Solution of the Schrödinger equation for bound states in closed form

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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 then 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

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

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 $k=1,2,3,\ldots$ 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 $\psi=[\psi(r_1),\psi(r_2),\ldots]^T$ and M is the bidiagonal matrix

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

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, $r_k = f(k)$, $k = 0,1,2,\ldots$. The function $f(k)$ must satisfy

$$0 \le f(0) < f(1) < f(2) < \cdots . \tag{8}$$

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

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

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

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

If one neglects the $O(1/k)$ contribution in Eq. (9), then $r_k \cong (ak+b)/\alpha_k$. The Rayleigh-Ritz principle[2] requires the energy to be stationary with variations of α, i.e., $\partial E/\partial\alpha = 0$. This condition applied to

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

gives

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

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

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

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 approach[3] 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)

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

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

$$\alpha = [\tfrac{1}{2}Kp(an+b)^p]\alpha[\ldots]^{1/(p+2)} . \tag{15}$$

Substituting this α in Eq. (14) brings

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

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
$\ln(r)$	3	2.2870	2.2897	2.2771
	4	2.5913	2.5957	2.5873
	5	2.8243	2.8299	2.8237
	1	1.8334		1.8117
	2	2.5506		2.5426
$\sqrt{r}$	3	3.0487		3.0465
	4	3.4475		3.4488
	5	3.7869		3.7909

[a]Taken 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

[a]From Eq. (18).
[b]From Eq. (19).
[c]From 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-root[5] and logarithmic[4] 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

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

for $V(r)=K\ln(r)$. We find $a=1.6712$ and $b=-0.368\,53$ for $V(r)=Kr^{1/2}$ and $a=1.5019$ and $b=-0.283\,30$ 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

$$E_n=1.889\,88(1.805\,23n-0.429\,15)^{2/3}\,. \tag{18}$$

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

$$E_n=1.889\,88(1.814\,25n-0.456\,19+0.018\,03/n)^{2/3}\,. \tag{19}$$

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., $c/n+d/n^2+\cdots$, is of the form

$$E_n=E(an+b)+O(1/n) \tag{20}$$

and vanishes for $n\to\infty$. This allows the application of the Cauchy criterion[2] 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 $c/n+d/n^2+\cdots$. It is interesting to observe that the form $E_n=E(an+b+c/n+\ldots)$ 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.

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