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The Yukawa and Hulthén potentials in quantum mechanics

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Abstract. The concept of kinetic potentials is used to construct a global geometrical approximation theory for the spectra of Schrödinger operators $H = -\Delta + vy$ in which the potential shape y is either (i) a transformation $y(r) = g(h(r))$ of a soluble potential $h(r)$ or (ii) a continuous mixture $y(r) = \int \rho(t)h(rt) dt$. The case in which y is the Yukawa potential and $h = -(e^r - 1)^{-1}$ is the Hulthén potential is discussed in detail. Simple formulae are derived for eigenvalue bounds which are compared to accurate data obtained by the direct numerical integration of Schrödinger's equation.

1. Introduction

In this paper we study the Yukawa potential $y(r)$ and the Hulthén potential $h(r)$. The shapes of these potentials are given respectively by the two formulae

$$y(r) = -\frac{e^{-r}}{r} \quad \text{and} \quad h(r) = -\frac{u}{e^{br} - 1} \quad (1.1)$$

where u and b are positive parameters. These potentials are very similar: they are both Coulomb-like for small r , and they both decay monotonically and (essentially) exponentially to zero for large r . The S -state eigenvalues \mathcal{E}_n of the Schrödinger operator $-\Delta + vh(r)$ corresponding to the Hulthén potential are known exactly and are given [1, 2] explicitly by the expression

$$\mathcal{E}_n = \mathcal{F}_n(v) = -\frac{(vu - n^2b^2)^2}{4n^2b^2} \quad n = 1, 2, 3, \dots \quad (1.2)$$

where the curves $(v, \mathcal{F}_n(v))$, $v \geq n^2b^2/u$, are called energy trajectories. We obviously have too many parameters in (1.2). Our policy will be to keep $y(r)$ fixed, and to adjust $h(r)$ by varying u and b . We then try to use the relationship between $y(r)$ and $h(r)$ to establish a corresponding relationship between the (unknown) spectrum $E_n = F_n(v)$ of the Yukawa Hamiltonian $-\Delta + vy(r)$ and the exact Hulthén spectrum (1.2).

We consider three distinct approaches: simple inequalities between $y(r)$ and $h(r)$ which we discuss in section 2; the Yukawa potential y represented as a smooth transformation $g(h)$ of the Hulthén potential (an application of the 'envelope method'), in section 4; and an approximation to the Yukawa potential as a continuous mixture of Hulthén potentials with different scales, in section 5. In section 3 we outline briefly the formulation of spectral theory in terms of 'kinetic potentials' which we need in sections 4 and 5.

Although the Hulthén eigenvalues for $l > 0$ may also be obtained to high accuracy [3], most of our effort will be directed towards exploiting the simple exact formula which we have for the S -states. For large values of the coupling v , the low-lying states are almost Coulombic and it becomes very effective to represent the Yukawa potential as a smooth (concave) transformation of $-1/r$: in this case, envelope representations lead to a simple upper-bound energy formula valid for *all* n and l ; this is given in section 4. We have already discussed the Yukawa potential in an earlier paper [4] on screened-Coulomb potentials. In that article we relied heavily on potential inequalities. In the present paper we shall review and clarify these inequalities and discuss in more detail the spectral implications of the representation $y = g(h)$. The newest aspect of the present paper is the extension of the notion of almost additivity for kinetic potentials to the case of continuous mixtures of the form $y(r) = \int a(t)h(r) dt$. Results are quoted for all these approaches, along with some accurate data obtained by the direct numerical integration of Schrödinger's equation.

The central idea of this work is to try to represent y smoothly in terms of h , and then to exploit geometry to discover how the corresponding spectra are related. The methods we use are quite general and, for the problem studied here, they lead naturally to a variety of simple formulae for both upper and lower energy bounds. The paper is in effect a tour of some aspects of spectral geometry presented in terms of an interesting example.

2. Simple inequalities

As we mentioned in [4], the inequality

$$y(r) = -\frac{e^{-r}}{r} \geq -\frac{1}{e^r - 1} = h(r) \quad (2.1)$$

in which $b = u = 1$ is certainly correct, but the spectral lower bound it provides is too weak to be interesting. The question which arises is: how to choose b and u so as to do better? In the Laurent expansions of $y(r)$ and $h(r)$ about $r = 0$, one gets the same coefficient of the Coulomb pole if $b = u$; meanwhile, the constant term is the same if $b = u = 2$. These choices lead one to consider the difference function $d(r) = h(r) - y(r)$ given by

$$d(r) = \frac{e^{-r}}{r} - \frac{2}{e^{2r} - 1} = \frac{e^{-r}}{r} - \frac{e^{-r}}{\sinh(r)}. \quad (2.2)$$

Since $\sinh(r) \geq r$, it follows that $d(r) \geq 0$. The graph of $d(r)$ shown in figure 1 demonstrates that $d(r) < 0.056$. Consequently, if $b = u = 2$, we have the potential inequalities

$$h(r) - 0.056 < y(r) < h(r) \quad (2.3)$$

and these immediately yield via (1.2) the following spectral inequalities which we found in [4]:

$$-\frac{(v - 2n^2)^2}{4n^2} - (0.056)v \leq E_n = F_n(v) \leq -\frac{(v - 2n^2)^2}{4n^2}. \quad (2.4)$$

These results look a little different from those quoted in [4] because we do not have the vestigial factor of $\frac{1}{2}$ in front of the kinetic energy operator in the Hamiltonians of the present paper. The energy bounds have a compelling simplicity, and for small v

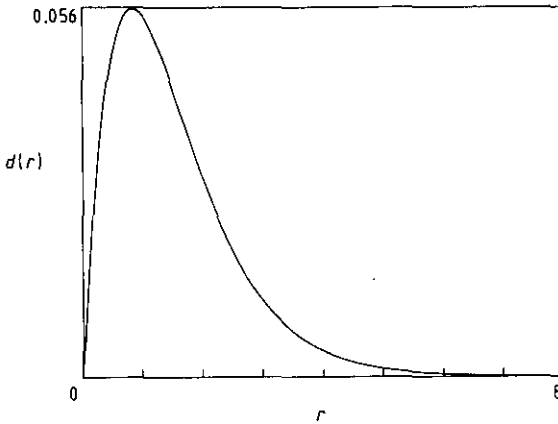


Figure 1. The difference function $d(r) = e^{-r}/r - u(e^{br} - 1)^{-1}$ between the Yukawa and Hulthén potentials. For the case $u = b = 2$ we have $0 \leq d(r) < 0.056$.

(and n) they can be very useful. We shall improve on both of them in sections 4 and 5. The use of the Laurent expansions to fix some of the parameters in the Hulthén potential, and the establishment of bounds on the difference function $d(r)$ will be helpful guides when we deal with approximations via continuous mixtures in section 5.

3. Kinetic potentials

In the abstract theory [5-8] of Schrödinger operators $H = K + V$ one thinks of the potential $V = vf$ as a perturbation of the positive-definite kinetic energy term $K = -\Delta$. If \mathcal{D}_n is an n -dimensional subspace of $L^2(\mathbb{R}^3)$ contained in the domain of H and contained in the angular-momentum subspace labelled by the spherical harmonic Y_l^m , then we can define the n th eigenvalue E_{nl} ($n = 1, 2, \dots$) by the min-max expression

$$E_{nl} = \inf_{\mathcal{D}_n} \sup_{\substack{\psi \in \mathcal{D}_n \\ \|\psi\|=1}} (\psi, H\psi). \tag{3.1}$$

Kinetic potentials arise when one effects the minimization in two stages. At the first stage, we scale the linear space \mathcal{D}_n so that we can fix the value of $(\psi, K\psi) = s$, then we minimize over all scales, that is to say, over all values of $s > 0$. Thus, if $\mathcal{D}_n = \text{Span}\{\phi_i\}_{i=1}^n$, and $\hat{\sigma}\phi_i(x) = \phi_i(\sigma x)$, $\sigma > 0$, then we define

$$\hat{\sigma}\mathcal{D}_n = \text{Span}\{\hat{\sigma}\phi_i\}_{i=1}^n \tag{3.2}$$

and

$$\mathbf{D}_n = \bigcup_{\sigma>0} \hat{\sigma}\mathcal{D}_n. \tag{3.3}$$

Of course, this union of scaled linear spaces is not itself a linear space. Now we are in a position to define kinetic potentials by the expression

$$\tilde{f}_{nl}(s) = \inf_{\mathbf{D}_n} \sup_{\substack{\psi \in \mathbf{D}_n \\ \|\psi\|=1 \\ (\psi, K\psi)=s}} (\psi, f\psi). \tag{3.4}$$

A kinetic potential (a contraction of the term *minimum mean iso-kinetic potential*) represents the result of min-max applied to the potential *shape* f : the coupling parameter v is not included. Only in the final stage of minimization do we recover the eigenvalue in terms of v , thus

$$E_{nl} = F_{nl}(v) = \min_{s>0} \{s + v\bar{f}_{nl}(s)\}. \quad (3.5)$$

It is not difficult to show [9, 10] that the kinetic potentials are *convex*, that they are ordered like the eigenvalues, that is to say, $F > G \Rightarrow \bar{f} > \bar{g}$, and that they have the following scaling properties:

$$\alpha f(tr) \rightarrow \alpha \bar{f}(s/t^2). \quad (3.6)$$

We can use calculus to invert (3.5) and express kinetic potentials in terms of the trajectory functions. Thus from (3.5) we have the transformation pairs

$$s = F_{nl}(v) - vF'_{nl}(v) \quad \bar{f}_{nl}(s) = F'_{nl}(v) \quad (3.7)$$

and

$$v^{-1} = -\bar{f}'_{nl}(s) \quad v^{-1}F_{nl}(v) = \bar{f}_{nl}(s) - s\bar{f}'_{nl}(s). \quad (3.8)$$

Fortunately, because of (3.7), we do not have to use the abstract definition (3.4) in order to construct component kinetic potentials from known trajectory functions. Meanwhile, the transformation (3.8) allows us to reconstruct the energy spectrum from the kinetic potentials.

In the case of the Coulomb potential (which we shall need in section 4) we obtain from (3.7) and the well known Coulomb spectrum $C_{nl}(v)$

$$c(r) = -r^{-1} \rightarrow C_{nl}(v) = -\frac{v^2}{4(n+l)^2} \rightarrow \bar{c}_{nl}(s) = -\frac{s^{1/2}}{(n+l)}. \quad (3.9)$$

For the S -states of the Hulthén potential (with a convenient scale parameter t included) we have from (1.2), (3.6) and (3.7)

$$h(r) = -\frac{1}{e^{tr} - 1} \rightarrow \bar{h}_{no}(s) = -\frac{1}{2} \left[\left(\frac{4s}{n^2 t^2} + 1 \right)^{1/2} - 1 \right]. \quad (3.10)$$

If the potential shape $f(r) = g(h(r))$ is a smooth transformation g of a soluble potential $h(r)$, then the kinetic potentials associated with $f(r)$ are given [9, 10] approximately by the simple formula

$$\bar{f}_{nl}(s) \approx g(\bar{h}_{nl}(s)). \quad (3.11)$$

If g is convex we get lower bounds ($\approx = \geq$) for *all* n and l , and if g is concave we get upper bounds ($\approx = \leq$) for *all* n and l . This result has [9] a very interesting geometrical interpretation in terms of envelopes: if we think of $f = g(h)$ as a function of h , then each tangent line to the graph of g is a shifted h -potential which is soluble and has a known energy trajectory; the *envelope* of this family of trajectories is precisely the trajectory we get when the RHS of (3.11) is substituted in (3.5).

This convenience of approximation in terms of kinetic potentials extends also to *sums* because it turns out [10] that the kinetic potentials are almost additive. More explicitly, the kinetic potentials corresponding to the sum of potential terms

$$f(r) = \sum_{i=1}^N a_i f^{(i)}(r) \quad (3.12)$$

are given [10] approximately by the expression

$$\bar{f}_{nl}(s) \approx \sum_{i=1}^N a_i \bar{f}_{nl}^{(i)}(s). \tag{3.13}$$

At the bottom of each angular-momentum subspace we get a *lower bound*, that is to say, for $n=1$ and each l we have $\approx = \geq$. For the higher radial excitations, this approximation, although no longer *a priori a bound*, remains very good. It is the extension of this result to integrals which we shall need to employ in section 5.

4. The Yukawa potential as a transformation of the Hulthén potential

In this section of the paper we find it convenient to work with the following definitions of y and h :

$$y(r) = -\frac{e^{-r}}{r} \quad \text{and} \quad h(r) = -\frac{1}{e^{br}-1}. \tag{4.1}$$

Consequently, if we express y as the transformation g of h then g becomes

$$g(h) = y \left[\frac{1}{b} \ln \left(1 - \frac{1}{h} \right) \right]. \tag{4.2}$$

We must now discuss the convexity of g . We find that $g''(h)$ may be written in the form $g'' = PQ$, where

$$P = \frac{e^{-r}(e^{br}-1)}{r^3 b^2 h^2 (h-1)^2} > 0$$

and

$$Q(r, b) = \{2 + (2+b)r + (1+b)r^2 - e^{br}[2 + (2-b)r + (1-b)r^2]\}. \tag{4.3}$$

A careful analysis of Q shows that $Q(r, 1) \leq 0$ and $Q(r, \sqrt{6}) \geq 0$ for all $r \geq 0$; but Q changes sign if $b \in (1, \sqrt{6})$. The formal proof of this claim is straightforward but long. Some functions $g(h)$ are shown in figure 2 for a selection of values of b from 1 to $\sqrt{6}$.

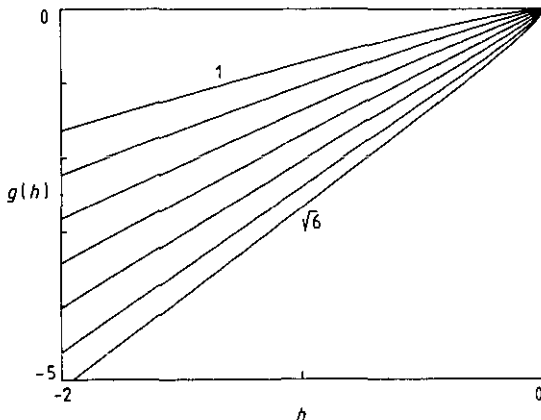


Figure 2. Graphs of $y = g(h)$, which expresses the Yukawa potential y as functions of the Hulthén potential $h(r) = -(e^{br}-1)^{-1}$ for $b = 1(0.25)2.25$, and $b = \sqrt{6}$. For $b = 1$, g is concave; for $b = \sqrt{6}$, g is convex; but for $b \in (1, \sqrt{6})$ the convexity of g is not definite.

The change in the convexity of $g(h)$ as b is varied is clearly illustrated in this figure, which, of course, is not offered as a proof of our claim.

We are now in a position to use our theory to obtain spectral approximations and bounds. For the S -states, according to (3.11), we simply use $g(\bar{h}_{n0}(s))$ in place of the unknown Yukawa kinetic potentials $\bar{y}_{n0}(s)$ in the general energy formula (3.5). It is interesting that we can, almost by sleight of hand, reparametrize the minimization in (3.5) in the following way. We change variables from s to r by the general equation

$$h(r) = \bar{h}_{nl}(s). \tag{4.4}$$

This is possible in principle because of the monotonicity [10] of both h and \bar{h}_{nl} . We then invert $\bar{h}_{nl}(s)$ to obtain s in terms of r ; and, at the same time, we observe that, in view of (4.4), $g(\bar{h}_{nl}(s)) = g(h(r)) = y(r)$, the original Yukawa potential. In the present example this only works for the S -states $l=0$ because these are the only states for which we have the exact kinetic potentials given by (3.10). Finally, we obtain the following special case of the energy formula (3.5):

$$E_{n0} \approx \min_{r>0} \left\{ \frac{n^2 b^2 e^{br}}{(e^{br} - 1)^2} + vy(r) \right\}. \tag{4.5}$$

We obtain our best lower bound when $b = \sqrt{6}$ (g is convex) and our best upper bound when $b = 1$ (g is concave); these bounds are valid for *all* n . In the limit as $b \rightarrow 0$ we recover the (S -state case) of the Coulomb envelopes used in [4]. In this case we can obtain upper bounds for *all* n and l because the Yukawa potential is a *concave* function of the soluble Coulomb shape $c(r) = -1/r$. The general formula for Coulomb envelopes is

$$E_{nl} \leq EC = \min_{r>0} \left(\frac{(n+l)^2}{r^2} + vy(r) \right). \tag{4.6}$$

In table 1 we exhibit some results obtained from (4.5) and (4.6). Accurate numerical data for the same set of eigenvalues will be shown later in table 2 of section 5.

Table 1. S -state eigenvalues of the Hamiltonian $H = -\Delta + vy(r)$ by Hulthén envelopes $y(r) = -e^{-r}/r = g(h(r))$, where $h(r) = -(e^{br} - 1)^{-1}$. The case $b = \sqrt{6}$ gives the best lower bound, and $b = 1$ gives the best upper bound. EC are upper bounds obtained from the Coulomb representation $y(r) = g(-1/r)$. Corresponding accurate numerical data EN are shown in table 2.

v	n	$b = \sqrt{6}$	$b = 2$	$b = 1$	EC
15	1	-42.708	-42.543	-42.294	-42.211
	2	-4.412	-3.852	-2.939	-2.611
30	1	-196.479	-196.312	-196.063	-195.979
	2	-31.925	-31.283	-30.302	-29.970
	3	-6.828	-5.642	-3.652	-2.921
70	1	-1156.491	-1156.324	-1156.074	-1155.991
	2	-242.105	-241.443	-240.446	-240.113
	3	-78.906	-77.457	-75.246	-74.499
	4	-28.349	-25.991	-22.233	-20.916
	5	-10.792	-7.900	-2.790	-0.796

In (4.5) and (4.6) the transformation function g no longer appears: only the establishment of energy *bounds* requires a study of the convexity of g . The expression (4.6), for example, can be used to approximate the spectrum of *any* potential $y(r)$ which can in principle be written as a smooth transformation g of $-1/r$.

5. The Yukawa potential as a continuous mixture of Hulthén potentials

The idea we explore in this section of the paper is to represent the Yukawa potential $y(r)$ in the form

$$y(r) = \int_0^\infty \rho(t)h(rt) dt \tag{5.1}$$

where $\rho(t)$ might be called the Hulthén transform of $y(r)$. The point of this is that we can then take advantage of the almost additivity of kinetic potentials by using an integral version of (3.13). However, we shall first deal with the potential.

The representation (5.1) immediately raises certain technical questions which we shall not deal with generally. Instead we consider the simpler approximation

$$y(r) \approx k(r) = \int_a^b uh(rt) dt \tag{5.2}$$

where u , a and b are constants. As we did in section 2 we demand correct behaviour near $r=0$. By comparing the Laurent expansions of $y(r)$ and $k(r)$ and equating the coefficients of $1/r$ and the constant terms we obtain the two conditions

$$u \ln(b/a) = 1 = u(b-a)/2. \tag{5.3}$$

Consequently we have only one free parameter, which we choose to be a . The approximation therefore becomes

$$y(r) \approx k(r) = \frac{2}{b-a} \int_a^b h(rt) dt \tag{5.4}$$

with b chosen to satisfy

$$b - 2 \ln(b) = a - 2 \ln(a) \quad a < 2 < b. \tag{5.5}$$

This prescription is well defined since the function $x - 2 \ln(x)$ is U shaped on $(0, \infty)$ and has a minimum at $x=2$. Again, following section 2, we look at the difference function $d(r) = k(r) - y(r)$. We find by computer experiments that for $a=0.688$ we have $|d(r)| < 0.011$. A graph of $d(r)$ is shown in figure 3. We may therefore write the potential inequalities

$$k(r) - 0.011 < y(r) < k(r) + 0.011. \tag{5.6}$$

We now turn to the kinetic potentials and the spectrum. The extension of (3.12) and (3.13) to the case of continuous mixtures of potentials with different scales leads immediately to the formula pair

$$k(r) = \int_0^\infty \rho(t)h(rt) dt \tag{5.7}$$

and

$$\bar{k}_{nl}(r) \approx \int_0^\infty \rho(t)\bar{h}_{nl}(r/t^2) dt \tag{5.8}$$

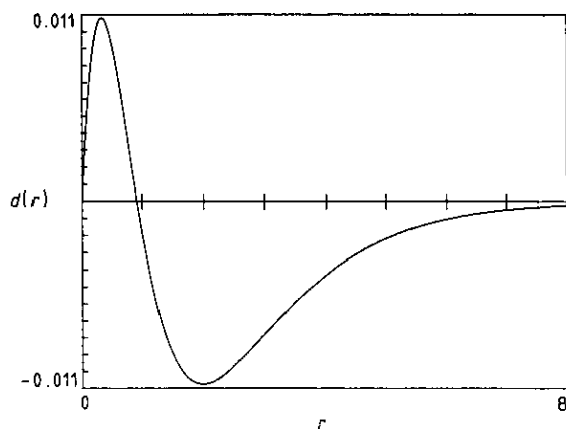


Figure 3. The difference function $d(r) = k(r) - y(r)$ between the Yukawa potential y and the continuous mixture of Hulthén potentials $k(r)$ given by (5.4). With $a = 0.688$ (and b fixed by the regularity condition (5.5)), we have $|d(r)| < 0.011$.

where (5.8) yields a lower bound for the bottom of each angular momentum subspace. By substituting the Hulthén S -state kinetic potentials (3.10) into (5.8) with $\rho(t)$ as in (5.4) we obtain from the general energy expression (3.5) the following approximation for the Yukawa spectrum:

$$E_{n0} \approx EA = \min_{s>0} \left\{ s + \frac{v}{b-a} \int_a^b \left[\left(\frac{4s}{n^2 t^2} + 1 \right)^{1/2} - 1 \right] dt \right\}. \quad (5.9)$$

We use the value $a = 0.688$ and the corresponding $b \approx 4.398\,427$ given by (5.5); with these assignments we know that $EA - (0.011)v$ is a lower bound for $n = 1$. In table 2 we exhibit the results EA given by (5.9), along with the lower bounds EL for $n = 1$, upper bounds given by (2.4), and some accurate values EN found by the direct numerical integration of Schrödinger's equation. The only adjustment we made was to choose a so as to optimize our approximation for $\rho(t)$ in (5.1) as a rectangular

Table 2. S -state eigenvalues of the Hamiltonian $H = -\Delta - v e^{-r}/r$. EA are given by (5.9) and are derived from the approximation to the Yukawa potential as a continuous mixture of Hulthén potentials; EL are the corresponding lower bounds for $n = 1$. EU are the upper bounds from the inequalities (2.4), and EN are accurate values obtained by direct numerical integration of Schrödinger's equation.

v	n	EL	EA	EU	EN
15	1	-42.680	-42.515	-42.250	-42.636
	2		-3.784	-3.063	-3.812
30	1	-196.600	-196.270	-196.000	-196.439
	2		-31.233	-30.250	-31.511
	3		-5.447	-4.000	-5.471
70	1	-1157.041	-1156.271	-1156.000	-1156.473
	2		-241.317	-240.250	-241.892
	3		-77.338	-75.111	-78.021
	4		-25.790	-22.563	-26.151
	5		-7.139	-4.000	-7.055

distribution on $[a, b]$. Clearly the integral version (5.8) of the sum (3.13) is an interesting approximation.

In table 3 we show some more results for an application to atomic physics. For this example we follow McEannan *et al* [11] who consider the outer electron of an atom with atomic number Z which has (approximately) the Hamiltonian

$$\mathbb{H} = -\frac{1}{2}\Delta - w e^{-\lambda r}/r \tag{5.10}$$

where

$$\lambda = \lambda_0 \alpha Z^{1/3} \quad w = \alpha Z \quad \lambda_0 = 1.13 \quad \alpha = (137.037)^{-1}. \tag{5.11}$$

In our notation we rescale and consider instead the Hamiltonian $H = -\Delta + v\gamma$, set $v = 2Z^{2/3}/\lambda_0$, and obtain the energy in kiloelectronvolts in terms of the eigenvalues E of H by the following formula: energy = $(255.4846)\lambda^2 E$. This factor is obtained by requiring the lowest eigenvalue $-\frac{1}{2}\alpha^2$ of \mathbb{H} with $\lambda = 0$ and $Z = 1$ to be equivalent to -13.6047 eV, the lowest energy of the hydrogen atom. In figure 4 we show graphs of the energy functions to be minimized in (5.9) for gold ($Z = 79$) and $n = 2, 3$ and 4. Our numerical results are shown as EA in table 3, along with $EL = EA - (0.011)v$ for $n = 1$, EU from the upper inequality of (2.4), and some numerical values EN from [11].

Table 3. S -state eigenvalues of three atoms. The approximations are as for table 2 save that the results are quoted in kiloelectronvolts and the numerical data EN are from [11].

Z	n	EL	EA	EU	EN
13	1	-1.4903	-1.4800	-1.4554	-1.488
	2		-0.549	-0.0191	
36	1	-14.2571	-14.2169	-14.1663	-14.24
	2		-1.6719	-1.5107	-1.692
	3		-0.1054	-0.00885	
79	1	-75.0055	-74.8908	-74.8044	-74.95
	2		-12.4029	-12.0837	-12.50
	3		-2.3938	-1.8903	
	4		-0.2130	-0.00172	

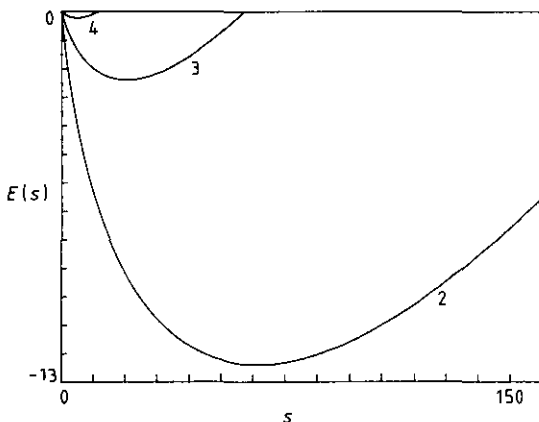


Figure 4. The energy functions $E_n(s)$ to be minimized in (5.9) for the application to gold ($Z = 79$) and $n = 2, 3$ and 4. The minima are the approximations EA to the Yukawa eigenvalues shown in table 3.

6. Conclusion

In this paper we have looked at various ways of relating the Yukawa potential y to the soluble Hulthén potential h . Two principal representations were explored: (i) smooth transformations $y(r) = g(h(r))$, and (ii) continuous mixtures $y(r) = \int \rho(t)h(rt) dt$. Such compositions of component soluble potentials can only be of use provided we can find some way of treating them. It turns out that both representations can be conveniently studied if we reformulate the min-max characterization of Schrödinger eigenvalues in terms of kinetic potentials. The variational task is thereby divided into two stages: kinetic potentials are the result of optimizing with respect to the potential *shape*; the final stage, involving the coupling parameter, is the minimization of a function of a single real variable and generates a semi-classical form for the original quantum-mechanical problem. The advantage of this is that, to a very good approximation, the kinetic potentials $\bar{y}(s)$ are built from the components, just like the potentials themselves; that is to say, respectively, (i) $\bar{y}(s) = g(\bar{h}(s))$, and (ii) $\bar{y}(s) = \int \rho(t)\bar{h}(s/t^2) dt$. Moreover, as we have seen, these general *approximations* are very often, at the same time, energy *bounds*.

Acknowledgments

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