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New Approach to Calculate Bound State Eigenvalues

EDGARDO GERCK

Instituto de Estudos Avançados, CTA, São José dos Campos, 12.200, SP, Brasil and Max Planck Institut für Quantenoptik, 8046, Garching, West Germany

JASON A. C. GALLAS

Departamento de Física, Universidade Federal de Santa Catarina, Florianópolis, 88.000, SC, Brasil and Max Planck Institut für Quantenoptik, 8046, Garching, West Germany

and

AUGUSTO B. d'OLIVEIRA

Instituto de Física, Universidade Federal Fluminense, Niterói, 24.000, RJ, Brasil

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Abstract A method of solving the radial Schrödinger equation for bound states is discussed. The method is based on a new piecewise representation of the second derivative operator on a set of functions that obey the boundary conditions. This representation is trivially diagonalised and leads to closed form expressions of the type $E = E(ab + b + c/n + \ldots)$ for the eigenvalues. Examples are given for the power-law and logarithmic potentials.

1. INTRODUCTION

This paper discusses a method of calculating the eigenvalues of the radial Schrödinger equation (in atomic units)

$$-\frac{1}{2}\frac{d^2}{dr^2}\tilde{\Psi} + V(r)\tilde{\Psi} = E\,\tilde{\Psi} \tag{1}$$

subject to the boundary conditions $\tilde{\Psi}(0) = \tilde{\Psi}(\infty) = 0$, where $V(r)$ may include the usual centrifugal terrn. A brief version of this work appeared recently[1].

The proposed approach is based on a new piecewise representation of the differential operator d^2/dr^2 from eq. (1) on the set

$$U_\alpha = \{\exp(-\alpha r),\ r.\exp(-\alpha r),\ r^2.\exp(-\alpha r)\} \tag{2}$$

Using this piecewise representation for d^2/dr^2 in the proposed appi-oach is equivalent to considering a continously and infinitely piecewise approximation $\Psi(r) = \sum_k \Psi_k(r)$ to the eigenfunction $\tilde{\Psi}(r)$ of eq. (1), where in each k-piece the $\Psi_k(r)$ is a linearcornbinationon the set U_{α_k} with $k \in N$:

$$\Psi_k(r) = (A_k + B_k r + C_k r^2)\exp(-\alpha_k r) \quad ; \; r_{k-1} \leq r \leq r_k$$

For any $\Psi(r)$ that is a linear combination on the set U_α, the unique two-point representation of the operator d^2/dr^2 is given by

$$\frac{d^2}{dr^2}\Psi(r) = \frac{2\alpha^2}{\exp(1)}\Psi(r - 1/\alpha) - \alpha^2\,\Psi(r) \tag{3}$$

as shown in sectíon 2. The ideal representation of the operator d^2/dr^2, i.e. the exact representation, would be given by its expánsion on the complete set of solutions of eq. (1). This set is of course infinite and, a priori, unknown. Wenote that the basis set U_α is clearly a good piecewise approxirnation to the ideal set if the parameter a is larger than zero. This is due to the fact that the U_α basis satisfies the boundary condition of eq. (1) at infinity.

The representation of the second derivative operator in U_α given by eq.(3) has severa1 uniqueproperties. Themainproperty is that this representation can be trivially diagonalized. Another characteristic aspect is that U_a (and hence $\Psi(r)$) depends on the free parameter a. This variational parameter will be determined by the method itself, through the stationary condition for E_n. This procedure will enable us to obtain analytical expressions for the eigenvalues of eq. (1), of the form $E_n = E(an + b + c/n + \ldots)$.

This paper is organized as follows. Section 2 presents the method for a general potential $V(r)$. Section 3 deals with the application of the method to power law and logarithmic potentials, together with a comparison of known results for some potentials now being studied as possible models of quark confinement (/2/ and references therein). The eigenvalues are given as a function of two parameters, a and b , in each case. The determination of these parameters in general is the subject of section 4. In section 5 the numerical accuracy of the eigenvalues, for the same examples as in section 3, is discussed and compared with known results. The last section contains a summary of the important features of the method.

2. THE METHOD

The method proposed here is based on the two-point piecewise representntion of the second derivative operator on the set U_α = $= \{\exp(-\alpha r), r.\exp(-\alpha r), r^2.\exp(-\alpha r)\}$, with $\alpha>0$. The main reasons for using this particular set are:

(i) Any element of U_a satisfies the boundary condition in eq. (1) at infinity.

(ii) The set $L(U_\alpha)$ of all the linear combinations of the elements of U_a is closed to the operation d^2/dr^2. This means that the second derivative of any linear cornbination of the elements of U_α is itse'lf a linear cornbination of the elements of U_α.

Foi- a function Ψ in $L(U_\alpha)$ the two-point representation of d^2/dr^2 can be found as the unique solution of the desired identity given by

$$\frac{d^2}{dr^2}\Psi(r) = p\,\Psi(r-q) + t\Psi(r) \tag{4}$$

where p, q and t are constants. These constants are uniquely calculated by requiring that eq.(4) be valid for each of the three functions of U_α. The constantsare

$$p = 2\,\alpha^2\,e^{-1} \tag{5}$$

$$q = 1/\alpha \tag{6}$$

$$t = -\,\alpha^2 \tag{7}$$

Equation (6) means that the distance between the two points must be

$$\Delta r = 1/\alpha \tag{8}$$

This representation of d^2/dr^2 on U_α is the cornerstone of this paper and is given by

$$\frac{d^2}{dr^2}\,\Psi(r) = \frac{2a^2}{e}\,\Psi(r-1/\alpha) - \alpha^2\,\Psi(r) \tag{9}$$

In this case, eq. (9) means that the second derivative of Y E $L(U_\alpha)$ is given exactly at any point r by a linear combination of the values of Y itself at the two points $r-1/\alpha$ and r, corresponding to property (ii) above. For a further discussion about the representation of d^2/dr^2 on U_α the reader is referred to the Appendix.

Introducing a grid r_k on the space coordinate $0 \leqslant r \leqslant \infty$ we may write $r_{k-1} - r_k - 1/\alpha_k$, where r_k is given by

$$r_k = f(k); \quad k = 0,1,2,... \tag{10}$$

with $f(0) \geqslant 0$ and with $r_k > r_{k-1}$ for any k. Note that f is an order preserving function, i.e. $k > j$ irnplies that $f(k) > f(j)$. This grid will be determined by the method itself.

The width of each k-piece given by $\text{Ar}_k = |f(k)-f(k-1)|$ satisfies eq. (8), i.e. $\Delta r_k \alpha_k = 1$, and may change with k since eq. (9) is a two-point formula.

From eqs. (8) and (10) it follows that

$$r_k = \frac{f(k)}{\Delta r_k \alpha_k} = \left[\frac{f(k)}{f(k)-f(k-1)}\right]\frac{1}{\alpha_k} \tag{11}$$

Since $f(k)$, $f(k-1)$ one can readily show that (see Appendix)

$$\frac{f(k)}{f(k)-f(k-1)} = ak + b + c/k + ... \tag{12}$$

where the several a, b, c, etc. are constants and $k = 1,2, ...$.

Equation (12) shows that for any function $f(k)$ the following is true:

(i) The higher k-order appearing in eq. (12) is one.

(ii) As point number k increases, eq. (12) is approximately linear in k.

For these reasons we may neglect the $O(1/k)$ contribution in eq. (12) and write

$$r_k = \frac{ak + b}{\alpha_k} \quad ; \quad k = 1, 2, 3, \ldots \tag{13}$$

This expression will play an important role in the following discussion. One should note that, in what follows, higher-order terms could have been used in eq. (13).

Armed with eqs. (9) and (13) we now turn to the problem of calculating the n-th eigenvalue of a given potential $V(r)$ in eq. (1). To this end we use the two-point representation of d^2/dr^2 given by eq. (9) in eq. (1) to consider the piecewise approximation

$$\psi^{(n)}(r) = \sum_k \psi^{(n)}(r) \quad \text{of} \quad \tilde{\psi}^{(n)} \qquad \text{where } \psi^{(n)}(r) \in L(U_{\alpha_k})$$

and α_k is yet a variational parameter, obtaining

$$-\frac{\alpha_k^2}{e}\, \psi^{(n)}(r_{k-1}) + \left[\frac{1}{2}\, \alpha_k^2 + V(r_k)\right] \psi^{(n)}(r_k) = E_r\, \psi^{(n)}(r_k) \tag{14}$$

for $k = 1, 2, \ldots$ where if $r_0 = 0$ then $\psi^{(n)}(r_0) = 0$ or if $r_0 \neq 0$ $\psi^{(n)}(r_0)$ is connected to the origin by eq. (A.5) (see Appendix). Equation (14) may also be written in matrix form: $M\Psi = E\Psi$ with $\Psi = (\Psi(r_1), \Psi(r_2), \ldots)^T$ and M a bidiagonal matrix given by

$$\begin{pmatrix} \frac{1}{2}\alpha_1^2 + V(r_1) & 0 & 0 & \cdots \\ -\alpha_2^2/e & \frac{1}{2}\alpha_2^2 + V(r_2) & 0 & \cdots \\ 0 & -\alpha_3^2/e & \frac{1}{2}\alpha_3^2 + V(r_3) & \\ \vdots & \vdots & \vdots & \end{pmatrix} \tag{15}$$

with no limit imposed on its order. This matrix is the representation of the Hamilton operator of eq. (1) and depends on the variational parameters a_1, a_2, ... with constraints.

We now note that, owing to the bidiagonal form of M, the n--eigenvector of M has the following form[3] :

$$\Psi^{(n)}(r_k) \begin{cases} = 0 \text{ if } k < n \\ \neq 0 \text{ if } k \geqslant r \end{cases} \tag{16}$$

and that all the eigenvalues of the eq. (14) are given trivially by the main diagonal of M, with no limit imposed on its order.

Using the eigenfunction form $\Psi^{(n)}(r_k)$ of eq. (16) for k=n in eq. (14) and recalling eq. (13) we get

$$E_n = \frac{1}{2}\alpha_n^2 + V\left(\frac{an+b}{\alpha_n}\right) \quad ; \quad n = 1,2, \ldots \tag{17}$$

where n is the radial quantum number.

Since $\Psi^{(n)}(r)$ is a function of the variational parameter the variational principle for E_n is $\partial E_n'/\partial\alpha = 0$ and can be directly applied to eq. (17) giving

$$\alpha_n + \frac{\partial}{\partial\alpha_n} V\left(\frac{an+b}{\alpha_n}\right) = 0 \tag{18}$$

The above equation also determines the parameters a of the basis U_α in any k-piece by means of eq. (A.8) from the Appendix and therefore corresponds to the variational principle $\partial E/\partial\alpha = 0$ applied to the whole $\Psi^{(n)}(r)$.

The general procedure being proposed here to obtain the bound states of eq. (1) begins by solving eq. (18) in order to determine the best α_n as defined above. By substituting this α_n in eq. (17) one obtains the eigenvalues as a *known function* of the constants a and b, namely

$$E_n = E(an + b) \tag{19}$$

The determination of a and b is discussed in section 4. We shall now compare eq. (19) for the power law and logarithmic potentials with known results.

3. APPLICATION TO THE POWER-LOW AND LOGARITHMIC POTENTIALS

To further clarify the proposed method we now apply it to some well-known eigenproblems. The results obtained are compared with the exact ones, whenever possible, or to approximations. For simplicity we only analyse s-states.

For the general power law potential $V(r) = K\,r^p$, with $p > -2$ and $p \neq 0$, eq. (17) gives (dropping the subscript n of a)

$$E_n = \frac{1}{2}\,\alpha^2 + K(an+b)^p/\alpha^p \tag{20}$$

From the stationary condition, $\partial E_n/\partial\alpha_n = 0$, it follows (compare with eq. (18)) that

$$\alpha = \left[Kp(an + b)^p\right]^{1/(p+2)} \tag{21}$$

Substituting back in eq. (20), one obtains

$$E_n = (Kp)^{2/(p+2)}(1/2 + 1/p)(an+b)^{2p/(p+2)} \tag{22}$$

as the bound state eigenvalues of the power law potential, or

$$E_n = \alpha^2(1/2 + 1/p) \tag{23}$$

in terms of α of eq. (21).

Using the same procedure for the logarithmic potential $V(r) = K\,\ell n(r)$, one obtains the eigenvalues

$$E_n = \frac{K}{2}\left[\ell n(e/K)\right] + K\,\ell n\,(an + b) \tag{24}$$

In Table 1 we given as functions of a and b, the solutions for some potentials which are nowadays of interest for a quark-quark confining model together with the general power law. The parameter a and b appearing in this table are calculated in section 4. However, as an example, the reader may recall that for $a = 1$ and $b = 0$ the Coulomb eigenvalues in Table 1 represent the correct bound-state spectrum for any order n.

In Table 1 two important functional relationships for the eigenvalues can be seen: with the scaling parameter K and with $(an+b)$. The remaining part of this section is devoted to a comparison of these two aspects of the function $E_n = E(an+b)$ with the known results. As a source of known results we use the work of Quigg and Rosner[2].

The K dependences of E_n given in Table 1 are all correct, as can very easily be verified by rescaling the Schrödinger equation (2).

The functional dependence of the eigenvalues with the quantum number as given in Table 1 is exact for the Coulomb, linear and harmonic potentials. For the other cases no exact solutionsare known. However, as can be seen from eqs. (4.33) and (4.59) from [2], our results indeed show the same quantum number dependence as the WKB ones. From the above comparison one sees that the proposed method reproduces the known functional dependences for the power law and logarithmic potentials with K and n.

For other potentials, the constants a and b could depend on the *scaling* constant K. However, and here we emphazise this point, the functional dependence $E_n = E(an + b)$ is always the same if the function $V(r)$ does not change. This can easily be verified from eqs. (17) and (18). This means that for any given potential $V(r)$ a scaling of the potential may only change a and b but not the function $E_n=E(an+b)$.

In the next section we discuss the calculation of a and b.

Potential	$V(r)$	α_n	E_n
Coulomb	$-K/r$	$K/[an + b]$	$-K^2/[2(an + b)^2]$
Harmonic	$K\ r^2$	$[2K(an + b)^2]^{1/4}$	$(2K)^{1/2}\ (an + b)$
Linear	$K\ r$	$[K(an + b)]^{1/3}$	$3/2)[K(an + b)/2]^{2/3}$
Square-root	$K\ r^{1/2}$	$[K(an+b)^{1/2}/2]^{2/5}$	$(5/2)(K/2)^{4/5}\ (an+b)^{2/5}$
Power-law	$K\ r^p$	$[Kp(an+b)^p]^{\left(\frac{1}{p+2}\right)}$	$[1/2 + 1/p]\ \alpha_n^2$
Logarithm	$K\ \ln(r)$	$(K)^{1/2}$	$K[\ln(e/K)]/2 + K\ \ln(an+b)$

Table 1: Summary of the results obtained by the proposed method for some potentials $V(r)$. E_n are the bound-state eigenvalues for $n = 1,2,\ldots$

4. CALCULATIONS OF A AND B

The procedure described in the previous sections leads to closed-form expressions of the type $E_n = E(an+b)$ for the eigenvalues.

To determine a and b, we study the behaviour of the first two eigenfunctions after the outer turning-point. In order to generate accurate eigenfunctions one usually needs $\Delta r << 1$. In general, however, this condition would conflict with the requirement $\Delta r = 1/\alpha$ in eq. (8). Instead of eq. (9) we therefore use the full three-point formula in U_α, given by eq. (A.1). The eq. (1) can be written in matrix form as $T\Psi = E\Psi$, where now T is tridiagonal. Since we already know the functional dependence of $\alpha_n = \alpha(an+b)$ and $E_n = E(an+b)$, the matrix equation $T\Psi = E\Psi$ has only two unknowns: a and b. This equation may be solved by any standard matrix technique or by using the continued fraction approach of Gerck und d'Oliveira . The later can be conveniently run in a programmable pocket calculator.

An alternative approach is self-evident: for any two eigenvalues E_i and E_j calculated by some numerical method we may set up a system of two equations, for $(ai+b)$ and $(aj+b)$, to obtain a and b.

In any one of the two suggested ways of determining a and b given above another advantage of the proposed method is clear: from

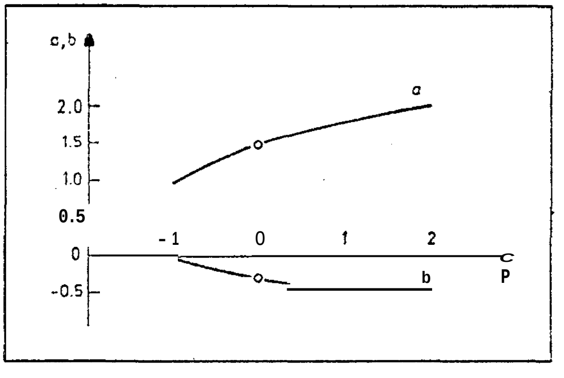

Fig.1 - Behaviour of the constants a and b in $E_n = E(an+b)$ for the power -law potential $V(r) = K r^p$ as a function of p.

the study of just two eigenfunctions or alternatively two eigenvalues the whole bound-state spectrum is obtained.

For the power law potential we show in Fig. 1 a plot of the pararneters a and b as a functions of the power p. This graph is illustrative of the general range of values of a and b.

5. NUMERICAL COMPARISON OF THE EIGENVALUES

To illustrate the accuracy of the eigenvalues calculated by the proposed rnethod, this section presents a short numerical comparison of the bound states E_n for the same potentials already discussed in section 3. The constants a and b were calculated using the three--point formulation from eq.(A.1) and applying to it the continued fraction approach from[4], The absolute error in a and b was chosen to be less thari 10^{-5}.

Table 2 presents the calculated values of a and b for some potentials. The eigenvalues E_n are readily obtained from Tables 1 and 2.

The calculated eigenvalues of the Coulomb and harmonic potentials coincide with the well-known exact results for any state ***n***.

Table 2: Values of the constants a and b in $E_n = E(an+b)$ from Table 1.

Potential	a	b
Coulomb	1.000000	.00000
Square-root	1.67120	-.36853
Linear	1.80523	-.42915
Harmonic	2.00000	-.50000
Logarithm	1.50198	-.28330

For the potentials $\ell n(r)$ and $r^{1/2}$ no exact solution is known. We therefore compare in Table 3 the first five calculated eigenvalues with those obtained from the WKB approximation and, when available, numerical results. It should be noted that the WKB result is not accurate for low n, as is well-known.

To show the effect of the constant c from eq. (12) in $E_n = E(an+b+c/n)$, we calculated this expression for the linear potential. The result is

$$E_n = (3/2)\, K^{2/3}\, (1.81425n - 0.45619 + 0.01803/n)^{2/3} \qquad (25)$$

For comparison the result for $E(an+b)$ is

$$E_n = (3/2)\, K^{2/3}\, (1.80523n - 0.42915)^{2/3} \qquad (26)$$

The first column of Table 4 gives the eigenvalues as calculated from eq. (26), the second column those from eq. (25), and the last two columns the exact and WKB results respectively. The exact results correspond to the zeros of the Airy functions[2]. As one can see the inclusion of c/n improves the eigenvalues. The contribution to E_n from higher order terms, i.e. $d/n^2 + \ldots$, can be inferred from the relative difference between $E(an+b)$ and $E(an+b+c/n)$. This is a general Cauchy-type criterion to estimate the intrinsic accuracy of the eigenvalues without referring to another result.

To close this section, we remark that although this paper is just intended to introduce the proposed method the eigenvalue expressions obtained in the cases of the square root and logarithmic potentials could be of interest on their own since there are no exact expressions available[5].

Table 3: Comparison between the first five eigenvalues for the square-root and logarithmic potentials.

$V(r)$	n	Present results	Numerical results[1]	WKB[1]
$\ell n(r)$	1	0.69777	0.69773	0.63123
	2	1.5009	1.5008	1.4785
	3	1.9405	1.9431	1.9305
	4	2.2448	2.2491	2.2407
	5	2.4778	2.4833	2.4771
$\sqrt{r}$	1	1.5961	-	1.5772
	2	2.2204	-	2.2135
	3	2.6540	-	2.6521
	4	3.0012	-	3.0024
	5	3.2967	-	3.3002

(1) From Ref./2/, in atomic units.

Table 4: Cornparison of the eigenvalues calculated by the proposed method, in two different approximations, withtheexact and WKB results for the linear potential $V(r) = r$.

n	$E(an+b)$[1]	$E(an+b+c/n)$[2]	Exact[3]	WKB[3]
1	1.8557	1.8558	1.8558	1.8416
2	3.2446	3.2446	3.2446	3.2385
3	4.3781	4.3817	4.3817	4.3781
4	5.3795	5.3867	5.3866	5.3843
5	6.2949	6.3055	6.3052	6.3037

(1) From eq. (26). (2) From eq. (25). (3) From Ref.2, in atomic units.

6. SUMMARY

We have presented a method to calculate the bound-states of the Schrödinger radial equation for a potential $V(r)$. The method is easy to apply and leads to an equation of the form $E_n = E(an+b+$ $+c/n \ldots)$ which may be approximated by $E_n = E(an+b)$. The constants a and b are calculated by means of the known functions

$$\alpha_n = \alpha(an+b) \text{ and } E_n .$$

The method is based on a new piecewise expansion of the second derivative operator in the set of functions I e ~ ~ (,r.exp()-αr), r^2.exp$(-\alpha r)\}$, with $\alpha>0$. This set satisfies the boundary condition at infinity and has the property that any function generated by linear combinations in it can have the second derivative *exactly* expressed at any point r as a linear combination of the values of the function itself at the points $r - \Delta r$, and $r + \Delta r$. Furthermore, for $\Delta r=1/\alpha$ only two values of the function are needed to express exactly its second derivative at one point. This last case leads to a bidiagonal matrix that is trivially diagonalized and produced a closed-form expression for the eigenvalues. By applying the stationary condition this expression gives also the optimum value for the a-parameter that makes the set used the best possible piecewise approximation, within the given exponentials, to the eigenfunctions.

Another feature of the rnethod is the sampling grid $f(k)$. The sampling grid has' a non-uniform sampling distance Δr_k and is determined through the constants a and b already mentioned.

The error of the method is determined instrinsically by the relative difference between $E(an+b)$ and $E(an+b+c/n)$, for example, for a particular state n. This corresponds to a Cauchy-type convergence criterion to judge when to stop the $an+b+c/n+\ldots$ sequence. As shown, although the full result of this method is given $E_n=E(an+b+c/n+\ldots)$ very good results are obtained by considering just $E_n=E(an+b)$.

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APPENDIX

Here we collect the following results required:

(I) representation of the operator d^2/dr^2 on U_α,

(Ii) expansion of $f(k)/f(k)-f(k-1))$ in powers of k and

(III) relationships for α_k and r_k.

I - Representation of d^2/dr^2 on U_α

The set of all possible linear cornbination in U_α is defined by $L(U_\alpha)$. Because d^2/dr^2 is a linear operator, the second derivative of any function of $L(U_\alpha)$ can be expressed as a linear combination of the second derivatives of the three elements of U_a.

The eigenfunctions considered in this paper are all piecewise linear combinations on the set U_α and they all belong to $L(U_\alpha)$. The representation of the operator d^2/dr^2 will therefore exactly represent the second derivative of the eigenfunctions if it is exact in U_α. Since U_α contains three functions, it is natural to look for a differentiation formula on U_α that may be expressed as a linear combination of thsee values of the function itself. Let the three values be symmetrically calculated, around the point r:

$$\frac{d^2}{dr^2}\Psi(r) = u\Psi(r-\Delta r) + v\Psi(r) + w\Psi(r+\Delta r) \tag{A.1}$$

where Δr has the usual meaning and u, v and w are constants yet to be, determined.

To calculate the three constants u, v and w one needs three equations. These equations are simply obtained by requiring that eq. (A.1) be satisfied for each of the three functions of U_a. The resulting systein of equations has a unique solution given by

$$u = (1 + \alpha\Delta r)/[(\Delta r)^2 \exp(\alpha\Delta r)] \tag{A.2}$$

$$v = \alpha^2 - 2/(\Delta r)^2 \tag{A.3}$$

$$w = (1-\alpha\Delta r)/\left[(\Delta r)^2 \exp(-\alpha\Delta r)\right] \tag{A.4}$$

For $\alpha\Delta r = 1$, eq. (A.4) gives $w = 0$ and eq. (A.1) coincides therefore with the two-point representation given by eq. (9).

Note that α may be a complex constant, and that thereforethe most general set of functions for which (A.1) is valid includes the trigonometric sine or cosine,

For later use we now calculate the representation of d^2/dr^2 on the set $V_\alpha = \{\exp(-\alpha r),\ r.\exp(-\alpha r)\}$ by the same procedure as above. The result is

$$\frac{d^2\Psi}{dr^2} = \frac{2\alpha}{(\Delta r)\exp(\alpha\Delta r)}\ \Psi(r-\Delta r) + \left[\alpha^2 - \frac{2\alpha}{\Delta r}\right]\Psi(r) \tag{A.5}$$

Since this equation is a two-point formula even for $\alpha\Delta r \neq 1$, it can be used to connect $\Psi^{(n)}(r_0)$ to $\Psi^{(n)}(0) = 0$ when $r_0 \neq 0$ as explained in the last item of this Appendix. For $\alpha\Delta r = 1$ eq. (A.5) coincides with eq. (A.1).

II. Expansion of $f(k)/(f(k)-f(k-1))$

Let $f(k)$, $k = 0,1,2,\ldots$ be a discrete sequence of numbers representing a grid on the space coordinate $0 \leq r < \infty$ as considered in section 2. The sequence $f(k)$ is then given by

$$0 \leq f(0) < f(1) < f(2) < \ldots < \infty$$

The quotient

$$\theta(k) = \frac{f(k)}{f(k)-f(k-1)} \quad ; \ k = 1,2,3, \ldots \tag{A.6}$$

plays an important role in the proposed approach. First is should be noted that $\theta(k)$ is well-defined, i.e. it has no singularities. Now, for an arbitrary integer M consider the minimal N-degree polynominal, $N \leq M - 1$, such that $f(k) = P^N(k)$ for $k = 1,2,\ldots,M$. This polynominal exists and is unique. Note that $f(k) - f(k-1) = Q^{N-1}(k)$, i.e. a polynominal of degree $N-1$. It then follows that

$$\theta(k) = \frac{P^N(k)}{Q^{N-1}(k)} = ak + b + c/k + \ldots \tag{A.7}$$

for $k = 1,2,\ldots,M$ and where a, b, c, etc. are constants. The above procedure may be repeated for $M' = M + 1$ and so on. This means that there is na imposed limit for M, and eq. (12) of section 2 for $k = 1,2,\ldots$ is obtained.

III, Relationships for α_k and r_k

From eqs. (8) and (13) it follows for α_k that

$$\alpha_{k+1} = \left[\frac{a(k+1) + b - 1}{ak + b}\right] \alpha_k \quad ; k = 1,2,\ldots \tag{A.8}$$

and for

$$r_{k+1} = \left[\frac{a(k+1) + b}{a(k+1) + b - 1}\right] r_k \quad ; \quad k = 1,2,\ldots \tag{A.9}$$

with

$$r_1 = \begin{cases} \left[\dfrac{a+b}{a+b-1}\right] r_0 & ; \text{ with } r_0 \neq 0, \text{ for } a = b \neq 1 \\ r_1 & ; \text{ with } r_0 = 0, \text{ for } a = b = 1 \end{cases} \tag{A.10}$$

As a general condition for $a+b$, from eqs. (A.9) and (A.10) one has

$$a + b \geqslant 1 \tag{A.11}$$

Note also the following property: for known a and b, all the α_k (or r_k) are determined as soon as only one a, say α_n (or r_n), is determined. This nieans that the best a_n in the n-th piece, as given by the stationary condition $\partial E_n/\partial\alpha_n = 0$ of eq. (18), fixes through $a_n r_n = an+b$ the best r_n and therèfore all the others

$r_k = 0 \leqslant r_0 \leqslant r_1 < \ldots < r_n \ \ldots$ and $\alpha_k = 0 < \alpha_1 \leqslant \alpha_2 \leqslant \ldots \leqslant \alpha_n \leqslant \ldots$

This is a remarkable feature of the piecewise representation used in this work.

As a final remark, from eqs. (A.10) and (14) it should be noted that if $a+b=1$ then $r_0=0$ implies that $\psi^{(n)}(r_0) = 0$, i.e. the boundary condition at the origin of eq. (1). However, if $a+b\neq 1$ the $r_0\neq 0$ and $\psi^{(n)}(r_0) \neq 0$. This means that one needs a connection formula between $\psi^{(n)}(r_0)$ and $\psi^{(n)}(0) = 0$. Since $\Delta r_0\alpha_0$ is free (although $\alpha_k\Delta r_k = 1$ for $k\neq 0$) one needs a two-point representation for d^2/dr^2 on the extra 0-th piece, with $0 \leqslant r \leqslant r_0$, that is also valid for $\alpha_0\Delta r_0 \neq 1$. This is accomplished with eq. (A.5).

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RESUMO

Um método para a solução da equação radial de Schrödinger para estados ligados é discutido. Baseia-se em uma nova representação seccional ("piecewise") do operador derivada segunda sobre um conjunto de funções que satisfazem as condições de contorno. Essa representação é diagonalizada trivialmente e conduz a expressões fechadas do tipo $E_n = E(an + b + c/n + \ldots)$ para os autovalores. Potenciais que são potências e logaritmos são usados como exemplos.