8). The calculated values of the energies for the 2s and 3p states are given in table 7, along with the values of the parameter b and the normalization constant A .

6. Summary

We have analysed the general structural properties of energy eigenfunctions of Yukawa and Hulthén potentials, in some local domains. The properties of these potentials, that they are exponentially damped for large r and have Coulombic form for small r , imply that the wavefunction tends to the spherical Hankel function for large r , and has some specific threshold properties for small r , mainly the cusp conditions. Based on these local properties, we develop some simple wavefunctions for many states, which incorporate these asymptotic and threshold properties. These essentially parameter-free wavefunctions give quite accurate values for the energies over a wide range of the screening parameter, for several states. They also provide a clear physical insight into the structure of the energy eigenfunctions in different domains. It is pointed out that the general virial relation between the kinetic energy and the potential terms, can be very useful, both as a test for the quality of the eigenfunctions, and for developing wavefunctions for excited states.

It is important to appreciate that these asymptotic and threshold properties are present in the energy eigenfunctions for a large class of potentials with exponential damping for large r and Coulombic behaviour for small r . Therefore, the simple forms of the wavefunctions we have suggested are relevant for a large class of potentials. The general nature of these properties and their implications deserves special attention.

References

- [1] Ecker G and Weizel W 1956 *Ann. Phys., Lpz.* **17** 126
- [2] Lam C S and Varshni Y P 1971 *Phys. Rev. A* **4** 1875
- [3] Ray P P and Ray A 1980 *Phys. Lett. A* **78** 443
- [4] Dutt R, Ray A and Ray P P 1981 *Phys. Lett. A* **83** 65
- [5] Dutt R and Mukherji U 1982 *Phys. Lett. A* **90** 395
- [6] Varshni Y P 1990 *Phys. Rev. A* **41** 4682
- [7] Smith C R 1964 *Phys. Rev. A* **134** 1235
- [8] Margenau H and Lewis M 1959 *Rev. Mod. Phys.* **31** 569
- [9] Harris G M 1962 *Phys. Rev.* **125** 1131
- [10] Krieger J B 1969 *Phys. Rev.* **178** 1337
- [11] Roussel K M and O'Connell R F 1974 *Phys. Rev. A* **9** 52
- [12] Greene R L and Aldrich C 1976 *Phys. Rev. A* **14** 2363
- [13] Stubbins C 1993 *Phys. Rev. A* **48** 220
- [14] Fessatidis V, Mancini J D, Haider Q, Zhou Y and Greco L 1998 *Phys. Lett. A* **242** 74
- [15] Iafrate G J and Mendelsohn L B 1969 *Phys. Rev.* **182** 244
- [16] Müller-Kristen H J W and Vahedi-Faridi N 1973 *J. Math. Phys.* **14** 1291
- [17] McEnnan J, Kissel L and Pratt R H 1976 *Phys. Rev. A* **13** 532
- [18] Mehta C H and Patil S H 1978 *Phys. Rev. A* **17** 34
- [19] Lai C S and Lin W C 1980 *Phys. Lett. A* **78** 335
- [20] Lai C S 1981 *Phys. Rev. A* **23** 455
- [21] Vrscay E R 1986 *Phys. Rev. A* **33** 1433

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- [22] Roy B and Roychoudhury R 1987 *J. Phys. A: Math. Gen.* **20** 3051
 - [23] Garavelli S L and Oliveira F A 1991 *Phys. Rev. Lett.* **66** 1310
 - [24] Gomes O A, Chacham H and Mohallem J R 1994 *Phys. Rev. A* **50** 228
 - [25] Rouse C A 1967 *Phys. Rev.* **159** 41
 - [26] Rogers F J, Graboske H C and Harwood D J 1970 *Phys. Rev. A* **1** 1577
 - [27] Nunez M 1993 *Phys. Rev. A* **47** 3620
 - [28] Kato T 1957 *Commun. Pure Appl. Math.* **10** 151
 - [29] Morse P M and Feshbach H 1953 *Methods of Theoretical Physics* (New York: McGraw-Hill)
 - [30] Bartlett J H, Gibbons J J and Dunn C G 1935 *Phys. Rev.* **47** 679