

Solution of the Schrödinger equation for bound states in closed form

Edgardo Gerck*

Laboratório de Estudos Avançados, CTA, 12200 S.J. dos Campos, SP, Brasil

Jason A. C. Gallas*

Departamento de Física da UFSC, 88000 Florianópolis, SC, Brasil

Augusto B. d'Oliveira

Instituto de Física, Univ. Federal Fluminense, 24000 Niterói, RJ, Brasil

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A method to calculate the bound-state eigenvalues of the Schrödinger equation is presented. The method uses a new diagonal representation of the Hamiltonian. The variational principle is applied to this diagonal representation and yields closed-form expressions of the form $E_n = E(an + b)$ for the eigenvalues. Examples are presented for some quark potentials of current interest.

This work presents a method to calculate the eigenvalues of the Schrödinger equation

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

subject to the boundary conditions $\psi(0) = \psi(\infty) = 0$, where $V(r)$ may include the usual centrifugal term. The formal approach used here is similar to the standard variational technique. However, rather than using a trial eigenfunction we use a suitable discrete representation of the second derivative operator on a convenient expansion set. By doing so we will be able to easily diagonalize the Hamiltonian matrix corresponding to Eq. (1).

The convenient basis set, which we use to expand the d^2/dr^2 operator, is

$$U = \{e^{-ar}, re^{-ar}, r^2e^{-ar}\}, \quad \alpha > 0.$$

This choice is partially motivated by the fact that a linear combination of the functions in U obey the boundary condition of the radial problem (1) at infinity. Having introduced U we ask the following question: For φ an arbitrary linear combination of the functions in U , is it possible to write $d^2\varphi/dr^2$ exactly as

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

a linear combination of the values of φ itself at only two points? The answer is positive and, following standard procedure,¹ we find the constants p , q , and t :

$$p = \frac{2\alpha^2}{e}, \quad q = \frac{1}{\alpha}, \quad t = -\alpha^2. \tag{3}$$

For later use we observe that the distance between the points at which the right-hand side of Eq. (2) has to be evaluated is

$$\Delta r = 1/\alpha. \tag{4}$$

We proceed by using Eq. (2) to approximate Eq. (1) as

$$-\frac{2\alpha_k^2}{e}\psi(r_{k-1}) + [\alpha_k^2 + V(r_k)]\psi(r_k) = E\psi(r_k), \tag{5}$$

where the index $k = 1, 2, 3, \dots$ refers to the partition of the coordinate space, as usual. Equation (5) can also be written in matrix form as $M\psi = E\psi$, where $\psi = [\psi(r_1), \psi(r_2), \dots]^T$ and M is the bidiagonal matrix

$$\begin{pmatrix} \alpha_1^2 + V(r_1) & 0 & 0 & \dots \\ -\frac{2\alpha_2^2}{e} & \alpha_2^2 + V(r_2) & 0 & \dots \\ 0 & -\frac{2\alpha_3^2}{e} & \alpha_3^2 + V(r_3) & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{pmatrix}. \tag{6}$$

From the particular form of M it is seen that its eigenvalues are already located on the main diagonal. The eigenvalues are therefore given by

$$E_n = \alpha_n^2 + V(r_n), \tag{7}$$

where α_n is still an unspecified constant. This equation is a diagonal representation of the Hamiltonian of Eq. (1), where n is the radial quantum number. The variational analog of Eq. (7) corre-

sponds to the diagonalization of the Hamiltonian for a given value of α_n . In order to obtain the eigenvalues, we therefore apply the Rayleigh-Ritz principle to Eq. (7). First, however, since for a given α_n we already fixed r_n through Eq. (4), we have to find the functional dependence $r_n = r_n(\alpha_n)$. This is done by determining how the several r_k points are distributed in the coordinate space. With no loss of generality we can assume the points r_k to be given by some analytical discrete function, say, $r_k = f(k)$, $k=0,1,2,\dots$. The function $f(k)$ must satisfy

$$0 \leq f(0) < f(1) < f(2) < \dots \quad (8)$$

This property guarantees that the quotient $f(k)/[f(k)-f(k-1)]$, $k=1,2,3,\dots$ has a Laurent expansion of the form

$$\frac{f(k)}{f(k)-f(k-1)} = ak + b + c/k + \dots, \quad (9)$$

where the several a, b, c , etc., are constants. If we recall that $r_k = f(k)$, it follows from Eq. (4) that

$$r_k = \frac{f(k)}{\Delta r_k \alpha_k} = \left[\frac{f(k)}{f(k)-f(k-1)} \right] \frac{1}{\alpha_k}, \quad k=1,2,\dots \quad (10)$$

If one neglects the $O(1/k)$ contribution in Eq. (9), then $r_k \cong (ak+b)/\alpha_k$. The Rayleigh-Ritz principle² requires the energy to be stationary with variations of α , i.e., $\partial E/\partial \alpha = 0$. This condition applied to

$$E_n = \alpha_n^2 + V \left[\frac{an+b}{\alpha_n} \right] \quad (11)$$

gives

$$2\alpha_n + \frac{\partial}{\partial \alpha_n} V \left[\frac{an+b}{\alpha_n} \right] = 0, \quad (12)$$

which must be solved for α_n .

Equations (11) and (12) are the main results of the present paper. For a given $V(r)$ the eigenvalues are obtained by solving Eq. (12) for α_n . Substitution of α_n in Eq. (11) then gives the desired eigenvalues as a function of the constants a and b .

The constants a and b in Eq. (11) are obtained by making the eigenfunctions satisfy the boundary conditions. To generate accurate eigenfunctions, one usually needs $\Delta r \ll 1$. However, this condition may conflict with the requirement $\Delta r = 1/\alpha$ of Eq. (4). We therefore use the full three-point representation of d^2/dr^2 in U , given by

$$\frac{d^2\varphi}{dr^2} = u\varphi(r-\Delta r) + v\varphi(r) + w\varphi(r+\Delta r) \quad (13)$$

with $u = (1+\alpha\Delta r)e^{-\alpha\Delta r}/(\Delta r)^2$, $v = \alpha^2 - 2/(\Delta r)^2$, and $w = (1-\alpha\Delta r)e^{\alpha\Delta r}/(\Delta r)^2$. Using this expansion we write Eq. (1) 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 has only two unknowns: a and b . Using a continued fraction calculational approach³ we obtained a and b for the examples to be discussed below with an absolute error of less than 10^{-5} . An alternative approach is, however, self-evident: For any two eigenvalues E_i and E_j calculated by some numerical method one may set up a system of equation $(ai+b)$ and $(aj+b)$ and solve for a and b . To conclude, we apply the method to calculate eigenvalues for some potentials which are nowadays in evidence as possible models of quark confinement.⁴

For the general power-law potential $V(r) = Kr^p$, $p > -2$ and $p \neq 0$, Eq. (11) gives (dropping the subscript n from α_n)

$$E_n = \alpha^2 + K(an+b)^p \alpha^{-p}. \quad (14)$$

From the condition that $\partial E/\partial \alpha = 0$ one obtains

$$\alpha = \left[\frac{1}{2} Kp(an+b)^p \right] \alpha^{1/(p+2)}. \quad (15)$$

Substituting this α in Eq. (14) brings

$$E_n = \alpha^2(1+2/p) = \left(\frac{1}{2} Kp \right)^{2/(p+2)} \left[1 + \frac{2}{p} \right] (an+b)^{2p/(p+2)}. \quad (16)$$

This formula gives the eigenvalues as a function $E_n = E(an+b)$ of the constants a and b . For the

TABLE I. Comparison between the first five eigenvalues for the square-root and logarithmic potentials.

$V(r)$	n	Present results	Numerical ^a results	WKB ^a
	1	1.0443	1.0443	0.9778
	2	1.8474	1.8474	1.8251
	3	2.2870	2.2897	2.2771
	4	2.5913	2.5957	2.5873
	5	2.8243	2.8299	2.8237
ln(r)	1	1.8334		1.8117
	2	2.5506		2.5426
	3	3.0487		3.0465
	4	3.4475		3.4488
	5	3.7869		3.7909

^aTaken from Ref. 4.

TABLE II. Comparison of the eigenvalues calculated by the proposed method, in two different approximations, with the exact and WKB results for the linear potential $V(r)=r$.

n	$E(an+b)^a$	$E(an+b+c/n)^b$	Exact ^c	WKB ^c
1	2.3380	2.3381	2.3381	2.3203
2	4.0879	4.0880	4.0879	4.0802
3	5.5161	5.5206	5.5206	5.5161
4	6.7778	6.7868	6.7867	6.7838
5	7.9311	7.9444	7.9441	7.9422

^aFrom Eq. (18).

^bFrom Eq. (19).

^cFrom Ref. (14).

cases with known exact solution [$V(r)=-K/r$, Kr , and Kr^2 with $K > 0$] Eq. (16) reproduces the correct scaling laws with K and n . In all other cases, for which the exact solution is not known, its scaling coincides with the WKB scaling [compare with Eqs. (4.33) and (4.59) of Ref. (4)]. From the eigenfunctions, as described above, we obtain $a=1$ and $b=0$ ($a=2$ and $b=-0.5$) for the Coulomb (harmonic) potential, as expected.

Motivated by the current interest in the square-root⁵ and logarithmic⁴ potentials and also by the fact that no exact solution is known for them, we study their eigenvalues in detail. From Eqs. (11) and (12) follows

$$E_n = \frac{1}{2}K \ln \left[\frac{2e}{K} \right] + K \ln(an+b) \quad (17)$$

for $V(r)=K \ln(r)$. We find $a=1.6712$ and $b=-0.36853$ for $V(r)=Kr^{1/2}$ and $a=1.5019$ and $b=-0.28330$ for the logarithmic potential, both $K > 0$. In Table I we show the first five eigenvalues for both potentials along with numerical and WKB results from Ref. 4.

Finally, we use the linear potential [$V(r)=r$] to investigate the effect of the c/n contribution in Eq. (11), which has hitherto been neglected. From Eq. (16) it follows that

$$E_n = 1.88988(1.80523n - 0.42915)^{2/3}. \quad (18)$$

With the c/n contribution also taken into account one obtains

$$E_n = 1.88988(1.81425n - 0.45619 + 0.01803/n)^{2/3}. \quad (19)$$

As is easily seen from Table II, the c/n term improves the eigenvalues. In general, note that the contribution to $E_n = E(an+b)$ from higher terms, i.e., $c/n + d/n^2 + \dots$, is of the form

$$E_n = E(an+b) + O(1/n) \quad (20)$$

and vanishes for $n \rightarrow \infty$. This allows the application of the Cauchy criterion² to estimate the relative accuracy of the eigenvalues. For example, the difference between $E(an+b)$ and $E(an+b+c/n)$ is a measure of the contribution from $c/n + d/n^2 + \dots$. It is interesting to observe that the form $E_n = E(an+b+c/n + \dots)$ for the linear potential corresponds to the asymptotic expansion of the zeros of the Airy function, which is the exact result.⁴ By dividing the eigenfunction in odd-even symmetry classes the method can also be extended to the one-dimensional Schrödinger equation. The eigenfunctions as well as this extension will be discussed elsewhere.

*Present address: Max-Planck Institut für Quantenoptik, Forschungsgelände, D-8046 Garching, West Germany.

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