# Finite-difference scheme to solve Schrödinger equations

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Comparisons are made among several three-node finite-difference schemes (FDS's) for solving time-independent Schrödinger equations. It is shown that the Mickens FDS is, although exact in some special cases, generally two orders lower than the Numerov FDS. An alternative FDS, the combined Numerov-Mickens FDS, is introduced. It has advantages of both the Numerov and the Mickens FDS's. Numerical comparison among these FDS's is presented.

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## I. INTRODUCTION

In physics, chemistry, and even some other natural sciences, it is always interesting and important to integrate Schrödinger equations numerically with both higher speed and accuracy. For the same reason, much interest is paid in solving the Schrödinger equations by using different finite-difference schemes (FDS's), even if they are one dimensional (1D) and time independent [1],

$$\psi''=F(x)\psi, \quad F(x)=2m[-E+V(x)]/\hbar^2 , \tag{1}$$

where $E$ is the energy eigenvalue, $m$ and $\hbar$ are the mass and Planck constant, respectively, and $V(x)$ is the potential function. The above equation can also result from physical problems having more than one space dimension, such as the three-dimensional motion of particles moving in a central force field [2,3].

In solving the 1D time-independent Schrödinger equation, great attention is paid to three-node finite-difference schemes, which can be solved by Gauss elimination with a rather small amount of computer storage and calculation [4]. Many of the three-node FDS's can be written as

$$-U_{n-1}+2DU_n-U_{n+1}=0, \quad U_n=U(x_n), \quad F_n=F(x_n) , \tag{2}$$

$$n=0,1,2,\ldots,N+1, \quad x_n=a+nh , \tag{3}$$

with $x_{0=a}$, $x_{N+1}=b$, where both $D$ and the relation between $U_n$ and $\psi(x_n)$ depend on the concrete FDS. For example, there are the central FDS [4–6]

$$U_n(\mathrm{C})=\psi_n, \quad D(\mathrm{C})=1+h^2F_n/2 , \tag{4}$$

the Numerov FDS (fourth-order) [4–7]

$$U_n(\mathrm{N})=(1-T_n)\psi_n, \quad D(\mathrm{N})=\frac{1+5T_n}{1-T_n} , \tag{5}$$

$$T_n=h^2F_n/12 , \tag{6}$$

and the Mickens FDS [8,9]

$$U_n(\mathrm{M})=\psi_n , \tag{7}$$

$$D(\mathrm{M})=\begin{cases}\cos(f_1h), & F_n=-f_1^2\le 0\\ \cosh(f_2h), & F_n=f_2^2\ge 0\end{cases} , \tag{8}$$

where $\psi_n=\psi(x_n)$. We know that the central and Numerov FDS's are approximations to second and fourth order in the mesh step length $h$, respectively [4–6]. When $F(x)$ remains constant in a region of $x$ (i.e., $F'=0$), the Mickens FDS is an exact FDS [8,9], for $U_n$ obtained by this FDS equals the exact values of $\psi(x_n)$, assuming that the rounding-off error is neglected. Therefore in this sense the Mickens FDS is better than both the central and Numerov FDS's when $F'=0$.

After realizing that the Mickens FDS is not an exact FDS when $F'(x)\neq 0$, one may naturally ask, to which order is the Mickens FDS an approximation? Does it always perform better than the central and Numerov FDS's? If not, can we construct an alternative FDS which is still a three-node one, remains an exact FDS when $F'=0$, and performs better than, or at least almost equally well as, the best of the above three FDS's in numerically solving (1) under any circumstances?

In the following we will answer the above questions. First we will determine how accurate the Mickens FDS is when $F'\neq 0$. Then we construct an alternative FDS. Finally the comparison among all the above-mentioned FDS's and a short summary will be presented.

## II. THEORY

It is easy to show that

$$\begin{aligned} &D(\mathrm{C})=1+6T_n , \\ &D(\mathrm{M})=1+6T_n+6T_n^2+0.4(6T_n^3)+\cdots , \\ &D(\mathrm{N})=1+6T_n+6T_n^2+6T_n^3+\cdots . \end{aligned} \tag{9}$$

 

In writing the second equality, we assume that $T_n < 1$, which can always be satisfied for any function $F(x)$ as long as $h$ is small enough. For convenience, we introduce a transition FDS with

$$U_n(\mathrm{T}) = \psi_n, \quad D(\mathrm{T}) = D(\mathrm{N}) , \tag{10}$$

i.e., the difference equations of the transition and the Numerov FDS's are the same, but their solutions have different meanings. $U_n$ in the transition FDS is just the solution $\psi_n$ of (1), as in the Mickens FDS, while $U_n$ in the Numerov FDS is $U_n(\mathrm{N}) = (1 - T_n)\psi_n$. Therefore the transition FDS bears a close resemblance to both the Numerov and the Mickens FDS's, which is just what we mean by "transition." Considering that $T_n = O(h^2)$, the Numerov FDS is a fourth-order FDS, and the only difference between the Numerov FDS and the transition FDS is the different illustrations of $U_n(\mathrm{N})$ and $U_n(\mathrm{T})$; one can derive readily the conclusion that the transition FDS is generally of second order.

Now note that

$$D(\mathrm{T}) = D(\mathrm{N}) = D(\mathrm{M}) + O(h^6) , \tag{11}$$

where $u = O(h^p)$ means that there exists some positive constant $C_1$, independent of $h$, such that $\lim_{h \to 0} |u/h^p| \leq C_1$. One might conclude that, in the regions where $F' \neq 0$, the Mickens FDS is generally of the same order as the transition FDS, i.e., each is a second-order FDS. Therefore the Mickens FDS is usually two orders lower than the Numerov FDS when $F' \neq 0$. But the former has an important advantage over the latter because the former is exact when $F' = 0$ [8,9].

From the Numerov and the Mickens FDS's, we introduce an alternative three-node FDS, which can be called a combined Numerov-Mickens FDS (CNMFDS), with

$$U_n(\mathrm{CNM}) = U_n(\mathrm{N}), \quad D(\mathrm{CNM}) = D(\mathrm{M}) . \tag{12}$$

Relations between the CNMFDS and the Mickens and the Numerov FDS's are clear: The difference equations (2) of the CNMFDS and the Mickens FDS are the same, which are different from that of the Numerov FDS in that $D(\mathrm{CNM})$ is different from $D(\mathrm{N})$ in a sixth-order term, for which one can write by using (12) and (9)

$$D(\mathrm{CNM}) = D(\mathrm{M}) = D(\mathrm{N}) + O(h^6) . \tag{13}$$

$U(\mathrm{CNM})$ and $U(\mathrm{M})$ have different illustrations. $U(\mathrm{CNM})$ is an approximation of $\psi_n$, while $U(\mathrm{M})$ is of $(1 - T_n)\psi_n$.

We now investigate the accuracy of the CNMFDS. First we consider the special case when $F(x)$ is independent of $x$, i.e., $F' = 0$. The difference equation of the Mickens FDS is an exact equation which discretizes the original differential equation (1). Therefore the difference equation multiplied by $(1 - T_n)$, which is a constant for any fixed $h$ when $F' = 0$, will also be exact as is the Mickens FDS. If we recall that this difference equation is the same as that of the CNMFDS, it is evident that the CNMFDS, like the Mickens FDS, is exact when $F' = 0$, and so in this case it is of much greater accuracy than the Numerov FDS. Second we consider the accuracy of the CNMFDS when $F' \neq 0$. From (13), the difference between $D(\mathrm{CNM})$ and $D(\mathrm{N})$ is of the sixth order, which is two orders higher than the order of the Numerov FDS. Hence the difference equation of the CNMFDS will preserve the accuracy of the difference equation of the Numerov FDS. As shown in (12), the relation between the wave function $\psi(x)$ and the discretized function $U_n$ in the CNMFDS is the same as that in the Numerov FDS. Therefore the CNMFDS is at least of the fourth order as is the Numerov FDS when $F' \neq 0$. Numerical experiments will show that, when $F' \neq 0$, the CMFDS is indeed of the fourth order and it performs sometimes much better than, or almost equally as well as, the Numerov FDS.

For further references, we rewrite the CNMFDS as

$$U_n(\mathrm{CNM}) = (1 - T_n)\psi(x_n), \quad T_n = h^2 F_n / 12 , \tag{14}$$

$$D(\mathrm{CNM}) = \begin{cases} \cos(f_1 h), & F_n = -f_1^2 \leq 0 \\ \cosh(f_2 h), & F_n = f_2^2 \geq 0 , \end{cases} \tag{15}$$

$$-U_{n-1}(\mathrm{CNM}) + 2D(\mathrm{CNM})U_n(\mathrm{CNM}) - U_{n+1}(\mathrm{CNM}) = 0 . \tag{16}$$

## III. NUMERICAL COMPARISONS

In this section, we will present two numerical comparisons among all of the FDS's mentioned above, although more comparisons are made in our actual calculations. We think that these two examples are typical enough to show potential uses of the CNMFDS in practical problems. The two examples are chosen not only for their importance but also for the clarity of their analytical solutions.

Our first example is a harmonic oscillator. The Schrödinger equation reads

$$\psi'' = (x^2 + 2l + 1)\psi, \quad l = 0, 1, 2, 3, \ldots , \tag{17}$$

which can be analytically solved by using Hermite polynomials [2]. The second example is the radial equation of a hydrogen atom, whose solution can be found in any standard textbook on quantum mechanics [2,3].

For determination, we only consider boundary-value problems and arbitrarily take $l = 5$ with

$$\psi = (15x - 20x^3 + 4x^5)\exp(-x^2/2) \tag{18}$$

in the first example and the normalized $4p$ state in the second. In the following, we set boundaries at $x = a$ and $x = b$, and calculate $\psi(x = a, b)$ from the corresponding analytical solution at $x = a, b$. We would like to point out that these selections will not restrict general conclusions.

We calculate the average absolute value of the error as

$$\epsilon = \sum_{n=1}^{N} |\psi_n - \psi_n^{(c)}| \Big/ N , \tag{19}$$

where $\psi_n = \psi(x_n)$, $x_n = a + nh$, $h = (b - a)/(N + 1)$, $\psi_n$ is the analytical value, and $\psi_n^{(c)}$ the value calculated by some concrete FDS. In Fig. 1, we calculate $\epsilon$ in the first example for different $N$ with $(a, b)$ to be either $(-2, 2)$ or $(0, 4)$. In Fig. 2, the dependence of $\epsilon$ on the number of nodes is shown for the hydrogen $4p$ state.

Other cases, such as a 1D time-independent

Schrödinger equation different from (14) and the H atom's or other choices of parameters $(a,b)$, are of course permitted. Although only two experiments are shown in the present paper, we find that they are generally in accordance with the numerous numerical experiments we have done. All of the calculations are performed with double precision on an AST386 computer (with 80287 coprocessor) using the FORTRAN language (Microsoft V3.30).

We first look at the errors of the transition FDS. They are close to that of the Numerov FDS when $N$ is small, which is more evident in Fig. 1. They are also close to that of the Mickens FDS when $N$ increases, and in fact the errors resulting from these two FDS's cannot be distinguished from each other in the figures. This can also be seen by using the definition of the transition FDS, recalling (11). According to the error in Fig. 1 from smallest to largest, the five FDS's are the CNM, Numerov, Mickens, transition, and second-order central FDS's, when $N$ is large ($h$ decreases). The CNMFDS is of the same order as the Numerov FDS but the error of the former is much less than that of the latter [in Fig. 1, $\epsilon(\mathrm{CNM})/\epsilon(\mathrm{N})\sim 0.1$]. It is worthwhile to point out in some other experiments (this can also be seen from a few data points shown in Fig. 2) that it is possible that the error in the CNMFDS may be a little larger than that in the Numerov FDS. But it is clearly shown that the order of the CNMFDS and the Numerov FDS is the same for $F'\neq 0$. Furthermore, in all the numerical experiments we have carried out, the CNMFDS works when $F'\neq 0$ almost equally well with, if not better than, the Numerov FDS.

Also shown in the figures is that the error of the Mickens FDS is less than that of the Numerov FDS when $N$ is small, which might not be so in our other experiments. In addition, when the error is too small, the rounding-off error could disturb drastically the performance of the CNMFDS and the Numerov FDS. In Fig. 1 this occurs when the error $\epsilon$ is somewhat smaller than $10^{-9}$.

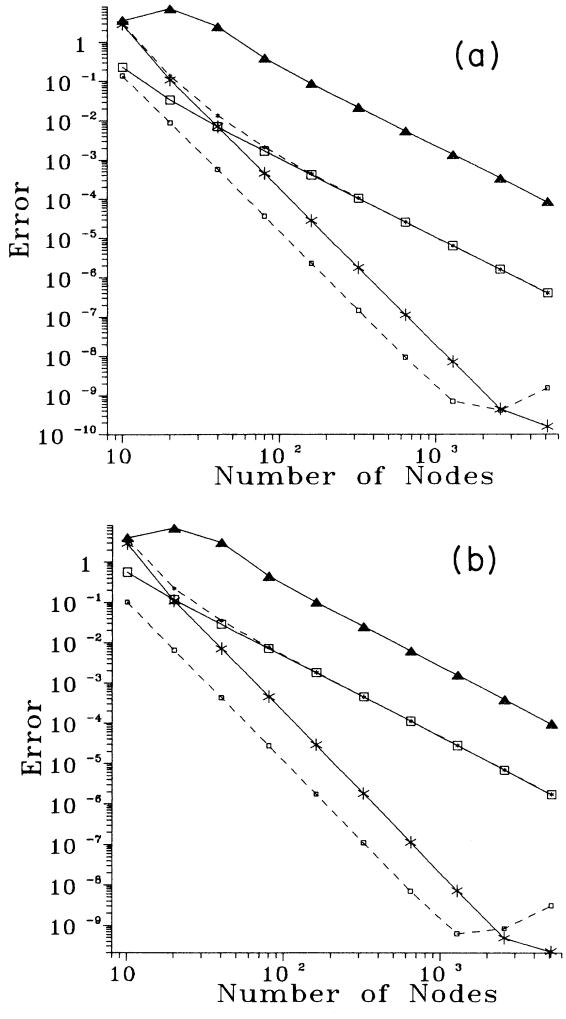


FIG. 1. The dependence of the average error [defined in text, see (19)] on the number of internal nodes $N$ for the fifth eigenfunction of the harmonic oscillator (unnormalized, see text): $-*-$, the Numerov FDS; $--\times--$, the transition FDS; $-\square-$, the Mickens FDS; $--\square--$, the CNMFDS; $-\blacktriangle-$, the central FDS. (a) $(a,b)=(-2,2)$. (b) $(a,b)=(0,4)$.

## IV. SUMMARY

We have compared a few FDS's which numerically solve the one-dimensional time-independent Schrödinger equation, such as the Numerov, Mickens, and central FDS's, as well as the transition FDS introduced in the present paper for illustration. It is found that the Mickens FDS, although exact when $F'=0$, is usually a second-order FDS when the potential function depends on the coordinate (i.e., $F'\neq 0$). An alternative FDS, the combined Numerov-Mickens FDS (CNMFDS), is presented. It possesses the advantages of both the Numerov and the Mickens FDS's in that it is a fourth-

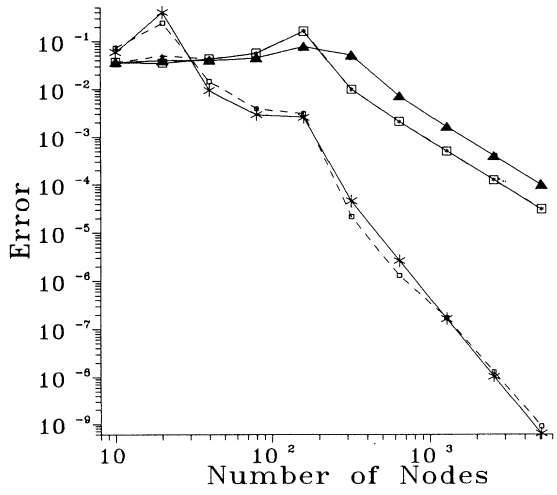


FIG. 2. The dependence of the average error [defined in text, see (19)] on the number of internal nodes $N$ for the normalized $4p$ state of the hydrogen atom: $-*-$, the Numerov FDS; $--\times--$, the transition FDS; $-\square-$, the Mickens FDS; $--\square--$, the CNMFDS; $-\blacktriangle-$, the central FDS. $(a,b)=(0.1,40.1)$.

order (exact) FDS when the potential function depends (does not depend) on the coordinate. Our numerical experiments show that in some cases the CNMFDS works at least equally well as the Numerov FDS, while in the other experiments it works much better than the latter. In this sense, the CNMFDS is better than the Numerov FDS as well as the other FDS's such as the Mickens and the central FDS's. We would like to stress that, although a complete numerical comparison of the CNMFDS and the Numerov FDS in different cases in crucial for getting an evaluation of the CNMFDS, some numerical experiments (only a few of them are shown in the present paper) do show that the CNMFDS has potential uses in practical calculations.

*Note added in proof.* One of our conclusions is that the Mickens FDS is of second order in the space step $h$. After our paper was submitted, the authors were informed that Professor R. E. Mickens has also been aware of this [10]. We thank Professor Mickens for pointing out this fact.

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