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Note

An Algorithm for the Solution of the Eigenvalue Schrödinger Equation

1. The one-dimensional radial eigenvalue Schrodinger equation may be written as

$$y''(r) = f(r)\, y(r) \tag{1}$$

$$0 < r < \infty, \tag{2}$$

where $f(r) = U(r) - E$, E is a real number denoting the energy and $U(r) = V(r) + l(l+1)/r^2$ is an effective potential for which

$$U(r) \to 0 \qquad \text{as} \quad r \to +\infty,$$

along with the boundary conditions,

$$\lim_{r \to 0} y(r) = 0 \qquad \text{and} \qquad \lim_{r \to \infty} y(r) = 0. \tag{3}$$

Such solutions exist for negative discrete eigenvalues of E_j. In this work the potential $U(r)$ is a real function.

More recently Papageorgious and Raptis [1] developed a new technique for determining the eigenvalues. They introduced a new function named *impedance* which is well known in transmission line theory. The properties of the new function are relevant to the problem in quantum mechanics.

2. Following the usual procedure of the piecewise perturbation numerical method [2], the domain $[r_0, r_k]$ is divided by the mesh points:

$$r_0, r_1, r_2, ..., r_k$$

into k arbitrary intervals:

$$[r_n, r_{n+1}], \qquad n = 0, 1, 2, 3, ..., k-1. \tag{4}$$

In addition we denote $\Delta r_n = r_{n+1} - r_n$.

Within each of these elementary intervals, we choose a polynomial $u_n(r)$ which approximates the true potential $u(r)$ over the interval. This piecewise polynomial approximating curve is usually called a "reference potential."

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The solution for this problem then satisfies the equation:

$$\begin{aligned} &y_0''(r) + (E - U_n) \qquad (y_0(r) = 0), \\ &r_n < r < r_{n+1}, \qquad n = 1, 2, 3, ..., k, \end{aligned} \tag{5}$$

where $U_n = U(r_n + h/2)$, which is the well-known Cauchy problem.

The analytical solutions of (5) are known by the perturbative theory as zeroth order-solutions $y_0(r)$. However, if we expand the solution $y(r)$ in a perturbation series as

$$\begin{aligned} &y(r) = y_0(r) + \lambda y_1(r) + \lambda^2 y_2(r) + \cdots \\ &r \in [r_n, r_{n+1}], \qquad 0 < \lambda \leqslant 1, \end{aligned} \tag{6}$$

where $y_0(r)$ is the zeroth-order solution, $y_1(r)$ is the first-order correction, $y_2(r)$ is the second-order correction, and so on.

If the series (6) are cut at the second-order terms and λ taken to be $\frac{1}{2}$, then the solution and its first derivative of the problem (1)–(2) can be approximated at the mesh points by the expressions

$$\begin{aligned} y(r_{n+1}) &= [X_1(\Delta r_n) - \tfrac{1}{2}C(\Delta r_n)\,\zeta(\Delta r_n)]\; y(r_n) + \Delta r_n X_2(\Delta r_n)\; y'(\Delta r_n) \\ y'(r_{n+1}) &= \omega_n^2\, \Delta r_n X_2(\Delta r_n)\; y(r_n) + [X_1(\Delta r_n) + \tfrac{1}{2}C(\Delta r_n)\,\zeta(\Delta r_n)]\; y'(\Delta r_n), \end{aligned} \tag{7}$$

where:

$$\begin{aligned} \omega_n &= \sqrt{|U_n - E|} \\ X_1 &= \cosh(\omega_n\, \Delta r_n) \\ X_2 &= \sinh(\omega_n\, \Delta r_n)/(\omega_n\, \Delta r_n) \\ C(\Delta r_n) &= [U(r_n + \Delta r_n/2) - U(r_n - \Delta r_n/2)](\Delta r_n)^2 \\ \zeta(\Delta r_n) &= [X_1(\Delta r_n) - X_2(\Delta r_n)]/(2\omega_n\, \Delta r_n)^2. \end{aligned}$$

Dividing the relations (8) we get, after some algebra,

(i) case for $U_n - E \geqslant 0$:

$$\frac{y'(r^{n+1})}{y(r_{n+1})} = \frac{8\omega_n^4 \tanh(\omega_n\,\delta) + [8\omega_n^3\,\delta + [U_2 - U_1]((\omega_n\,\delta - \tanh(\omega_n\,\delta))](y'(r_n)/y(r_n))}{[8\omega_n^3\,\delta - [U_1 - U_2](\omega_n\,\delta - \tanh(\omega_n\,\delta)] + 8\omega_n^2\,\delta\tanh(\omega_n\,\delta)(y'(r_n)/y(r_n))}; \tag{8}$$

(ii) case for $U_n - E < 0$:

$$\frac{y'(r_{n+1})}{y(r_{n+1})} = \frac{-8\omega_n^4 \tan(\omega_n\,\delta) + [8\omega_n^3\,\delta + [U_2 - U_1](\omega_n\,\delta - \tan(\omega_n\,\delta))](y'(r_n)/y(r_n))}{[8\omega_n^3\,\delta - [U_1 - U_2](\omega_n\,\delta - \tan(\omega_n\,\delta)] + 8\omega_n^2\,\delta\tan(\omega_n\,\delta)(y'(r_n)/y(r_n))}; \tag{9}$$

where

$$\delta = \Delta r_n, \qquad U_2 = U(r_n + \Delta r_n/2), \qquad U_1 = U(r_n - \Delta r_n/2).$$

We define, now, the function

$$z(r) = jy'(r)/y(r), \tag{10}$$

which is called "*the impedance*," where $y'(r) = dy(r)/dr$ and $j = \sqrt{-1}$.

For reasons of numerical calculations, since $y(r)$ and $y'(r)$ are real functions and by letting $z(r) = jZ(r)$, we have

$$Z(r) = y'(r)/y(r). \tag{11}$$

The function $Z(r_{n+1}) = y'(r_{n+1})/y(r_{n+1})$, which can be calculated at the point r_{n+1} by using the recursion relations (8) and (9), gives useful information about the physics of the problem (1)–(3).

As described in [1], we consider an intermediate point r_c and the apply the recursion relations (8) and (9). Starting from r_0 outwards to r_c we calculated $Z^L(r_c)$ (i.e., the impedance to the left) and starting from r_k inwards to r_c we calculate $Z^R(r_c)$ (i.e., the impedance to the right). The eigenvalue is given by

$$Z^L(r_c) + Z^R(r_c) = 0. \tag{12}$$

For a trial eigenvalue E we have the value of the function $F(E)$,

$$F(E) = Z^L(r_c) + Z^R(r_c), \tag{13}$$

where the roots of the algebraic equation $F(E) = 0$ are the eigenvalues.

In order to calculated $Z^L(r_c)$ and $Z^R(r_c)$ for a given value of E, we have to start the integration with the initial values of $Z^L(r_0)$ and $Z^R(r_k)$. These values are calculated from the equation

$$Z^L(0) = y'(0)/y(0) \tag{14}$$

and, since by definition $y(0) = 0$, we have $Z^L(0) = \infty$.

For numerical reasons we start the ourward integration at r_0 close to the origin and we use $Z(r_0)$ equal to a very large number.

The inward integration is starting from a point r_k such that for $r > r_k$ the potential is negligible. The initial value of r_k has been taken from the asymptotic solution of $y(r)$ and $y'(r)$. Since

$$y(r) \simeq \exp(-\sqrt{-E}r), \qquad y'(r) \simeq -\sqrt{-E}\exp(-\sqrt{-E}r),$$

we get $Z(r_k) \simeq -\sqrt{-E}$.

The intermediate point r_c can be taken at any point in the range (r_0, r_k). However, for numerical purposes, we avoid taking values of r_c either close to the

TABLE I

Absolute Error in Units of 10^{-9}
(Real Time of Computation in Seconds) Optic Potential

	$h=\frac{1}{8}$		$h=\frac{1}{32}$		$h=\frac{1}{128}$	
j	SF-PNM	New method	SF-PNM	New method	SF-PNM	New method
0	606 (6.6)	387 (1.2)	2 (25.6)	0 (4.1)	0 (102.1)	0 (16.1)
6	127921 (45.3)	29400 (0.8)	509 (184.6)	117 (3.0)	1 (737.5)	0 (12.0)
12	442048 (80.8)	93022 (1.3)	1845 (324.4)	395 (5.0)	7 (1270.1)	0 (20.0)

Note. $r_0=0.0$, $r_c=2.0$, $r_k=15$, and $l=0$.

r_0, because we have very large numbers of $Z^L(r_c)$ and $Z^R(r_c)$, or close to r_k, because we have very small numbers of $Z^L(r_c)$ and $Z^R(r_c)$, resulting in inaccurate eigenvalues.

3. In order to test the validity of the present method we apply it as follows:

Case I. We solve the problem (1)–(3) with $l=0$, where $V(r)$ is:

(i) an optical potential:

$$V(r)=U_0/(1+t)-(U_0/a_0)\,t/(1+t)^2 \qquad (15)$$
$$t=\exp[(r-R_0)/a_0],$$

TABLE II

Absolute Error in Units of 10^{-8}
(Real Time of Computation in Seconds) Morse Potential (i)

	$h=\frac{1}{8}$		$h=\frac{1}{32}$		$h=\frac{1}{128}$	
j	SF-PNM	New method	SF-PNM	New method	SF-PNM	New method
0	377387 (4.3)	42739 (0.6)	1512 (33.3)	174 (2.0)	6 (132.9)	0 (7.6)
10	2069927 (93.1	387047 (0.6)	10193 (291.3)	2050 (2.2)	40 (1220.3)	8 (8.8)
18	222420 (206.0)	40897 (1.1)	1164 (655.8)	237 (4.4)	6 (2541.6)	2 (17.6)

Note. $r_0=0.0$, $r_c=2.0$, $r_k=10$, and $l=0$.

TABLE III

Absolute Error in Units of 10^{-8}
(Real Time of Computation in Seconds) Morse Potential (ii)

	$h=\frac{1}{8}$		$h=\frac{1}{32}$		$h=\frac{1}{128}$	
j	SF-PNM	New method	SF-PNM	New method	SF-PNM	New method
0	573824 ((4.1)	734303 (0.6)	23241 (16.4)	3135 (2.1)	90 (63.1)	12 (7.7)
12	27167893 (43.1)	6797535 (0.6)	204000 (190.4)	41158 (1.9)	833 (776.8)	170 (7.5)
24	932187 (90.6)	638940 (1.0)	8288 (331.3)	1674 (3.8)	34 (1735.8)	8 (15.2)

Note. $r_0 = 0.0$, $r_c = 2.0$, $r_k = 10$, and $l = 0$.

where $U_0 = 50\ \mathrm{fm}^{-2}$, $R_0 = 7$ fm, $a_0 = 0.6\ \mathrm{fm}^{-1}$; and

(ii) a Morse potential:

$$U(r) = U_0 t(t-2) \qquad t = \exp[a_0(R_0 - r)], \tag{16}$$

where:

(a) $U_0 = 188.4355A^{-2}$, $a_0 = 0.711248A^{-1}$, $R_0 = 1.9975A$ and

(b) $U_0 = 605.559A^{-2}$, $a_0 = 0.988879A^{-1}$, $R_0 = 2.40873A$ [5].

TABLE IV

Absolute Error in Units of 10^{-6}
(Real Time of Computation in Seconds) Morse Potential (i)

	$h=\frac{1}{8}$		$h=\frac{1}{32}$		$h=\frac{1}{128}$	
j	SF-PNM	New method	SF-PNM	New method	SF-PNM	New method
0	3644 (8.3)	391 (1.2)	14 (32.6)	1 (4.1)	0 (129.8)	0 (16.1)
8	21607 (76.6)	4031 (1.1)	103 (292.5)	20 (4.0)	0 (1171.6)	0 (16.0)
16	6270 (158.3)	1144 (1.2)	32 (551.3)	6 (4.7)	0 (2206.0)	0 (18.8)

Note. $r_0 = 0.0$, $r_c = 2.0$, $r_k = 20$, and $l = 5$.

TABLE V

Absolute Error in Units of 10^{-6}
(Real Time of Computation in Seconds) Morse Potential (ii)

	$h=\frac{1}{8}$		$h=\frac{1}{32}$		$h=\frac{1}{128}$	
j	SF-PNM	New method	SF-PNM	New method	SF-PNM	New method
0	55233 (8.5)	7260 (1.9)	229 (32.6)	30 (5.0)	0 (129.9)	0 (21.6)
10	295383 (87.2)	46733 (1.2)	2081 (358.2)	419 (4.7)	8 (1427.7)	1 (18.8)
22	54376 (191.2)	30184 (1.2)	474 (758.8)	96 (4.7)	2 (3026.4)	0 (18.9)

Note. $r_0=0.0$, $r_c=2.0$, $r_k=20$, and $l=5$.

Case II. We solve the problem (1)–(3) with $l=5$, where $V(r)$ is a Morse potential of the form (16) with U_0, R_0, and a_0 are the same as in Case I.

The reference eigenvalues computed: (a) for the optical potential from the analytic result of Bencze [4]; (b) for the Morse potential and for the Case I from the equation

$$e_k = -D[1 - a\, D^{-1/2}(k+\tfrac{1}{2})]^2; \tag{17}$$

(c) for the Morse potential and $l=5$, from SFPNM with second correction and $h=\frac{1}{128}$ in (a) and $h=\frac{1}{64}$ in (b) (we use this method because there are not published values from the theoretical calculations (named true values) in this case).

Eigenvalues E_j, obtained on the Micro-Vax at various step sizes h using the present new method and the step function perturbative numerical method (SF-PNM) of Adam, Ixaru, and Corciovei [3], are collected in Table I–V. The table entries are:

(a) the values of the absolute error in the calculated eigenvalue

$$\Delta_j = |E_{\text{computed}} - E_{\text{exact}}|; \tag{18}$$

(b) the computing time.

It can be seen that the new method is more efficient than the method SF-PNM in terms of the accuracy and computing time.

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