

# Improved Regula Falsi Method for Solving the Schrödinger Equation with a Piecewise Constant Potential

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An improved regula falsi scheme is introduced for the solution of the Schrödinger equation with stepped potentials. The scheme significantly reduces the number of iterations needed for eigenvalue evaluations. © 1987 Academic Press, Inc.

## 1. INTRODUCTION

The solution of the one-dimensional Schrödinger equation is of major importance in quantum mechanics (see, e.g., [1]). Many 3-D systems can be reduced to 1-D ones by standard techniques such as the separation of variables. Moreover, quasi 1-D systems have recently attracted considerable attention [2]; Localization problems and tunnelling are treated mainly in 1-D disordered lattices [3]. Since the number of cases for which analytic solutions are available is rather small, a general numerical scheme could be very helpful. A simple approach is to replace the potential  $V(x)$  of the Schrödinger equation by a piece-wise constant function (the procedure is an old one, being periodically rediscovered; see [4]) for which the solution is obtained by merging together the known solutions of each interval. In addition to being an approximation to the general case, it can simply yield the main qualitative feature of any problem. In particular, for problems where the actual potential is unknown but for its general form, the use of a stepped potential [5] brings out their relevant properties and enables us to understand their physical nature.

An important application of the piecewise constant potential is the mathematically identical optical problem [6] where it is called the “staircase” or “multilevel” method.

The numerical procedure designed to get the eigenvalues of the piecewise con-

stant Schrödinger equation is treated here. Since it calls for the computation of the zeroes of a complicated function, a special attention was given to reduce computing costs. Instead of the standard Newton–Raphson and regula falsi methods, a new improved scheme was used. In this scheme, although only one calculation of the function per step was needed, a quadratic convergence for the second and third iterations was still guaranteed.

## 2. THE PROCEDURE

We consider the eigenvalues of the one dimensional Schrödinger equation

$$-\frac{\hbar^2}{2m} \psi'' + V\psi = E\psi, \quad a \leq x \leq b \tag{1}$$

with the homogeneous boundary conditions

$$\begin{aligned} \eta_0 \psi'(a) + \sigma_0 \psi(a) &= 0, \\ \eta_1 \psi'(b) + \sigma_1 \psi(b) &= 0, \end{aligned} \tag{2}$$

where  $\eta_0, \sigma_0, \eta_1, \sigma_1$  are any given real constants. The interval  $[a, b]$  is divided into  $N$  subintervals by introducing the mesh  $[4, 6]$  points  $a = a_0 < a_1 < \dots < a_{N-1} < a_N = b$  and  $V(x)$  is replaced by a stepped function  $\bar{V}(x)$  defined as

$$\bar{V}(x) = V_i, \quad a_{i-1} \leq x \leq a_i, \quad i = 1, \dots, N. \tag{3}$$

If  $N$  is large enough,  $\max_{1 \leq i \leq N} |a_i - a_{i-1}|_{N \rightarrow \infty} \rightarrow 0$  and  $V_i$  approximates  $V(x)$  at  $a_{i-1} \leq x \leq a_i$  for all  $i$ , the eigenvalues of

$$-\frac{\hbar^2}{2m} \psi'' + \bar{V}(x) \psi = E\psi \tag{4}$$

converge to those of Eq. (1). For a finite  $N$ , Eq. (4) is an approximation whose eigenvalues improve with  $N$ .

At the  $n$ th subinterval the solution of (4) is

$$\psi_n = A_n e^{k_n x} + B_n e^{-k_n x}, \tag{5}$$

where

$$k_n^2 = \frac{2m(V_n - E)}{\hbar^2}. \tag{6}$$

Using the continuity of  $\psi, \psi'$  one gets,

$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = T_{N-1} T_{N-2} \dots T_1 \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = T \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \tag{7}$$

where

$$T_n = \frac{1}{2} \begin{pmatrix} e^{(\theta_n - \bar{\theta}_{n+1})} \left(1 + \frac{\theta_n}{\bar{\theta}_{n+1}}\right) & e^{-(\theta_n + \bar{\theta}_{n+1})} \left(1 - \frac{\theta_n}{\bar{\theta}_{n+1}}\right) \\ e^{(\theta_n + \bar{\theta}_{n+1})} \left(1 - \frac{\theta_n}{\bar{\theta}_{n+1}}\right) & e^{(\bar{\theta}_{n+1} - \theta_n)} \left(1 + \frac{\theta_n}{\bar{\theta}_{n+1}}\right) \end{pmatrix} \quad (8)$$

and  $\bar{\theta}_{n+1} = k_{n+1} a_n$ ,  $\theta_n = k_n a_n$ .

The transfer matrix  $T$  is related to the transfer matrix  $R$  of [3] by

$$T = \frac{1}{4} \begin{pmatrix} e^{(\bar{\theta}_{N+1} - \theta_N)} \left(1 + \frac{\bar{\theta}_{N+1}}{\theta_N}\right) & e^{-(\theta_N + \bar{\theta}_{N+1})} \left(1 - \frac{\bar{\theta}_{N+1}}{\theta_N}\right) \\ e^{(\theta_N + \bar{\theta}_{N+1})} \left(1 - \frac{\bar{\theta}_{N+1}}{\theta_N}\right) & e^{(\theta_N - \bar{\theta}_{N+1})} \left(1 + \frac{\bar{\theta}_{N+1}}{\theta_N}\right) \end{pmatrix} R \\ \times \begin{pmatrix} e^{(\bar{\theta}_1 - \theta_0)} \left(1 + \frac{\bar{\theta}_1}{\theta_0}\right) & e^{-(\theta_0 + \bar{\theta}_1)} \left(1 - \frac{\bar{\theta}_1}{\theta_0}\right) \\ e^{(\theta_0 + \bar{\theta}_1)} \left(1 - \frac{\bar{\theta}_1}{\theta_0}\right) & e^{(\theta_0 - \bar{\theta}_1)} \left(1 + \frac{\bar{\theta}_1}{\theta_0}\right) \end{pmatrix}, \quad (9)$$

where  $\theta_0 = k_0 a_0$ ,  $\bar{\theta}_1 = k_1 a_0$ ,  $\theta_n = k_n a_n$ ,  $\bar{\theta}_{n+1} = k_{n+1} a_n$ ,  $k_0^2 = k_{N+1}^2 = 2m(-E)/\hbar^2$ .

The use of the boundary conditions (Eq. (2)) leads to

$$f(E) = \beta_1(t_{11} a_0 + t_{12} \beta_0) - \alpha_1(t_{21} \alpha_0 + t_{22} \beta_0) = 0, \quad (10)$$

where

$$\frac{A_1}{B_1} = \frac{e^{-k_1 a_0} (\eta_0 k_1 - \sigma_0)}{e^{k_1 a_0} (\eta_0 k_1 + \sigma_0)} = \frac{\alpha_0}{\beta_0}; \quad \frac{A_N}{B_N} = \frac{e^{-k_N a_N} (\eta_1 k_N - \sigma_1)}{e^{k_N a_N} (\eta_1 k_N + \sigma_1)} = \frac{\alpha_1}{\beta_1}. \quad (11)$$

Equation (10) can be solved for the eigenvalues by a standard Newtonian scheme. However, since we may need a relatively large number of constants  $V_i$  to achieve good accuracy,<sup>1</sup> an algorithm that reduces the number of computations of  $f$ ,  $f'$  would be useful. In the next section an improved version of the regula falsi method is presented and its efficiency for the model is demonstrated in solving an equation with a two-step potential (Sect. 4).

<sup>1</sup> An estimate of the number ( $N$ ) of subdivisions needed for a given accuracy can be obtained by perturbation theory. If the  $i$ th interval length is denoted by  $h_i$ , which is assumed to be small, 1st order perturbation theory gives for the error in the  $l$ th eigenvalue,

$$\Delta E_l \leq \sum_i \int_{a_{i-1}}^{a_i} (V(x) - V_i) \psi_l^2 dx.$$

This can easily be shown to be  $O((\max_i h_i)^2)$ .

## 3. THE NUMERICAL METHOD

We denote by  $s$  the exact solution of  $f(x) = 0$ , i.e.,  $f(s) = 0$ . It may be calculated iteratively by any Newton-type algorithm. Let  $x_0$ ,  $x_n$ ,  $\varepsilon$  be the first approximation, the  $n$ th iteration and its error (defined as  $(x_n - s)$ ), respectively,  $f_n = f(x_n)$  and  $f'_n = f'(x_n)$ .

The standard Newton-Raphson method given by

$$x_{n-1} = x_n - \frac{f_n}{f'_n} \quad (12)$$

guarantees an error relation of the type

$$\varepsilon_{n+1} = O(\varepsilon_n^2). \quad (13)$$

Thus, two computations of  $f$ ,  $f'$  at  $x_n$  are necessary for quadratic convergence.

In the regula falsi scheme, one replaces  $f'_n$  by a simple finite difference expression to get

$$x_{n+1} = x_n - \frac{(x_n - x_{n-1}) f_n}{f_n - f_{n-1}}, \quad (14)$$

$$\varepsilon_{n+1} = O(\varepsilon_n^{(1+\sqrt{5})/2}). \quad (15)$$

Thus, following the first two computation of  $f_0$ ,  $f'_0$  only one additional calculation (of  $f_n$ ) per iteration is needed to obtain convergence of the order of  $(1 + \sqrt{5})/2$  in the regula falsi method. Two consecutive iterations provide an order of  $((1 + \sqrt{5})/2)^2 \simeq 2.6 > 2$ . Thus, it is preferable to use this scheme rather than the classical Newton-Raphson one (Eqs. (12), (13)).

In this work we present an improved method, better than both previous schemes. We aimed at replacing  $f'_n$  in Eq. (12) by a different approximation  $\tilde{f}'_n$ , based upon the already known values of  $f_n$ ,  $f_{n-1}$ ,  $f'_{n-1}$  that would provide a quadratic convergence for a single function computation. By a procedure similar to that explained in Appendix B we choose

$$\tilde{f}'_n = \frac{2(f_n - f_{n-1})}{x_n - x_{n-1}} - f'_{n-1} \quad (16)$$

to get

$$x_{n+1} = x_n - \frac{(x_n - x_{n-1}) f_n}{2(f_n - f_{n-1}) - (x_n - x_{n-1}) f'_{n-1}}. \quad (17)$$

An error analysis of Eq. (17) given in Appendix A indeed shows such a convergence.

We are trying to avoid calculating  $f'_n$  (except for  $f'_0$  whose computation is a necessity) since in general this reduces the number of function evaluations. Hence, Eq. (17) can be used just once (for  $n = 1$ ). However, a quadratic convergence at the next step at the price of one evaluation is still possible: we compute  $f_2$  and approximate  $f'_2$  by

$$\tilde{f}'_2 = \alpha f'_0 + \beta f_0 + \gamma f_1 + \delta f_2, \quad (18)$$

where the choice of  $\alpha, \beta, \gamma, \delta$  (obtained in Appendix B) does yield

$$\varepsilon_3 = O(\varepsilon_2^2) \quad (19)$$

Thus, after performing just four evaluations (of  $f'_0, f_0, f_1, f_2$ ) one reduces an initial error  $\varepsilon_0$  to  $O(\varepsilon_0^8)$ . If convergence is not yet completed, the remaining needed iterations may be carried out by the usual parabolic regula falsi scheme or by an extension of the scheme given by Eq. (18).

The parabolic scheme [7] is given by

$$x_{n+1} = x_n - \frac{f_n(x_{n-2} - x_n)(x_{n-1} - x_n)(x_{n-2} - x_{n-1})}{(f_{n-1} - f_n)(x_n - x_{n-2})^2 - (f_{n-2} - f_n)(x_{n-1} - x_n)^2} \quad (20)$$

and provides an error relation

$$\varepsilon_{n+1} = O(\varepsilon_n^3), \quad (21)$$

where  $\alpha$  satisfies

$$\alpha^3 - \alpha^2 - \alpha - 1 = 0 \quad (22)$$

giving  $\alpha \simeq 1.84$ . The expressions obtained in the extended improved scheme become cumbersome, but always guarantee a quadratic convergence.

#### 4. AN EXAMPLE

Rewriting Eq. (1) in appropriate units, one gets

$$-\psi'' + V\psi = E\psi. \quad (23)$$

To check the stepped potential model (SPM) with the improved numerical method, we chose  $V = -x$  and approximated it by a two step function:

$$V(x) = \begin{cases} V_1, & 0 \leq x < a_1, \\ V_2, & a_1 \leq x \leq 10. \end{cases} \quad (24)$$

The numerical values of  $V_1, V_2$ , and  $a_1$  were chosen to give the best fit of the exact eigenvalues. The latter were obtained by numerically solving Eq. (23) with  $V = -x$

TABLE I

The Calculated Eigenvalues for Several Values of  $a_1, V_1, V_2$  and the Exact Eigenvalues (Eq. (23) with the Boundary Condition  $\psi(0) = \psi(10) = 0$ )

$a_1$	$V_1$	$V_2$	$E_1$	$E_2$	$E_3$	$E_4$	$E_5$	$E_6$
5	-2.5	-7.5	-7.2	-6.2	-4.6	-2.6		
5	-1.0	-9.0	-8.7	-7.6	-5.9	-3.6	-0.96	
5	-3.5	-6.5	-6.2	-5.3	-3.8			
5	-2.5	-8.5	-8.2	-7.2	-5.5	-3.3		
6	-2.7	-8.5	-8.0	-6.5	-4.1			
Exact			-7.7	-5.9	-4.5	-3.2	-2.1	-0.9

(the Airy equation – see, e.g., [8]). Results are presented in Table I. The comparison shows that the best fit occurs for  $V_1 = -2.5, V_2 = -7.5$  and  $a_1 = 5$  as could have been expected.

The comparison between the three different numerical schemes appears in Table II for a specific case ( $a_1 = 5, V_1 = 2.5, V_2 = -7.5$ ). The improvement is self evident.

APPENDIX A

Let  $x_{n+1}, \tilde{x}_{n+1}$  be defined as

$$\begin{aligned}
 x_{n+1} &= x_n - \frac{f_n}{f'_n}, \\
 \tilde{x}_{n+1} &= x_n - \frac{f_n}{\tilde{f}'_n},
 \end{aligned}
 \tag{A1}$$

TABLE II<sup>a,b,c</sup>

The Performance of the Three Different Numerical Schemes ( $a_1 = 5, V_1 = -2.5, V_2 = -7.5$ )

Scheme	Newton Raphson	Regula Falsi	Improved R.F.
Total Number of evaluations	36	27	22

<sup>a</sup> The search for the eigenvalues of the specific example was performed within the interval  $V_2 < E < V_1$ . The starting guess for the lowest value  $E_i$  was taken as  $(V_2 + 0.05)$ . For all  $i$ , once  $E_i$  was computed, the starting guess for  $E_{i+1}$  was  $(E_i + 0.4)$ . If this guess overshoot or led back to  $E_i$ , it was immediately adjusted.

<sup>b</sup> The convergence test was  $|x_{n+1} - x_n| \leq 5 \times 10^{-10}$ ;  $x_n, x_{n+1}$  being two consecutive approximations to any  $E_i$ .

<sup>c</sup> The total number of computations for all four eigenvalues are given.

where  $\tilde{f}'_n$  is an approximation to  $f'_n$ . Denote the difference  $\tilde{f}'_n - f'_n$  by  $\delta$ . Then

$$\tilde{\varepsilon}_{n+1} = \tilde{x}_{n+1} - s = \left( x_n - \frac{f_n}{f'_n} - s \right) + \frac{f_n}{f'_n} - \frac{f_n}{f'_n + \delta} \quad (\text{A2})$$

which, provided  $\varepsilon_n$  is small enough, leads to

$$\tilde{\varepsilon}_{n+1} = O(\varepsilon_n^2) + \frac{f_n \delta}{f'_n(f'_n + \delta)} = O(\varepsilon_n^2) + O(\varepsilon_n \delta) \quad (\text{A3})$$

since  $f_n = O(\varepsilon_n)$ .

Thus, a necessary and sufficient condition for  $\tilde{f}'_n$  to provide quadratic convergence is  $\delta = O(\varepsilon_n)$ . If we choose

$$\tilde{f}'_n = \frac{2(f_n - f_{n-1})}{x_n - x_{n-1}} - f'_{n-1} \quad (\text{A4})$$

and replace  $f_{n-1}$ ,  $f'_{n-1}$  by their Taylor expansions around  $x_n$  we get

$$\tilde{f}'_n = f'_n - \frac{(\varepsilon_{n-1} - \varepsilon_n)^2}{3} f'''_n + O(\varepsilon_{n-1}^2) \quad (\text{A5})$$

or

$$\delta = \tilde{f}'_n - f'_n = O(\varepsilon_{n-1}^2) = O(\varepsilon_n). \quad (\text{A6})$$

Hence, provided the  $(n-1)$ th iteration is of a quadratic nature, the choice (A4) guarantees a quadratic convergence for the  $n$ th iteration as well.

## APPENDIX B

Assume that  $f'_{n-2}$ ,  $f_{n-2}$ ,  $f_{n-1}$ ,  $f_n$  are known by previous consecutive computations and that  $\varepsilon_{n-1} = O(\varepsilon_{n-2}^2)$ ,  $\varepsilon_n = O(\varepsilon_{n-1}^2)$ . We define

$$\tilde{x}_{n+1} = x_n - \frac{f_n}{\tilde{f}'_n} = x_n - \frac{f_n}{\alpha f'_{n-2} + \beta f_{n-2} + \gamma f_{n-1} + \delta f'_n} \quad (\text{B1})$$

and search for  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\delta$  that would give the best approximation to  $f'_n$ . This is done by expanding  $f'_{n-2}$ ,  $f_{n-2}$ ,  $f_{n-1}$  around  $x_n$  and choosing  $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\delta$  that would cancel the terms containing  $f_n$ ,  $f'_n$ ,  $f'''_n$  and would also set the coefficient of  $f'_n$  to 1.

The values obtained are

$$\begin{aligned} \alpha &= \frac{x_{n-1} - x_n}{x_{n-2} - x_{n-1}}, & \beta &= \frac{(x_{n-1} - x_n)(2x_{n-1} + x_n - 3x_{n-2})}{(x_{n-1} - x_{n-2})^2(x_{n-2} - x_n)}, \\ \gamma &= \frac{(x_{n-2} - x_n)^2}{(x_{n-1} - x_n)(x_{n-1} - x_{n-2})^2}, & \delta &= \frac{3x_n - 2x_{n-1} - x_{n-2}}{(x_{n-2} - x_n)(x_{n-1} - x_n)}. \end{aligned} \quad (\text{B2})$$

Their substitution in Eq. (B1) leads to

$$\tilde{f}'_n \triangleq \alpha f'_{n-2} + \beta f'_{n-1} + \gamma f'_n = f'_n + O(\varepsilon_n) \quad (\text{B3})$$

and therefore to quadratic convergence.

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