Dynamical-group approach to the Hulthén potential

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High-accuracy approximations of the bound-state energies of the Hulthén potential are obtained by means of algebraic perturbation calculations which are based upon the dynamical-group structure SO(2,1).

I. INTRODUCTION

The Hulthén potential[1] has been used in a number of areas in physics, ranging from nuclear physics[2,3] to atomic physics.[4] In atomic units the potential is given by

$$V(r) = -Z\lambda e^{-\lambda r}/(1 - e^{-\lambda r}) , \qquad (1.1)$$

where λ is the screening parameter and Z can be regarded as the charge of the nucleus. Its main advantage is that it yields closed analytic solutions for the s waves.[5] Amongst the various methods which have been proposed in order to evaluate bound-state energies of the Hulthén potential (1.1) for $l \neq 0$ (Ref. 6), the Padé approximation methods[7] yield fairly accurate results.

In the present paper we shall study the nonzero angular momentum states in the context of algebraic perturbation theory. Therefore we present an approach which is based on the Lie algebra of the group SO(2,1), which is well known to be the dynamical group for a number of spherically symmetric potentials.[8] Also for s waves the Hulthén potential has been treated already from the SO(2,1) algebraic point of view.[9] Recently, a nonperturbative scaling variational method based on SO(2,1) has been formulated by Gerry et al.[10] and applied to a class of screened Coulomb potentials.[11] As it is the case in their work, we shall also introduce a so-called tilting transformation that relates between physical states and the group states which constitute a basis of the relevant unitary irreducible representations of SO(2,1). It will be demonstrated that all the matrix elements of the energy functional can be expressed in closed form. Then the energy matrix, in which the unknown bound-state energies occur on diagonal as well as on off-diagonal positions, is numerically diagonalized by means of a Gauss-Seidel iteration scheme.[12] The tilting parameter is thereby adjusted in order to accelerate the convergence of the perturbation expansions. This same technique has been applied previously to the Schrödinger equation for the exponential-cosine screened Coulomb potential.[13] In the present case of the Hulthén potential we again obtain very accurate results, and this in spite of the appearance of a transcendental function in the denominator of the potential. At the end of the paper our results are listed for certain typical values of the screening parameter λ.

II. ALGEBRAIC FORMULATION

The noncompact SO(2,1) Lie algebra is realized in terms of the radial vector r and the momentum p as follows:[14]

$$K_1 = \tfrac{1}{2}(rp^2 - r), \quad K_2 = \mathbf{r} \cdot \mathbf{p} - i, \quad K_3 = \tfrac{1}{2}(rp^2 + r) , \qquad (2.1)$$

where $\mathbf{p} = -i\nabla$. Introducing the ladder operators $K_\pm = K_1 \pm iK_2$, we shall utilize the Hermitian SO(2,1) representation in which the compact generator K_3 is diagonal. Denoting by $|lmn\rangle$ the orthonormal basis states of the representation space, the irreducible representation is completely determined by

$$K_3 |lmn\rangle = n |lmn\rangle ,$$

$$K_\pm |lmn\rangle = \sqrt{(l+1 \pm n)(\pm n - l)} |lmn \pm 1\rangle ,$$

$$L^2 |lmn\rangle = (K_3^2 - K_1^2 - K_2^2)|lmn\rangle = l(l+1)|lmn\rangle$$

$$(n \in \{1,2,3,\dots\}, \; l \in \{0,1,\dots,n-1\} ,$$

$$m \in \{-l, -l+1, \dots, l\}) , \qquad (2.2)$$

where $n = n_r + l + 1$, n_r the radial quantum number and l being the orbital angular momentum.

The Schrödinger equation with the Hulthén potential (1.1) can be rewritten on multiplication with $r[1 - \exp(-\lambda r)]$ as

$$\Omega(E)|\psi\rangle = 0 , \qquad (2.3)$$

$$[\tfrac{1}{2}(1 - e^{-\lambda r})rp^2 - \lambda Z e^{-\lambda r} r - E(1 - e^{-\lambda r})r]|\psi\rangle = 0 .$$

On account of the realization (2.1) the energy functional $\Omega(E)$ can be written as

$$\Omega(E) = \tfrac{1}{2}[1 - e^{-\lambda(K_3 - K_1)}](K_3 + K_1)$$

$$+ (E - \lambda Z)e^{-\lambda(K_3 - K_1)}(K_3 - K_1) - E(K_3 - K_1) . \qquad (2.4)$$

Next, we carry out a tilting transformation so that the Schrödinger equation (2.3) becomes

$$\bar{\Omega}(E,\theta)\,|\,\bar{\psi}\rangle \ , \tag{2.5}$$

where

$$|\,\bar{\psi}\rangle = e^{-i\theta K_2}\,|\,\psi\rangle \tag{2.6}$$

and

$$\bar{\Omega}(E,\theta) = e^{-i\theta K_2}\Omega(E)e^{i\theta K_2} \ . \tag{2.7}$$

Through the use of the Baker-Hausdorff-Campbell formula

$$e^{-i\theta K_2}(K_3 \pm K_1)e^{i\theta K_2} = e^{\pm\theta}(K_3 \pm K_1) \tag{2.8}$$

it is easily verified that

$$\bar{\Omega}(E,\theta) = \left[\frac{1}{2\omega} - \omega E\right]K_3 + \left[\frac{1}{2\omega} + \omega E\right]K_1$$

$$+ \left[-\frac{1}{2\omega} + \omega(E - \lambda Z)\right]e^{-\omega\lambda(K_3 - K_1)}K_3$$

$$+ \left[-\frac{1}{2\omega} - \omega(E - \lambda Z)\right]e^{-\omega\lambda(K_3 - K_1)}K_1 \ , \tag{2.9}$$

wherein

$$\omega = e^{-\theta} \ . \tag{2.10}$$

A method to obtain in closed form the matrix elements of the exponential operator on the right-hand side of (2.9) in the SO(2,1) group state basis, has been established by Bargmann.[15] The application of this method yields

$$\langle n'l\,|\,e^{-\omega\lambda(K_3-K_1)}\,|\,nl\rangle = \langle nl\,|\,e^{-\omega\lambda(K_3-K_1)}\,|\,n'l\rangle$$

$$= \frac{1}{\Gamma(n'-n+1)}\left[\frac{\Gamma(n'-l)\Gamma(n'+l+1)}{\Gamma(n-l)\Gamma(n+l+1)}\right]^{1/2}\left[1+\frac{\omega\lambda}{2}\right]^{-n'-n}\left[\frac{\omega\lambda}{2}\right]^{n'-n}$$

$$\times {}_2F_1\left[l+1-n, -n-l; 1+n'-n; \frac{\omega^2\lambda^2}{4}\right] \quad (n' \geq n) \ , \tag{2.11}$$

whereas from (2.2) we immediately obtain that

$$\langle n'l\,|\,K_3\,|\,nl\rangle = n\delta_{n'n} \ , \tag{2.12}$$

$$\langle n'l\,|\,K_1\,|\,nl\rangle = \langle nl\,|\,K_1\,|\,n'l\rangle$$

$$= \tfrac{1}{2}\sqrt{(n-l)(n+l+1)}\,\delta_{n'n+1} \quad (n' > n) \ . \tag{2.13}$$

Notice that we have dropped everywhere the irrelevant quantum label m. The function ${}_2F_1(a,b;c;z)$ represents a hypergeometric series which in (2.11) always reduces to a polynomial. Finally, the matrix elements of the energy functional $\bar{\Omega}(E,\theta)$ can be calculated on account of the completeness relation for the SO(2,1) group states.

III. PERTURBATION EXPANSION

A first approximation to the bound-state energies can be obtained by considering only the diagonal terms of the energy matrix $\bar{\Omega}(E,\theta)$, hence by solving

$$\langle nl\,|\,\bar{\Omega}(E,\theta)\,|\,nl\rangle = 0 \tag{3.1}$$

with respect to E. However, the solution being θ dependent, it has been shown by Feranchuk and Komarov[16] that the choice

$$\left[\frac{\partial E_{nl}^{(0)}(\theta)}{\partial \theta}\right]_{(\theta=\theta_{nl})} = 0 \tag{3.2}$$

yields attractive results for the approximations of zeroth order.

Here we want to correct the lowest-order estimates by treating the nondiagonal elements as perturbation terms. Let us therefore notice that all the matrix elements of

$\bar{\Omega}(E,\theta)$ are linear with respect to E. Hence, we write

$$\langle n'l\,|\,\bar{\Omega}(E,\theta)\,|\,nl\rangle = a_{n'n} + Eb_{n'n} \ . \tag{3.3}$$

Since the operator $\bar{\Omega}(E,\theta)$ leaves the l value unchanged, its nth eigenstate $|\,\bar{\psi}nl\rangle$ associated with a particular l value, can be expanded in terms of the SO(2,1) group states as follows:

$$|\,\bar{\psi}_{nl}\rangle = \sum_{i=l+1}^{\infty} c_i\,|\,il\rangle \ . \tag{3.4}$$

The substitution of (3.3) into (2.5) yields

$$\sum_{i=l+1}^{\infty}\sum_{j=l+1}^{\infty}(a_{ji} + b_{ji}E_{nl})c_i\,|\,jl\rangle = 0 \ , \tag{3.5}$$

and, since the group states belong to a basis, all the coefficients accompanying basis states should vanish. For $j = n$ we solve the secular equation (3.5) with respect to E_{nl},

$$E_{nl} = -\frac{\Sigma_i a_{ni}c_i}{\Sigma_i b_{ni}c_i} \ , \tag{3.6}$$

whereas for $j \neq n$ we solve it with respect to the unknown c_j;

$$c_j = -\frac{\Sigma_{i,j(i\neq j)}a_{ji}c_i + \Sigma_{i,j(i\neq j)}b_{ji}c_iE_{nl}}{a_{jj} + b_{jj}E_{nl}} \quad (j\neq n) \ . \tag{3.7}$$

Equations (3.6) and (3.7) have the appropriate form in order to establish an iteration algorithm for the calculation of E_{nl}. Denoting the pth order approximations of E_{nl} and of the coefficients c_j, respectively, by $E_{nl}^{(p)}$ and $c_j^{(p)}$, the following Gauss-Seidel iteration scheme is proposed:

TABLE I. Energy eigenvalues E_{nl} in atomic units as a function of the screening parameter λ for 1s-3d states and for $Z=1$. In square brackets are shown the ω value and the number of iterations. In parentheses are given for an s state the exact energy value and for a p or d state the Padé approximation result taken from Ref. 7.

λ	1s	2s	2p	3s	3p	3d
0.025	−0.487 577 7	−0.112 811 5	−0.112 760 4	−0.043 758 9	−0.043 707 1	−0.043 603 0
	[1.0,15]	[2.0,15]	[1.48,15]	[3.0,15]	[2.95,30]	[2.5,15]
	(−0.487 578 1)	(−0.112 812 5)		(−0.043 758 7)	(−0.043 707)	(−0.043 603)
0.050	−0.475 312 1	−0.101 248 5	−0.101 042 5	−0.033 368 7	−0.033 165 0	−0.032 753 2
	[1.0,35]	[2.0,25]	[1.485,15]	[3.0,25]	[2.95,30]	[2.5,15]
	(−0.475 312 5)	(−0.101 250 0)	(−0.101 044 3)	(−0.033 368 1)	(−0.033 165)	(−0.032 753)
0.100	−0.451 249 0	−0.079 996 9	−0.079 179 4	−0.016 807 0	−0.016 053 7	−0.014 484 2
	[1.0,40]	[2.0,25]	[1.49,15]	[3.015,25]	[3.0,15]	[2.5,15]
	(−0.451 250 0)	(−0.080 000 0)	(−0.079 179)	(−0.016 805 6)	(−0.016 054)	(−0.014 484)
0.150	−0.427 810 7	−0.061 245 3	−0.059 441 5	−0.005 879 7	−0.004 466 4	−0.001 396 5
	[1.0,40]	[2.005,25]	[1.51,15]	[3.015,25]	[3.025,15]	[3.0,15]
	(−0.427 812 5)	(−0.061 250 0)		(−0.005 868 0)	(−0.004 466)	(−0.001 391)
0.200	−0.404 993 5	−0.045 001 4	−0.041 886 0	−0.000 560 7		
	[1.005,40]	[2.005,25]	[1.52,15]	[3.02,25]		
	(−0.405 000 0)	(−0.045 000 0)	(−0.041 886)	(−0.000 555 6)		
0.300	−0.361 231 7	−0.020 001 4	−0.013 790 0			
	[1.01,30]	[2.01,25]	[1.53,25]			
	(−0.361 250 0)	(−0.020 000 0)				

$$E_{nl}^{p}=-\frac{\sum_i a_{ni}c_i^{(p)}}{\sum_i b_{ni}c_i^{(p)}} \quad (p \geq 0) \ ,$$

$$c_j^{(p)}=-\left[\sum_{\substack{i,j \\ i<j}} a_{ji}c_i^{(p)}+\sum_{\substack{i,j \\ i<j}} b_{ji}c_i^{(p)}E_{nl}^{(p-1)}+\sum_{\substack{i,j \\ i>j}} a_{ji}c_i^{(p-1)}+\sum_{\substack{i,j \\ i>j}} b_{ji}c_i^{(p-1)}E_{nl}^{(p-1)}\right]\Big/(a_{jj}+b_{jj}E_{nl}^{(p-1)}) \quad (j \neq n, \ p \geq 1) \ , \qquad (3.8)$$

$$c_n^{(p)}=1 \quad (p \geq 1) \ ,$$

whereby the initial c values are given by

$$c_j^{(0)}=\delta_{jn} \ . \qquad (3.9)$$

For each value of the free tilting parameter θ for which the scheme (3.8) and (3.9) is convergent the property $\lim_{p \to \infty} E_{nl}^{(p)}=E_{nl}$ is satisfied. Nevertheless, the rate of convergence is expected to be θ dependent. This fact is confirmed by the numerical calculations which are discussed in the next section.

IV. NUMERICAL RESULTS AND DISCUSSION

The iterative scheme expounded in the previous section has been used to calculate the bound-state energy values for certain typical values of the screening parameter λ. Although the scheme (3.8)–(3.9), when it is convergent, theoretically produces the correct eigenvalue E_{nl} in the limit $p \to \infty$, we have to introduce in practice one more

TABLE II. Energy eigenvalue E_{nl} in atomic units as a function of the screening parameter λ for states with $n=4$. The results shown in square brackets and in parentheses have the same meaning as in Table I.

λ	4s	4p	4d	4f
0.025	−0.020 001 7	−0.019 949 0	−0.019 846 2	−0.019 691 1
	[4.0,25]	[4.0,20]	[4.0,15]	[4.0,15]
	(−0.020 000 0)	(−0.019 949)	(−0.019 846)	(−0.019 691)
0.050	−0.011 253 3	−0.011 058 3	−0.010 667 4	−0.010 061 9
	[4.01,25]	[4.0,25]	[4.0,15]	[4.0,15]
	(−0.011 250 0)	(−0.011 058)	(−0.010 667)	(−0.010 062)
0.075	−0.005 007 5	−0.004 622 4	−0.003 834 6	−0.002 556 3
	[4.015,25]	[4.1,25]	[4.1,25]	[4.0,15]
	(−0.005 000 0)	(−0.004 622)	(−0.003 834)	(−0.002 556)
0.100	−0.001 253 2			
	[4.02,25]			
	(−0.001 250 0)			

constraint. Indeed, due to the exponential occurring in the potential, the off-diagonal energy matrix coefficients a_{ij} and b_{ij} do not vanish in general, although, far away from the diagonal, they become neglectable. Hence, for calculational purposes, since it is impossible to evaluate to all orders p an infinity of $c_j^{(p)}$ coefficients, we have built in a cutoff on the energy matrix such that it reduces to a band matrix. On the other hand, it has been verified that the rate of convergence of the iteration procedure strongly depends upon the tilting angle θ and, hence, upon the chosen value of the parameter ω. This fact necessitates the derivation for each particular case of an optimum value of that parameter. It turns out that the optimum depends not only upon the value of the screening parameter but also upon the state under consideration.

In Tables I and II the results which have been obtained by the present technique are listed and compared either with exact values or with the results obtained by a Padé approximation method.[7] Indeed, for the s states the bound state energies for $Z = 1$ are known to be given by the simple formula[5]

$$E_{n0} = -\frac{1}{8n^2}(2 - \lambda n^2)^2 . \qquad (4.1)$$

Also, all the calculations have been carried out by restricting the energy matrix (3.3) to a nineteen-band matrix, which means that these coefficients a_{ij} and b_{ij} for which $|j - i| > 9$ have been set equal to zero. In the tables we also show the number of iterations required and the optimal ω value. It should be remarked that for s states this optimal value is close to the theoretical value which one obtains in the case of a pure Coulomb potential from the ansatz (3.2). Also, we have noticed that the convergence rate is more ω sensitive in the case of s states than it is for higher l values. Hence, we could expect that the accuracy of our approximations is much higher for the latter states, a fact which seems to be confirmed since the Padé approximation results are almost everywhere exactly reproduced. In view of the low calculational efforts required, the present technique therefore turns out to be very useful for obtaining high accuracy approximations of the bound-state energies of the Hulthén potential for $l \neq 0$.

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