EIGENVALUE PROBLEM FOR SCHRÖDINGER EQUATION USING NUMEROV METHOD

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În aceeastă lucrare este prezentată o metodă originală de rezolvare a ecuației lui Schrödinger unidimensională, folosind potențialul Wood-Saxon, cu ambele puncte de întoarcere interior respectiv exterior care poate fi utilizată şi în alte domenii (de exemplu în spectroscopie moleculară), precum şi soluția numerică a acesteia. Acestea se referă la alegerea pasului, schimbarea pasului, iterația valorilor proprii, fixarea limitelor inferioară respectiv superioară a valorilor proprii, determinarea unui interval de integrare necesar pentru coordonata de poziție, un exemplu numeric cu potențialul Wood–Saxon şi o comparație a Metodei Numerov cu alte metode.

In this paper we present an original method to solve the one-dimensional Schrödinger equation in Wood Saxon potential, with both an inner and outer classical turning point which can be used in other fields (for example molecular spectroscopy) and also the its numerical solution. These involve choice of a step size, changing step size, iteration on the eigenvalue, setting upper and lower bounds on the eigenvalue, determining a useful range of the coordinate for the numerical integration, a numerical example with Wood–Saxon potential and a comparation between Numerov method and other methods.

Keywords: one-dimensional Schrödinger equation,Wood Saxon potential, eigenvalue, Numerov method, classical turning point.

1. Introduction

Over the past couple of decades, new algoritms have improved the accuracy and efficiency with a few orders comparable of the original Numerov method for resonant state and highest oscillatory solution, by finding better discretization or extending the interval of periodicity.

In these algoritms we found Taylor series expansion [1], [2], continuity of the logarithmic derivative [2], bisection method [3] used for finding zero of the nonlinear equation $f(x)=0$, a few types of discretizations [1]-[5], trigonometrically-fitting method [4], [5] (TFM) which overcome the traditional Obrechkoff one-step method (or called as the non-TFM) for its poor-accuracy in

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the resonant state, and Wood Saxon potential. Numerical solution of the one-dimensional Schrödinger equation in a Wood-Saxon potential has seen application in electrochemistry.

Numerov's method is the highest order method which is at the same time a three-point method. Lower-order methods such as the Runge-Kutta method (error of order $h^4 y^{(4)}$) lead to smaller net intervals h, and hence longer integrations times and more roundoff errors. Methods involving more than three adjacent function values should be avoided, since they are frequently unstable. If the Noumerov method with a given step size h has insufficient accuracy, the remedy lies in decreasing the step size, not in going to some other method.

2. Numerov method; theory

Method of Numerov is the most popular scheme to integrate the one-dimensional Scrödinger equation:

$$y'' = f(x)y(x),\ f(x) = V(x) - E,\ x \in [a,b] \tag{1}$$

with nonsingular potential $V(x)$. In order to solve it we used a three point scheme of the form:

$$y(x+h) - 2y(x) + y(x-h) = \beta_0 (y''(x+h) + y''(x-h)) + \beta_1 y''(x) \tag{2}$$

where:

$$\beta_0 = h^2/12,\ \beta_1 = 5h^2/6 \tag{3}$$

and h represent the step size. The values of β_0 and β_1 where obtained from the condition that Eq. (2) may be integrated exactly, polynomials whose degree is as high as possible. In fact, the algoritm (2) and (3) integrates exactly the functions $1, x, x^2, x^3, x^4$ and x^5.

It should be noted, however, that the general behaviour of the solution of Eq.(1) is better described in terms of the exponential functions. Indeed, take some subinterval [a_1,b_1] of [a,b] on which approximate $V(x)$ by a constant $\overline{V}$. The Eq. (1) is then approximated by $\overline{y''} = \overline{f}\,\overline{y}, \overline{f} = \overline{V} - E$ which has the general solution:

$$\overline{y} = A_0 \exp\left(\sqrt{\overline{f}}\,x\right) + B_0 \exp\left(-\sqrt{\overline{f}}\,x\right) \tag{4}$$

It means that the algorithm (2) and (3) is accurate enough for Eq.(1) if the step size h is so small that the exponential functions can be approximated safely by fifth order polynomials. Therefore the larger $\overline{f}$ is the smaller should be the step size to be used and this is the basis of repeated criticism of the standard Numerov scheme when it is used to integrate Eq. (1) at higher energies.

We shall discuss the various problems encountered, and methods used to solve the eigenvalue problem for Scrődinger equation:

• How to chose a step size, how to decide when the step size needs changing, and how to carry out this change. A midpoint formula is develop for use with the Numerov method.

• How to iterate on the eigenvalue when already close to it. The usual variational method is put into a convenient form,and a formula is developed for the derivative of the wavefunction, to be used with the Numerov method (it should be noted that the Numerov method itself does not give the derivative at all).

• How to narrow down the search for the desired eigenvalue (with N a given number of nodes) in the initial stages.

• How to decide on a range of the independent variable *x* for the numerical integration.

In order to establish the statement of the problem, and a quick review of the Numerov method we consider the form of one-dimensional Scrödinger equation:

$$\frac{d^2y}{d^2x} = f(x)y(x) \tag{5}$$

where

$$f(x) = (2M/\hbar^2)[V(x) - E]. \tag{6}$$

Here $V(x)$ is the potential energy function, M is the reduced mass of the problem, and $\hbar^2$ is Planck's constant divided by 2π. The potential $V(x)$ approaches zero in the limit of large positive x, it is negative for intermediare values of x, and becomes positive and large for small positive x. Formally speaking, we desire a solution $y(x)$ which is bounded and square-integrable on the positive x axis, with $y(0) = 0$. In practice, we need not consider values near $x = 0$ at all, since $y(x)$ becomes exponentially small in that region, due to the "repulsive core" of the potential $V(x)$. The energy E in Eq. (6) is an eigenvalue, to be determined so that the solution $y_N(x)$ of Eq. (5) is not only square-integrable (and therefore approaches zero as x approaches infinity), but has exactly N nodes (zeros) on the positive x axis.

The eigenvalue E_N in question are negative. For any E, eigenvalue or not, there are two values of x, called the *classical turning points*, at which:

$$f(x) = 0. \tag{7}$$

The desired solution $y(x)$ has increasing exponential behavior for $0 < x < x_1$, oscillatory behavior between the two turning points [where $f(x)$ is negative], and decreasing exponential behavior for $x > x_2$. We shall concentrate on the problem of numerical integration of the differential Eq. (5), without

worrying about the eigenvalue problem aspects; that is, we assume that $f(x)$ is a given function, which is large and positive for small x, becomes negative in the range $x_1 < x < x_2$ [where x_1 and x_2 are the solutions of Eq. (7)], and then becomes positive again, approaching a constant positive value as x approaches infinity. In order to establish notation for later use, we review *Numerov method* briefly here, and follow this with a brief reminder why this is the method of choice. We start from the Taylor expansion of $y(x+h)$ around the point x,

$$y(x+h) = \sum_{n=0}^{\infty} \frac{h^n}{n!} y^{(n)} \tag{8}$$

where $y^{(n)}$ is the n'th derivative if $y(x)$ evaluated at the point x. We obtained:

$$\frac{1}{2}[y(x+h)+y(x-h)] = \mathrm{y} + \frac{1}{2}h^2 y^{(2)} + \frac{h^4}{4!} y^{(4)} + \frac{h^6}{6!} y^{(6)} + ... \tag{9}$$

and, differentiating twice,

$$\frac{1}{2}[y^{(2)}(x+h)+y^{(2)}(x-h)] = y^{(2)} + \frac{1}{2}h^2 y^{(4)} + \frac{h^4}{4!} y^{(6)} + ... \ . \tag{10}$$

We now multiply Eq. (10) by the factor $\frac{1}{12}h^2$, and substract the result from Eq. (9). This eliminates the term proportional to $y^{(4)}$. We replace the second derivative $y^{(2)}$, wherever it occurs, by $f(x)y(x)$ according to Eq. (5). Introducing the notation

$$T(x) = \frac{h^2}{12} f(x) = \frac{h^2}{12} \frac{2M}{\hbar^2} [V(x) - E] \tag{11}$$

we thus arrive to the *basic formula of the Numerov method*

$$[1 - T(x+h)]y(x+h) + [1 - T(x-h)]y(x-h) = [2 + 10T(x)]y(x) - \frac{h^6}{240} y^{(6)} + ... \tag{12}$$

If $y(x)$ and $y(x-h)$ are known, $y(x+h)$ can be found directly from this equation if the error term, proportional to $y^{(6)}$, is ignored; the values of $T(x)$ are known, of course.

3. Changing net size

In the case of large positive values of the potential $V(x)$ for small x, we must start the integration with a rather small net size h. Unless we are prepared to change net size as we go out, we will then waste a lot of machine time in the region where $f(x)$ is small in absolute value. It is therefore necessary to decide, during the course of the integration, whether the net size can be increased with safety, whether it must perhaps be decreased, and to program in the necessary

steps for carrying out these operations. In the neighborhood of a point x at which $f(x)$ is positive and varying slowly, the solution $y(x)$ has roughly exponential behavior $\exp(\pm ax)$ with $a \cong \sqrt{f(x)}$ and in a region of negative $f(x)$, the behavior of $y(x)$ is oscillatory, of type $\sin(kx-b)$ with $k \cong \sqrt{-f(x)}$. In either case, we obtain the estimate:

$$y^{(6)} \approx [f(x)]^3 y(x) \tag{13}$$

We substitute this estimate into the error term of Eq. (12), and use the notation (11):

$$Relative\ error\ per\ step = \frac{Error..in..y(x+h)}{y(x)} \approx -\frac{72}{10}[T(x)]^3 \tag{14}$$

The relative error per step that we are prepared to tolerate depends on the total number of the steps we anticipate having to take, and on the accuracy with which we wish to know the final wavefunction. The number of steps we shall have to take is proportional to the number of nodes N in the wavefunction, since a given accuracy in $y(x)$ decides in the main the number of half-wavelengths can be estimated as $N+1/2$ for our purpose.

As an example, suppose we anticipate having to take some 500 steps altoghether, and we wish to know the function $y(x)$ to 1% accuracy. We can then tolerate relative errors of up to 2×10^{-5}, witch by Eq. (14) means $|T(x)|\leq 0.001$ is a safe upper limit. These estimate depend on integrating in such a way that error made at a given step does not tend to perpetuate itself, with compound interest, during subsequent steps. It should be noted that the condition deduced from the estimate (14) is a condition on $T(x)$, on the coefficient in the differential equation, not on the solution $y(x)$ directly. This highly desirable behavior is associated with the linearity if the differential Eq. (5), and is sometimes not brought out clearly in books on numerical analysis where the emphasis is frequently on the solution of nonlinear differential equations. Since the condition which determines the choice of step size is on $T(x)$, the regions of x in which different step sizes are required can be determined as soon as $T(x)$ is known for all x to sufficient accuracy, as soon as we have a trial value of the energy E [which appears in Eq. (11)] sufficiently close to the true value of E. Thus, in principle, $t(x)$ need not be tested at every point during the integration; but in practice, such a test takes little time. The only step-size changes of interest are halving and doubling of the step size. $T(x)$ should be calculated in minimum time. The effective way of doing so is to store, in core memory, the values of:

$$Y(x) = h^2 2MV(x)/12\hbar^2 \tag{15}$$

for all netpoints $x_n = nh$ on the finest net size h. The computation of $T(x)$ for this net size is then a straight table-lookup followed by substraction of a constant:

$$T(x) = Y(x) - h^2 2ME/12\hbar^2 \tag{16}$$

If we restrict net-size changes to doubling and halvings, and if h in Eq. (15) is the finest net size ever used, then the effect of net-size changes amounts to multiplication of the right side of Eq. (16) by an appropriate power of 4, a fast operation in a binary machine. If h is chosen as indicated, the possible net-size halving during the course of the integration will never lead us to a net size h' smaller than h, and there will never be a need for interpolations in the table of $Y(x)$.

Doubling the net size is trivial: all we need to do is to carry along, during the integration, $y(x-2h)$ as well as $y(x-h)$.When h is doubled, as a result of a test on $T(x+h)$, the value of $y(x-2h)$ is stored into the position reserved for $y(x-h)$, $T(x)$ is multiplied by 4, and $T(x-h') = T(x-2h)$ are obtained by table-lookup followed by multiplication by a new power of 4.

Halving the net size, at first sight, is more troublesome.If we decide that the absolute value of $T(x+h)$ is too large for comfort, and to introduce the halved net size $h' = h/2$, we require $y(x-h') = y(x-\frac{h}{2})$ to continue the integration. The value of $y(x)$ known to us are $y(x-h)$ and $y(x)$. We thus require an accurate formula for midpoint interpolation-accurate to the same order as the Numerov method itself –for otherwise we lose the advantage of the Numerov method. Letting $x_0 = x - \frac{h}{2}$ be the point at which we desire to know y, our problem can be restarted as follows: find $y(x_0)$, given values of $y(x_0+h')$ and $y(x_0-h')$, and given that $y(X)$ satisfies the differential equation (5). The solution, though exceedingly simple, does not, to our knowledge, appear in the literature: it consist in using the basic formula of the Numerov method, Eq. (12), to solve for it $y(x)$. The accuracy is then obviously the same as the accuracy of the Numerov method.No additional function values need be stored and net-size halving is now as simple as net-size doubling. For the sake of the record,we write down *the midpoint interpolation formula* explicitly (in the error term, we replace $2+10T(x)$ by 2):

$$y(x) = \frac{[1-T(x+h)]y(x+h) + [1-T(x-h)]y(x-h)}{2+10T(x)} + \frac{h^6 y^{(6)}}{480} + \ldots . \tag{17}$$

4. Iteration on the eigenvalue when we are close and a derivative formula

The lowest eigenvalue of the Hamiltonian E is approximated by the mean value $\frac{\langle v(x)|Hv(x)\rangle}{\langle v(x)|v(x)\rangle}$. One obtain $E=\frac{\int v(x)\left[-\frac{\hbar^2}{2M}(d^2/dx^2)+V(x)\right]v(x)dx}{\int v^2(x)dx}$ and finally

$$\frac{2ME}{\hbar^2}\cong\frac{\int v(x)\left[-d^2/dx^2+2MV(x)/\hbar^2\right]v(x)\}dx}{\int v^2(x)dx} \tag{18}$$

Written in this form, the expression is rather awkward. We have seen already that and must integrate outwards for small values of the coordinate x, and inwards for large x. We let Q be a trial value for the energy E, hopefully close to the true value of E. Then integrate the differential equation:

$$\frac{d^2v}{dx^2}=\frac{2M}{\hbar^2}[V(x)-Q]v(x)\equiv f_Q(x)v(x) \tag{19}$$

first outwards from some sufficiently small value of x until we reach a joining point $x=x_0$, then inwards from some sufficiently largue value of x until we reach the same joining point.The outwards integration is started in such a way that we obtain the exponentially increasing solution, the inwards integration is started in such a way that we obtain the exponentially decreasing solution.In either solution,there is one free multiplicative constant.We can, and do, read just this constant at the end so that $v(x)$ turns out to be continuous at $x=x_0$, the joining point.In practice, x_0 is chosen to be the minimum of the potential $V(x)$. The fact that this $v(x)$ is not yet the true solution to the eigenvalue problem manifest itself as a discontinuity in the first derivative $v'(x)$ at $x=x_0$. The lefthand value v'_L obtained from the outwards integration fails to equal the righthand value v'_R obtained from the inwards integration. The second derivative d^2v/dx^2 therefore has a delta-function singularity at $x=x_0$, which makes a finite contribution to the integral in the numerator of (18). Except for this delta function contribution, the result would be just Q, the trial value for the energy, as can be seen by substituting (19) into (18). Putting things together, we obtain the simple iteration formula:

$$\frac{2ME}{\hbar^2}\cong\frac{2MQ}{\hbar^2}-\frac{v(x_0)(v'_R-v'_L)}{\int[v(x)]^2dx} \tag{20}$$

The Simpson-rule sums necessary for the evaluation of the integral in the denominator can be accumulated during the process of solving the differential

Eq. (19), and can be multiplied by the appropriate factors to make $v(x)$ continuous at $x = x_0$, without any problem. However, Eq. (20) is useless unless we have an accurate value for the derivative $dv/dx = v'(x)$. The Numerov method by itself fails to give us such a value; in fact, the Numerov method is built on the fact that the first derivative does not appear explicitly in the differential equation.

One method is to integrate the second derivative d^2v/dx^2 numerically; however, this is both awkward and productive of numerical inaccuracies.

A better method, which is new to our knowledge, can be developed by using reasoning similar to that of the Numerov method itself. We star by developing a low-accuracy formula, so as to show the basic idea; we then improve the method so as to get a derivative formula with an error term of order $h^9v^{(9)}$.

Returning to the *Taylor – series expansion* (8), we compute:

$$A_1 \equiv \frac{1}{2}[y(x+h) - y(x-h)] = hy' + \frac{h^3}{3!}y^{(3)} + \frac{h^5}{5!}y^{(5)} + ... \tag{21}$$

Taking into account the *second derivative* on both sides, and multiplying by $h^2/6$, we obtain:

$$B_1 \equiv \left(\frac{h^2}{12}\right)[y''(x+h) - y''(x-h)] = \frac{h^3}{6}y^{(3)} + \frac{h^5}{36}y^{(5)} + ... \tag{22}$$

We substract (22) from (21) and use the differential equation to replace y'' by $f(x)y(x)$, to obtain the first derivative formula:

$$hy' = [1 - T(x+h)]y(x+h) - [1 - T(x-h)]y(x-h) + (7/360)h^5y^5 + ... \tag{23}$$

Here $T(x)$ is defined by (11) with $f(x) = f_Q(x)$ defined by (19). The error term in (23) may be sufficiently small in some cases. It is, however, of order $h^5y^{(5)}$ porrer than the basic error of the Numerov method. At substantially no expense in machine time, the accuracy of the *first derivative*, and hence of Eq. (20), can be improved significantly, simply by using function values at $x + 2h$ and $x - 2h$. We define:

$$A_2 = \frac{1}{2}[y(x+2h) - y(x-2h)] \tag{24}$$

and

$$\begin{aligned} B_2 &= \frac{1}{12}h^2[y''(x+2h) - y''(x-2h)] = \\ &= T(x+2h)y(x+2h) - T(x-2h)y(x-2h) \end{aligned} \tag{25}$$

We then write down the Taylor expansion of A_1, A_2, B_1, and B_2, carrying terms up to order $h^9v^{(9)}$ inclusive. We eliminate the terms proportional to $k^ky^{(k)}$

with k =3,5,7 and solve for hy'. The procedure is tedious but straight forward; we quote only the result which is:

$$hy' = \frac{16}{21}\left(-A_1 + \frac{37}{32}A_2 - \frac{37}{35}B_1 - \frac{17}{40}B_2\right) - \frac{4016}{35}\frac{h^9 y^{(9)}}{9!} + ... \tag{26}$$

Thus, by integrating a mere two steps beyond the joining point $x = x_0$, we can determine the value of the first derivative to an accuracy substantially better than the basic accuracy of the Numerov method. We now have *an iteration scheme of second order* for the eigenvalue E: starting from a *trial eigenvalue* Q, near to E, we find an improved approximation to E from Eq. (20). The improvement is second order, the error of E is proportional to the square of the error of the trial value Q, once Q is close enough. The iteration is terminated conveniently when we begin to hunt, when the new correction $E - Q$ is both sufficiently small for safety and no smaller than the previous correction in absolute value. The one unnecessary iteration can be saved after a bit of experience, by setting a straight upper limit on $|E - Q|$, and terminating as soon as $|E - Q|$ falls below this upper limit.

The iteration procedure described in the preceding section works only if the trial energy Q is already quite close to the true eigenvalue E_N lies certainly between them:

$$Q_1 < E_N < Q_2 \tag{27}$$

We then try the value:

$$Q = (Q_1 + Q_2)/2 \tag{28}$$

and ascertain whether Q lies above or below the desired E_N ($[Q_1, Q_2]$ being a "probe interval"). If Q lies above E_N, we replace Q_2 by Q and repeat the process; if Q lies below E_N, we replace Q_1 by Q and repeat the process. At each stage, we gain exactly one binary digit of accuracy in the energy. Unless Q_1 and Q_2 are very bad limits indeed, a few stages of halving suffice to get us close enough to E_N. The first step to ascertain where Q lies in relation to E_N is to count the nodes of the trial function $v(x)$ generated by (19). As we generate $v(x)$, we count each node and accumulate. If the node count, at any stage, exceeds N, then the trial value Q was too high. Conversely, if at the end of generating $v(x)$, the node count is below N, then Q was too low. Since we generate $v(x)$ in two stages, so to speak, first by integrating out, then by integrating in, a bit of care is required to avoid double counting of nodes occurring right at the joining point x_0.

We have found the following *simple scheme quite adequate to ensure convergence*:

(1) Ascertain whether the number of nodes in $v(x)$ equals N; if not, proceed with halving.

(2) If the node count agrees, proceed to evaluate the second-order correction $E-Q$ from (20) and (26); the sign of the correction is right, even if the magnitude is far off.Thus, if $E-Q$ turns out to be positive, Q was too low, and we replace Q_1 by Q; if $E-Q$ turns out to be negative, Q was too high, and we replace Q_2 by Q.

(3) Now compute the new $E=Q+(E-Q)$ predicted by the second-order iteration scheme. If this new value of E lies between Q_1 and Q_2,it is safe to use. If not, next trial value is determined by Eq. (28). In this way, we combine the *safety of halving scheme* with the *speed of the second-order iteration*.

5. Setting upper and lower bounds on the eigenvalue

The halving method requires bounds Q_1 and Q_2 on the true eigenvalue E_N. We discuss here methods of setting such bounds. The simpliest case, and the one occurring most of the time, is that we already posses a list of true eigenvalues E_M with $M=N-1,N-2,N-3,....,N-k$, say. Clearly $Q_1=E_{N-1}$ is a lower bound for E_N. Ordinary *polynomical extrapolation* of the list E_M to some depth $j\le k$ [in practice, $j=Min(k,4)$ is adequate] yields a prediction for E_N, which we denote by W_N. We then put:

$$Q_1=E_{N-1},\quad Q_2=E_{N-1}+2\left(W_N-E_{N-1}\right) \tag{29}$$

Unless the polynomical extrapolation is utterly unjustified, the factor 2 in Eq. (29) ensure that Q_2 lies above the true E_N. Furthermore, when we start the halving procedure with this Q_1 and Q_2, the first value tried, by (28), is the predicted value, $Q=W_N$. If the prediction is accurate, this trial value is close enough to the truth to permit use of the second-order iteration scheme, which then yields full convergence in 3 or 4 steps.

Use of (29) requires at least two known eigenvalues, E_{N-1} and E_{N-2}. Thus, an alternative procedure is required at the beginning of the run. The simplest choice is:

$$Q_1=Min[V(x)],\quad Q_2=0 \tag{30}$$

These are perfectly safe *upper and lower bounds* on all bound-state energies. There are two troubles, however:

(1) Quite a few halving steps may be required if such generous bound are used.

(2) The choice of the range of integration (minimum and maximus values of x) for finding $v(x)$, depends on the trial energy. A range of integration suitable for $Q = \frac{1}{2} Min[V(x)]$ the first trial value generated from the choice (30) by means of (28), is a most unsuitable range of integration for the desired eigenvalue E_N, particulary. So if $N = 0$ if we wish to start by generating the ground state. Thus, if (30) is used, the range of integration must be readjusted during the halving process until we are down to the right number of nodes.

Better limits than (30) are available if we want to generate all eigenvalues E_N from $N = 0$ onwards. $Q_1 = Min[V(x)]$ is then a fairly close lower bound for the true E_0, but $Q_2 = 0$ would be a very bad upper bound. A simple scheme consistes in approximating $V(x)$ near its minimum by a quadratic polynomial (oscillator potential) and determining the ground state energy of this oscillator, $h\nu/2$ .We then set $Q_2 = Q_1 + h\nu$, the extra factor 2 serving as a safety measure. An alternative is to use Eq. (20) with a simple trial function:

$$v(x) = \exp[-a(x - x_0)^2] \tag{31}$$

The two methods can be combined by determining the parameter a in (30) from the oscillator-potential fitting, the function (31) being just of the right form for the ground-state wavefunction of an oscillator potential. With a bit of experience, it is possible to make a reasonable guess at the zero-point energy $E_0 - Min[V(x)]$ and to set a generous upper limit Q_2 which is nonetheless far nearer to the true E_0 than the trivial choice, without going to all the trouble of evaluating (18) numerically for the function (30).Once the lowest eigenvalue E_0 is known, a safe upper limit for the eigenvalue E_1 is:

$$E_1 \le Q_2 = E_0 + 3\{E_0 - Min[V(x)]\} \tag{32}$$

The factor 3 is exactly right for a square-well potential, and is an overestimate for all other potentials; for an oscillator potential, the correct factor would be 2, to that 3 is a perfectly safe choice for an upper limit. Once E_0 and E_1 are known, *extrapolation* becomes possible with more and more accuracy as further eigenvalue very rapid convergence.

The outwards integration must start at a value of x less than the inner turning point x_1; the inwards integration must start at a value of x larger than the outer turning point x_2. In this section, we discuss the choice of these starting points, and hence the choice of the total range of integration for the wavefunction. We also discuss how the integrations are started so as to get the desired solution, the exponentially increasing solution for the outwards integration, the exponentially decreasing solution for the inwards integration. We discuss the

second point first; that is, let us suppose we have chosen a staring value of x, call it $x = a$, for outward integration. Clearly $v(a)$ can be set arbitrarily, since one multiplicative factor is free. To get going with the Numerov method, we require an approximation to $v(a+h)$ for the exponentially increasing solution. The first thing to realize is that quite sizeable errors are permitted here. An erroneous choice of $v(a+h)$ has the effect of admixing, to the desired exponentially increasing solution, a component proportional to the other, exponentially decreasing solution. As we integrate out from *a* towards the turning point x_1, this erroneous component becomes smaller. Whereas the desired component increases in value.

To the crude approximation need here, the differential equation (5) is satisfied by:

$$v(x) \cong v(a)\exp[W(x)] \tag{33}$$

where

$$W(x) = \int_a^x \sqrt{f(x)}dx\,. \tag{34}$$

This is one step cruder than the usual *WKB approximation*, but is good enough for us here.We now become even cruder, by replacing the integral from relation (34) by its *trapezoidal-rule approximation*.The result is the following estimate for $v(a+h)$:

$$v(a+h) \equiv v(a)\exp[\sqrt{3T(a)} + \sqrt{3T(a+h)}] \tag{35}$$

where $T(x)$ is defined by (11), and is the quantity we require in any case for the Noumerv method. We note that $f(x)$, and hence $T(x)$, are positive outside the classical turning points, so that the square roots in (35) are real numbers. The positive square roots should be used for the exponentially increasing solution, to get from *a* to *a+h*, and the negative square roots should be use for the exponentially decreasing solution, to get from the outermost point $x = b$ to $x = b - h$, at the start of the inwards integration. We note that there is no difference, in the Numerov method, whether one integrates inwards or outwards; the basic equation (12), can be solved for $y(x-h)$ as it can for $y(x+h)$. It remains to decide on suitable values of *a* and *b*. If *a* is too close to the inner turning point x_1, we fail to generate enough of the desired wavefunction; if *a* is too far from x_1, we not only waste machine time by generating the wave function (we miss an appreciable part of the exponential tail) in a region where its value is exceedingly small and of no conceivable physical interest, but we can also get into scaling troubles: even modern machines, with floating-point facilities, do not allow an infinite range of the floating-point exponent. And once we are well and truly into the exponential region, it becomes all too easy to get into underflow

troubles even on present machines. Supppose we wish to chose the inner starting point $x = a$ so that $v(a)$ is smaller than the value at the turning point, $v(x_1)$, by a factor exp(A), with A given *a priori*. For example, we might choose $A = 16$, corresponding to a factor of roughly 10^7. We now use the estimate Eqs. (33), (34) to get the condition on *a*:

$$\int_a^{x_1} \sqrt{f(x)}dx = A \tag{36}$$

The integrand is zero at the upper limit, the classical turning point x_1. We again replace the integral by trapezoidal-rule approximation, and keep going downwards through $x_1 - h, x_1 - 2h, x_1 - 3h, ..., x_1$-h, until the accumulated sum exceeds A. The terms in the sum are of form $\sqrt{2T(x_i)}$ where $T(x)$ is defined by Eq. (11). Te uppermost value of x, $x = b$, is determined similary, the condition being:

$$\int_{x_2}^{b} \sqrt{f(x)}dx = A \tag{37}$$

Since $f(x) = f_Q(x)$ depends on the value of the trial energy Q, the turning points x_1, x_2 as well as the cutoff points *a* and *b*, depend on the value of Q. As Q increases, the outer turning point x_2 and the outer cutoff point *b* move further out (increase in value), whereas the inner turning point x_1 and the inner cutoff point *a* move inwards (decrease in value).In principle, *a* and *b* ought to be recalculated when the trial energy Q changes.

6. Numerical example and discussion of results

We take into account the *Woods-Saxon potential*:

$$V(x) = V_{WS}(x) = \frac{u_0}{(1+q)} + \frac{u_1 q}{(1+q)^2} \tag{38}$$

where $q = \exp\left(\frac{x - x_0}{a}\right)$, with $u_0 = V_0 = -50$, $a = 0.6$, $x_0 = 7$ and $u_1 = -u_0 / a$. We consider Eq. (1) for this potential in rather large domain of energies, $E_{\min}$ = - 50, $E_{\max}$ =1010. For negative energies we solve the bound state problem, with the boundry conditions

$$y(0) = 0, \quad y(x) = \exp\left(-\sqrt{-E}\right) \tag{39}$$

for large values of x. For positive energies one has the so called open channel problem. This consists either to determine the phase shifts $\delta(E)$ or to find those

E's at which δ equals $\pi/2$. We actually solve the latter problem, known as " the resonance problem" when the eigenenergies lie under the potential barrier. The *boundary conditions* for this problem:

$$y(0)=0, \quad y(x)=\cos(\sqrt{E}x) \tag{40}$$

for large x. The *domain* of numerical integration is [0,15]. One of the authors (C. Tatu) has developed a software application in Fortran programming language for Numerov method begining with the three point scheme and the iteration scheme of second-order.

The numerical example consiste in the integration of the differential equation using Wood-Saxon potential:

$$V_{WS}=V(r)=\frac{-V_0}{1+\exp[(r-R)/a]} \tag{41}$$

where $r=x$, V_0 = potential depth, R = width of the potential, and a = surface thickness. After compilation of this program he used in Linux OS a Gnuplot software for graphical representation of $V(x)$ (Wood-Saxon potential) and $y(x)$ function (Figs. 1 and 2, 3, 4, respectively). Some eigenvalues, errors and number of iterations are presented in Table 1.

Table 1.

	Eigenvalues	Errors	Xmatch-Xi	Iterations
1	-49.45778872900700	9.24D-10	-0.00000000140718	35
2	-48.14843004409380	2.09D-08	1.27513E-09	35
3	-46.29075410649230	1.52D-07	-8.43995E-10	35
4	-43.09683190659410	6.34D-07	8.98532E-10	35
5	-41.23260969553620	1.92D-06	-3.37735E-10	35
6	-38.12278984299330	4.75D-06	-1.41659E-10	35
7	-34.67232334252640	1.01D-05	-6.84757E-11	35
8	-30.91226692618510	1.94D-05	4.50828E-10	35
9	-26.87348318285510	3.43D-05	-1.66361E-10	36
10	-22.58865865646650	5.64D-05	-2.12436E-10	36
11	-18.09477582683750	8.75D-05	-2.12082E-10	36
12	-13.43699793696420	1.29D-04	-8.28638E-11	37
13	-8.676261823904500	1.80D-04	3.68863E-11	37
14	-3.908469327185230	2.37D-04	2.91823E-11	38

In the case when the Woods-Saxon potential (Fig.1) is negative for $x<x_1$, is also negative and has increasing exponential for $x_1<x<x_2$ and becomes positive an decresing exponential for $x>x_2$, where x_1, x_2 are the classical turning points (solutions of $f(x)=0$, with $f(x)=V(x)-E$).

In Figs. 2-4 we present the dependence of function $y(x)$ (from equation (1): $y'' = f(x)y(x)$), for $N = 1$, $N = 2$ and $N = 14$ nodes.

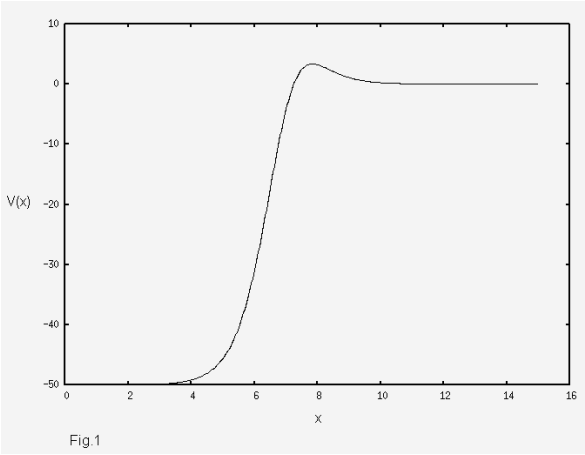

Fig 1. The dependence of Woods-Saxon potential $V(x)$ on the coordinate x.

As can be seen it will have an oscillatory behavior until turning point and an exponential behaviour after it.

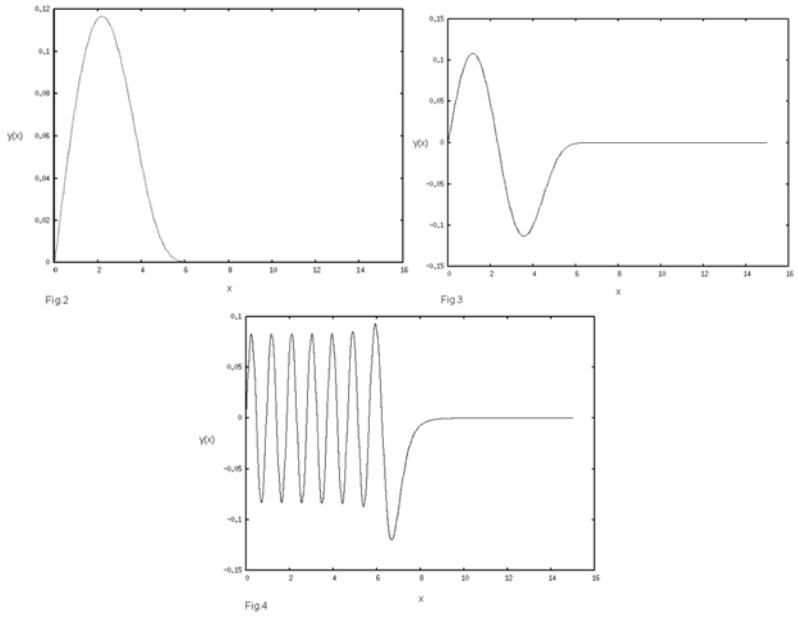

Fig. 2, 3, 4. The dependence of function $y(x)$, for: 2) $N = 1$, 3) $N = 2$ and 4) $N = 14$ nodes.

7. Conclusions

Starting from Taylor expansion, we use the convergence scheme with halving method (*bisection method*) starting from a trial energy value Q (to find the real energy E). The halving method require bounds Q_1, Q_2 on the true eigenvalue E_N .Once E_0 and E_1 are known the polinomical extrapolation of the list E_M becomes possible. At the integration we replace the integral using the trapezoidal-rule approximation. These involve choice of a step size, changing step size, iteration on the eigenvalue, setting upper and lower bounds on the eigenvalue, setting upper and lower bounds on the eigenvalue, determining a useful range of the coordinate for the numerical integration, a numerical example with Wood–Saxon potential and a comparation between Numerov method and other methods.

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