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A Simple Accurate Method for the Numerical Solution of the Schrödinger Equation

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Abstract. We present here a simple accurate method for the numerical integration of the radial Schrödinger equation. The formula considered contains free parameter are defined in order to integrate exponential functions. Numerical results also indicate that the new methods are much more accurate than other well known explicit methods.

1 Introduction

In many scientific areas there is a real need for the numerical solution of the Schrödinger equation. Some of these areas are the nuclear physics, the physical chemistry, the theoretical physics and chemistry (see [13,27]).

There is much activity in the area of the solution of the one-dimensional Schrödinger equation. The result of this activity is the development of a great number of methods (see [1-4], [5-30]).

The one dimensional Schrödinger equation has the form:

$$y''(x) = [l(l+1)/x^2 + V(x) - k^2]y(x). \quad (1.1)$$

where k^2 is a real number denoting *the energy*, l is a given integer and V is a given function which denotes *the potential*. The function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \rightarrow 0$ as $x \rightarrow \infty$. The boundary conditions are:

$$y(0) = 0 \quad (1.2)$$

and a second boundary condition, for large values of x , determined by physical considerations.

Boundary value methods based on either collocation or finite differences are not very popular for the solution of (1.1) due to the fact that the problem is posed on an infinite interval. Initial value methods, such as shooting, also need to take into account the fact that $|y'(x)|$ may be very large near $x = 0$. The aim of this paper is to derive more efficient integrators to solve equation (1) in a shooting approach.

One of the most popular methods for the solution of (1.1) is **Numerov's method**. This method is only of order four, but in practice it has been found to have a superior performance to certain higher order four-step methods. The reason for this, as proved in [21], is that the Numerov method has the same phase-lag order as the four-step methods but it has a larger interval of periodicity. Another disadvantage of the four-step methods is that with these methods we need more starting values. These reasons suggest that the investigation of linear multistep methods is not a fruitful way of deriving efficient high order methods.

An alternative approach to deriving higher order methods for (1.1) was given by Cash and Raptis [2]. In [2], a sixth order Runge-Kutta type method with a large interval of periodicity was derived. This method has a phase-lag of order six (while Numerov's method has phase-lag of order four) and a much larger interval of periodicity than the method of Numerov. More recently Simos [28] has derived a sixth order method with phase-lag of order eight and with a large interval of periodicity.

The purpose of this paper is to develop a simple and accurate exponentially fitted numerical method for the solution of the radial Schrödinger equation. The new method is explicit and has a phase-lag of order infinity (phase-fitted). We have applied the new methods to *the resonance problem* (which arises from the one-dimensional Schrödinger equation) with two different types of potential. Note that *the resonance problem* is one of the most difficult to solve of all the problems based on the one-dimensional Schrödinger equation because it has highly oscillatory solutions, especially for large resonances (see section 4). We note, also, that we present an explicit method which is very simple in programming.

2 Exponential multistep methods

In this section we explain the derivation of the exponentially fitted methods.

For the numerical solution of the initial value problem

$$y^{(r)} = f(x, y), \quad y^{(j)}(A) = 0, \quad j = 0, 1, \dots, r-1 \quad (2.1)$$

the multistep methods of the form

$$\sum_{i=0}^k a_i y_{n+i} = h^r \sum_{i=0}^k b_i f(x_{n+i}, y_{n+i}) \quad (2.2)$$

over the equally spaced intervals $\{x_i\}_{i=0}^k$ in $[A, B]$ can be used.

The method (2.2) is associated with the operator

$$L(x) = \sum_{i=0}^k [a_i z(x + ih) - h^r b_i z^{(r)}(x + ih)] \quad (2.3)$$

where z is a continuously differentiable function.

Definition 1 The multistep method (2.2) called algebraic (or exponential) of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \dots, x^{p+r-1}$ (or $\exp(v_0 x), \exp(v_1 x), \dots, \exp(v_{p+r-1} x)$ where $v_i, i = 0, 1, \dots, p+r-1$ are real or complex numbers).

Remark 1 (see [34]) If $v_i = v$ for $i = 0, 1, \dots, n$, $n \leq p+r-1$ then the operator L vanishes for any linear combination of $\exp(vx), x\exp(vx), x^2\exp(vx), \dots, x^n\exp(vx), \exp(v_{n+1}x), \dots, \exp(v_{p+r-1}x)$.

Remark 2 (see [34]) Every exponential multistep method corresponds in a unique way, to an algebraic multistep method (by setting $v_i = 0$ for all i).

Lemma 1 (For proof see [34] and [35]) Consider an operator L of the form (2.3). With $v \in \mathbb{C}$, $h \in \mathbb{R}$, $n \geq r$ if $v = 0$, and $n \geq 1$ otherwise, then we have

$$L[x^m \exp(vx)] = 0, \quad m = 0, 1, \dots, n-1, \quad L[x^n \exp(vx)] \neq 0 \quad (2.4)$$

if and only if the function φ has a zero of exact multiplicity s at $\exp(vh)$, where $s = n$ if $v \neq 0$, and $s = n - r$ if $v = 0$, $\varphi(w) = \rho(w)/\log^r w - \sigma(w)$, $\rho(w) = \sum_{i=0}^k a_i w^i$ and $\sigma(w) = \sum_{i=0}^k b_i w^i$.

Proposition 1 (For proof see [18] and [21]) Consider an operator L with

$$L[\exp(\pm v_i x)] = 0, \quad j = 0, 1, \dots, k \leq \frac{p+r-1}{2} \quad (2.5)$$

then for given a_i and p with $a_i = (-1)^r a_{k-i}$ there is a unique set of b_i such that $b_i = b_{k-i}$.

In the present paper we investigate the case $r = 2$.

3 The new method

Consider the method:

$$\bar{y}_{n+1} = 2y_n - y_{n-1} + h^2 y_n'' \quad (3.1)$$

$$\bar{y}_n = y_n - ah^2(\bar{y}_{n+1}'' - 2y_n'' + y_{n-1}'') \quad (3.2)$$

$$y_{n+1} + a_1 y_n + y_{n-1} = h^2[b_0(\bar{y}_{n+1}'' + y_{n-1}'') + b_1 \bar{y}_n''] \quad (3.3)$$

where, for example, $y_{n+1}'' = f(x_{n+1})y_{n+1}$ with $x_{n+1} = x_n + h$, $f(x_{n+1}) = l(l+1)/x_{n+1}^2 + V(x_{n+1}) - k^2$.

We have chosen to consider this family of methods because it has four free parameters. This is sufficient to allow the construction of methods which integrate more exponential functions than the analogue Runge-Kutta-type method, with algebraic order six, proposed by Raptis and Cash [20].

We require that the family of methods (3.1)-(3.3) should integrate exactly any linear combination of the functions:

$$\{\exp(\pm vx), x \exp(\pm vx), x^2 \exp(\pm vx), x^3 \exp(\pm vx)\}. \quad (3.4)$$

To construct a method of the form (3.1)-(3.3) which integrates exactly the functions (3.4), we require that the method (3.1)-(3.3) integrates exactly (see section 2):

$$\{\exp(\pm v_0 x), \exp(\pm v_1 x), \exp(\pm v_2 x), \exp(\pm v_3 x)\} \quad (3.5)$$

and then put:

$$v_0 = v_1 = v_2 = v_3 = v. \quad (3.6)$$

Demanding that (3.1)-(3.3) integrates (3.5) exactly, we obtain the following system of equations for b_0, b_1, a and a_1

$$-a_1 + b_0 w_j^2 (w_j^2 + 2) + b_1 w_j^2 - a b_1 w_j^6 = 2 \cosh(w_j) \quad (3.7)$$

where $w_j = v_j h, j = 0, 1, 2, 3$.

Solving for $b_i, i = 0, 1$, for a and a_1 we obtain:

$$\begin{aligned} a_1 &= \frac{-3(3w^2 + 16) \cosh(w) + w(w^2 + 33) \sinh(w)}{24}, \\ b_0 &= \frac{5w \cosh(w) - (w^2 + 5) \sinh(w)}{8w^3}, \\ b_1 &= \frac{-w(7w^2 + 10) \cosh(w) + (w^4 + 17w^2 + 10) \sinh(w)}{8w^3}, \\ a &= \frac{3w \cosh(w) - (w^2 + 3) \sinh(w)}{3w^2[-w(7w^2 + 10) \cosh(w) + (w^4 + 17w^2 + 10) \sinh(w)]}. \end{aligned} \quad (3.8)$$

The above formulae are subject to heavy cancellations for small values of $w = vh$. In this case it is much more convenient to use the following series expansion for the coefficients b_i , $i = 0(1)3$ of the method:

$$\begin{aligned}
 a_1 &= -2 + \frac{w^8}{20160} + \frac{w^{10}}{453600} + \frac{w^{12}}{23950080}, \\
 b_0 &= \frac{1}{12} - \frac{w^4}{3360} - \frac{w^6}{90720} - \\
 &\quad - \frac{w^8}{5322240} - \frac{w^{10}}{518918400} - \frac{w^{12}}{74724249600}, \\
 b_1 &= \frac{5}{6} + \frac{w^4}{1680} + \frac{w^6}{4536} + - \\
 &\quad + \frac{23w^8}{2661120} + \frac{w^{10}}{6486480} + \frac{61w^{12}}{37362124800}, \\
 a &= -\frac{1}{300} - \frac{w^2}{4200} - \frac{w^4}{236250} + \frac{277w^6}{291060000} + \\
 &\quad + \frac{18847w^8}{189189000000} + \frac{31463w^{10}}{8939180250000} - \frac{13888499w^{12}}{60786425700000000}.
 \end{aligned} \tag{3.9}$$

The local truncation error of the above scheme is given by

$$L.T.E.(h) = -\frac{(y_n^{(6)} + y_n^{(4)})h^6}{240} + O(h^8). \tag{3.10}$$

If $v = i\phi$, then the family of methods (4) is exact for any linear combination of the functions:

$$\{\sin(\phi x), \cos(\phi x), x\sin(\phi x), x\cos(\phi x), x^2\sin(\phi x), x^2\cos(\phi x), x^3\sin(\phi x), x^3\cos(\phi x)\} \tag{3.11}$$

4 Stability and phase-lag analysis

If we apply the method (3.1)-(3.3) to the scalar test equation $y'' = -\phi^2 y$, we obtain the difference equation

$$y_{n+1} - 2Q(H^2)y_n + y_{n-1} = 0 \tag{4.1}$$

where

$$Q(H^2) = -\frac{a_1}{2} - \frac{H^2(2b_0 + b_1)}{2} + \frac{b_0 H^4}{2} + \frac{ab_1 H^6}{2} \tag{4.2}$$

and $H = \phi h$.

The stability polynomial of the difference equation (4.1) is given by

$$C(t; H^2) = t^2 - 2Q(H^2)t + 1. \quad (4.3)$$

If we substitute the coefficients b_0 , b_1 , a_1 and a given by (3.8) (with $w = vh$ and $v = i\phi$) into (4.3) we obtain the following stability polynomial:

$$C(t; H^2) = t^2 - 2\cos(H)t + 1. \quad (4.4)$$

We have the following definitions:

Definition 2 [13] *A symmetric two-step method with stability polynomial given by (4.3) is said to have a non-zero interval of periodicity $(0, H_0^2)$ if, for all $H^2 \in (0, H_0^2)$, the roots of the stability polynomial satisfy*

$$t_1 = e^{i\theta(H)}, \quad t_2 = e^{-i\theta(H)} \quad (4.5)$$

where θ is a real function of $H = \phi h$.

Definition 3 [29-30] *A method is said to be phase fitted (or complete in phase) if it has a phase-lag of order ∞ .*

Remark 3 *A method is said to be phase fitted if $Q(H^2) = \cos(H)$.*

Remark 4 *A symmetric two-step method with stability polynomial given by (4.3) has an interval of periodicity $(0, H_0^2)$ if, for all $H^2 \in (0, H_0^2)$, $1 \pm Q(H^2) > 0$.*

For the method derived in section 2 we find that, for the values of coefficients given by (3.8), $1 \pm Q(H^2) = 1 \pm \cos(H) > 0$ for all $H^2 \in (0, \infty) - \{H^2 : H = q\pi, q = 1, 2, \dots\}$ and $Q(H^2) = \cos(H)$ i.e. the method is phase fitted.

5 Numerical illustrations

In this section we present some numerical results to illustrate the performance of our new methods. We consider the numerical integration of the Schrödinger equation:

$$y''(x) = (W(x) - E)y(x) \quad (5.1)$$

in the well-known case where the potential $V(x)$ is the Woods-Saxon potential

$$V(x) = V_W(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{[a(1+z)^2]} \quad (5.2)$$

with $z = \exp[(x - X_0)/a]$, $u_0 = -50$, $a = 0.6$ and $X_0 = 7.0$. In order to solve this problem numerically we need to approximate the true (infinite) interval of integration $[0, \infty)$ by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $0 \leq x \leq 15$. We consider (5.1) in a rather large domain of energies, i.e., $E \in [1, 1000]$. The problem we consider is the so-called *resonance problem*.

5.1 The Resonance Problem Woods-Saxon Potential

In the case of positive energies $E = k^2$ the potential dies away faster than the term $l(l+1)/x^2$ and equation (1.1) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right)y(x) = 0, \quad (5.3)$$

for x greater than some value X .

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx), n_l(kx)$ are the **spherical Bessel and Neumann functions** respectively. Thus the solution of equation (1) has (when $x \rightarrow 0$) the asymptotic form

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AC[\sin(kx - \pi l/2) + \tan \delta_l \cos(kx - \pi l/2)] \end{aligned} \quad (5.4)$$

where δ_l is the **phase shift** that may be calculated from the formula

$$\tan \delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \quad (5.5)$$

for x_1 and x_2 distinct points on the asymptotic region (for which we have that x_1 is the right hand end point of the interval of integration and $x_2 = x_1 - h$, h is the stepsize) with $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$.

Since the problem is treated as an initial-value problem, one needs y_0 and y_1 before starting a two-step method. From the initial condition, $y_0 = 0$. It can be shown that, for values of x close to the origin, the solution behaves like $y(x) \sim cx^{l+1}$ as $x \rightarrow 0$, where c is an independent constant. In view of this we take $y_1 = h^{l+1}$ [2,21]. With these starting values we evaluate at x_1 of the asymptotic region the phase shift δ_l and the normalization factor C from the above relations.

For positive energies one has the so-called resonance problem. This problem consists either of finding the **phase shift** $\delta(E) = \delta_l$ or finding those E , for $E \in [1, 1000]$, at which δ equals $\pi/2$. We actually solve the latter problem, known as "*the resonance problem*" when *the positive eigenenergies lie under the potential barrier*.

The boundary conditions for this problem are:

$$\begin{aligned} y(0) &= 0, \\ y(x) &\sim \cos[\sqrt{E}x] \text{ for large } x. \end{aligned}$$

The domain of numerical integration is $[0, 15]$.

In our numerical illustration we find the positive *eigenenergies* or *resonances*. For comparison purposes we use the following fourth order explicit methods:

Method MI: Numerov's method made explicit of Chawla [31].

Method MII: Explicit Numerov-type method with minimal phase-lag of Chawla and Rao [32].

Method MIII: Explicit Numerov-type method with minimal phase-lag of Simos [33].

Method MIV: New exponentially-fitted method.

We note here tha the Numerov's method made explicit of Chawla [31] gives must better results when compares with the Numerov's method.

The numerical results obtained for the four methods, with stepsizes equal to $h = \frac{1}{2^n}$, were compared with the analytic solution of the Woods-Saxon potential resonance problem, rounded to six decimal places. Figures 1-4 show the errors $Err = -\log|E_{calculated} - E_{analytical}|$ of the eigenenergies $E_0 = 53.588872$ - $E_3 = 989.701916$ for several values of n .

The performance of the present method is dependent on the choice of the fitting parameter v . For the purpose of obtaining our numerical results it is appropriate to choose v in the way suggested by Ixaru and Rizea [7]. That is, we choose:

$$v = \begin{cases} (-50 - E)^{1/2} & \text{for } x \in [0, 6.5] \\ (-E)^{1/2} & \text{for } x \in (6.5, 15] \end{cases} \quad (5.6)$$

For a discussion of the reasons for choosing the values 50 and 6.5 and the extent to which the results obtained depend on these values see [7, pp. 25].

5.2 Modified Woods-Saxon Potential

In Figures 5-8 some results for $Err = -\log|E_{calculated} - E_{analytical}|$ of the eigenenergies $E_0 = 61.482588$ - $E_3 = 1002.768393$, for several values of n , obtained with another potential in (5.1) are shown. This potential is

$$V(x) = V_W(x) + \frac{D}{x} \quad (5.7)$$

where V_W is the Woods-Saxon potential (5.2). For the purpose of our numerical experiments we use the same parameters as in [7], i.e. $D = 20$, $l = 2$.

Since $V(x)$ is singular at the origin, we use the special strategy of [7]. We start the integration from a point $\epsilon > 0$ and the initial values $y(\epsilon)$ and $y(\epsilon + h)$ for the integration scheme are obtained using a perturbative method (see [6]). As in [7] we use the value $\epsilon = \frac{1}{4}$ for our numerical experiments.

For the purpose of obtaining our numerical results it is appropriate to choose v in the way suggested by Ixaru and Rizea [7]. That is, we choose:

$$v = \begin{cases} \frac{[V(a_1)+V(\epsilon)]}{2} & \text{for } x \in [\epsilon, a_1] \\ \frac{V(a_1)}{2} & \text{for } x \in (a_1, a_2] \\ V(a_3) & \text{for } x \in (a_2, a_3] \\ V(15) & \text{for } x \in (a_3, 15]. \end{cases}$$

where a_i , $i = 1, \dots, 3$ are fully defined in [7].

All computations were carried out on an IBM PC-AT compatible 80486 using double precision arithmetic (16 significant digits precision).

6 Conclusion

We investigate here the explicit exponentially fitted methods. We note that the explicit numerical methods are the most simple methods for programming purposes and for this reason very simple for application in any problem.

The method proposed in this paper is the first explicit exponentially-fitted method. This method is much more accurate than the Numerov-type methods of Chawla [31], Chawla and Rao [32] and Simos [33].

The crucial concern when solving the Schrödinger equation is that the numerical method should integrate exactly the functions (3.4) with m and p as large as possible, as shown by [7] and [21].

As predicted by the analysis, method MIV is the most accurate of all the methods for the problems tested.

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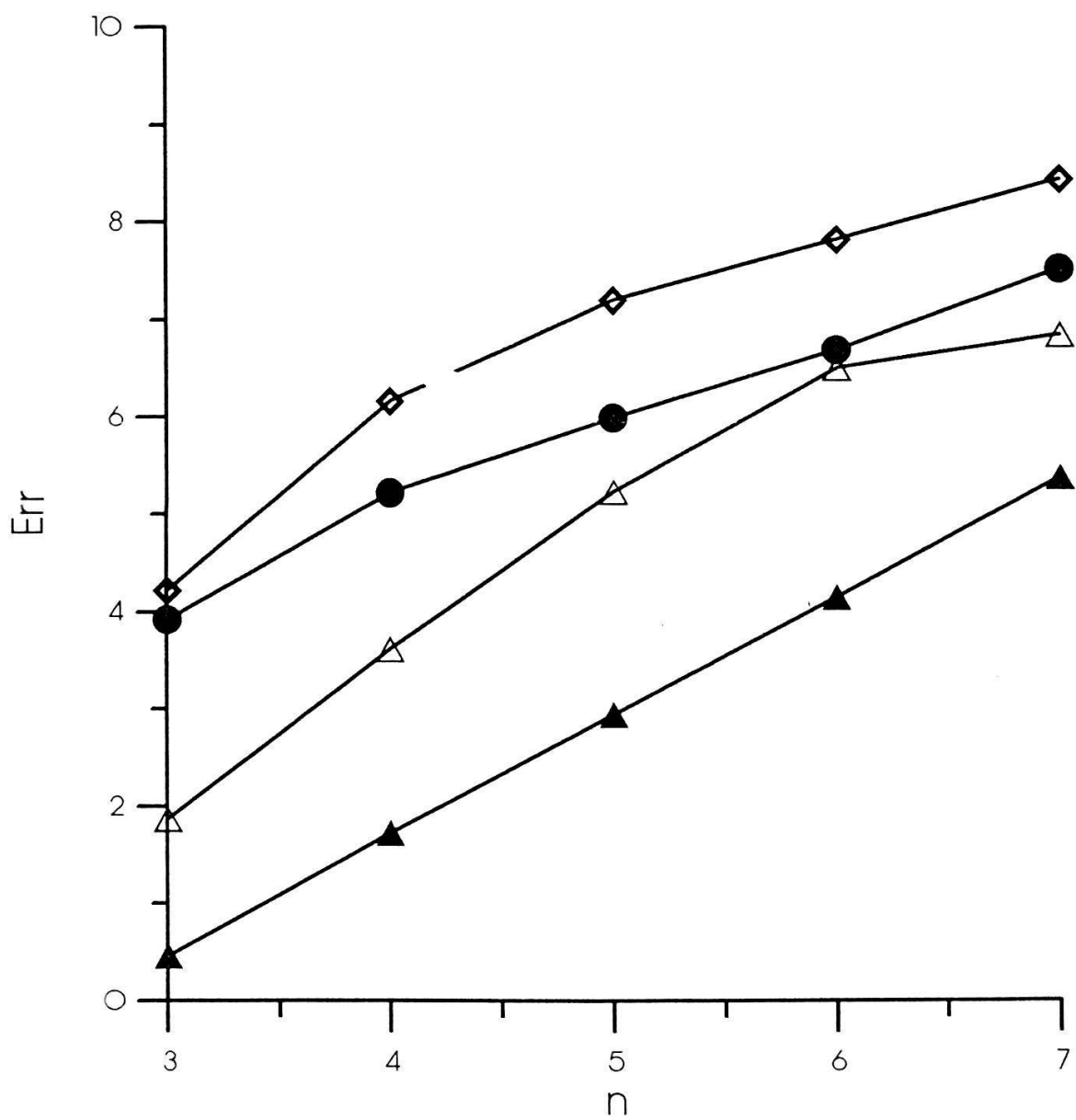


Figure 1: Values of Err for several values of n for the resonance $E=53.588872$

- ▲— Method MI
- △— Method MII
- Method MIII
- ◇— Method MIV

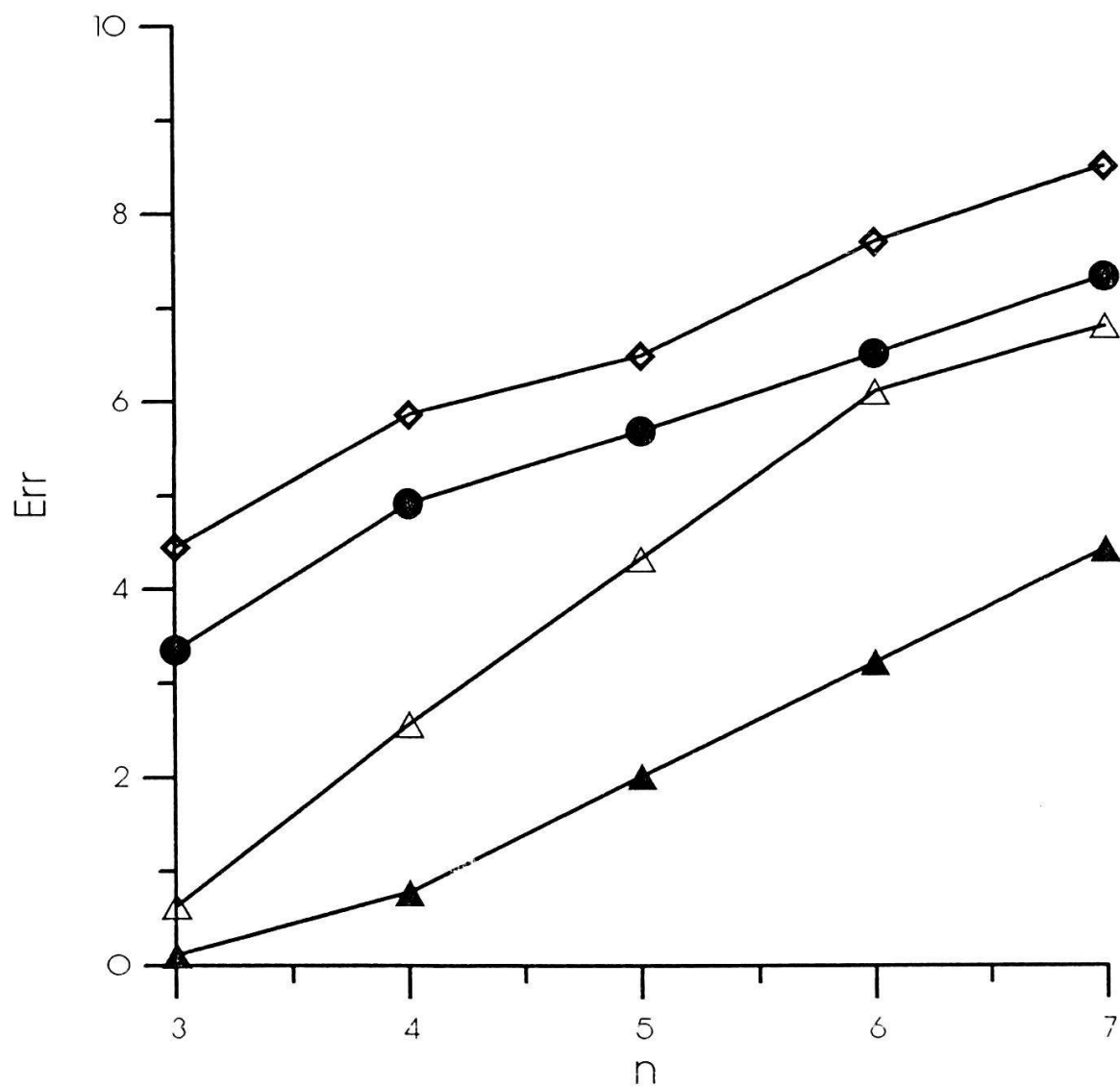


Figure 2: Values of Err for several values of n for the resonance $E=163.215341$

- ▲— Method MI
- △— Method MII
- Method MIII
- ◇— Method MIV

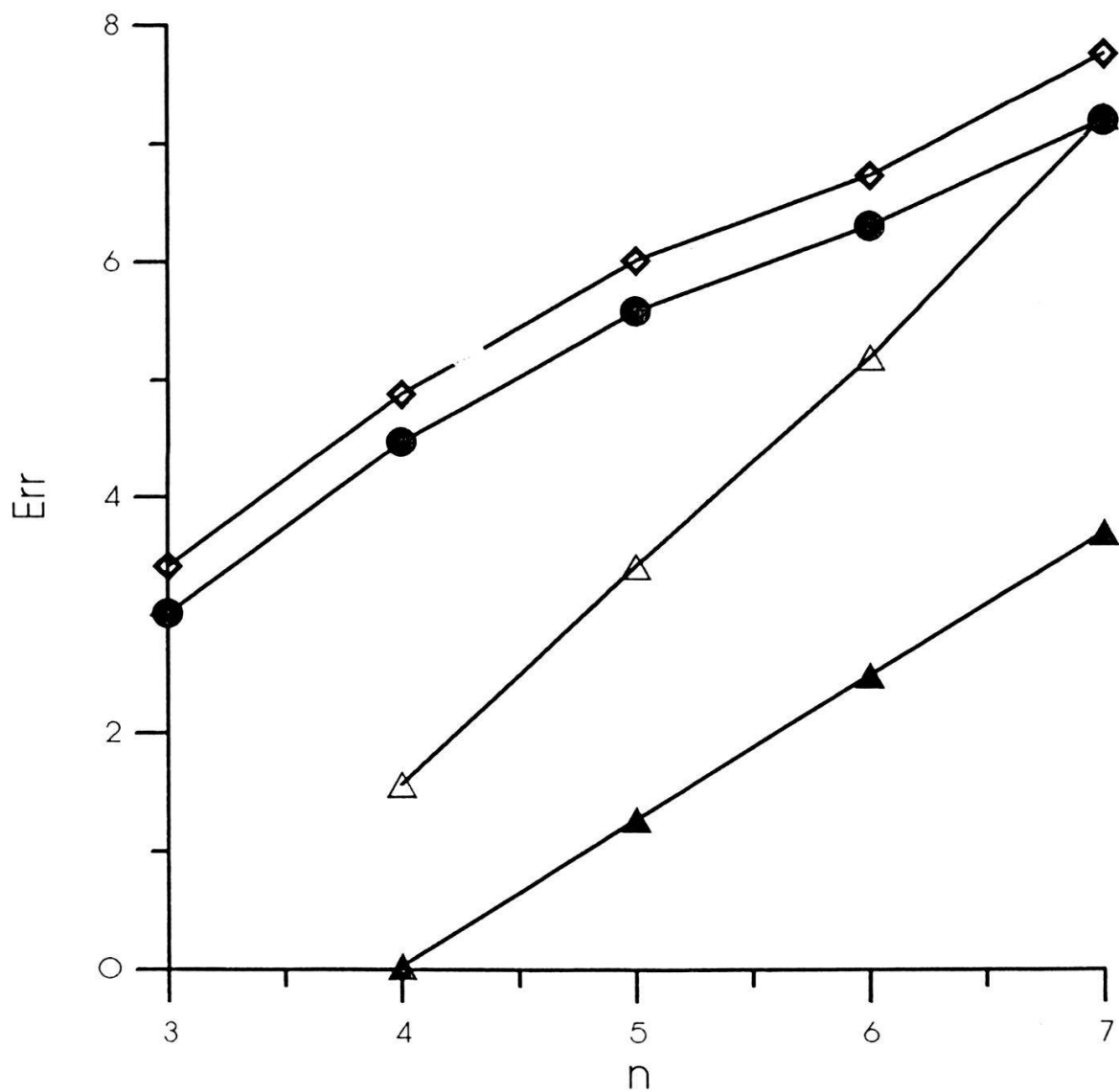


Figure 3: Values of Err for several values of n for the resonance $E=341.495874$. The non-existence of a value for a method indicates that Err is negative.

- ▲ Method MI
- △ Method MII
- Method MIII
- ◆ Method MIV

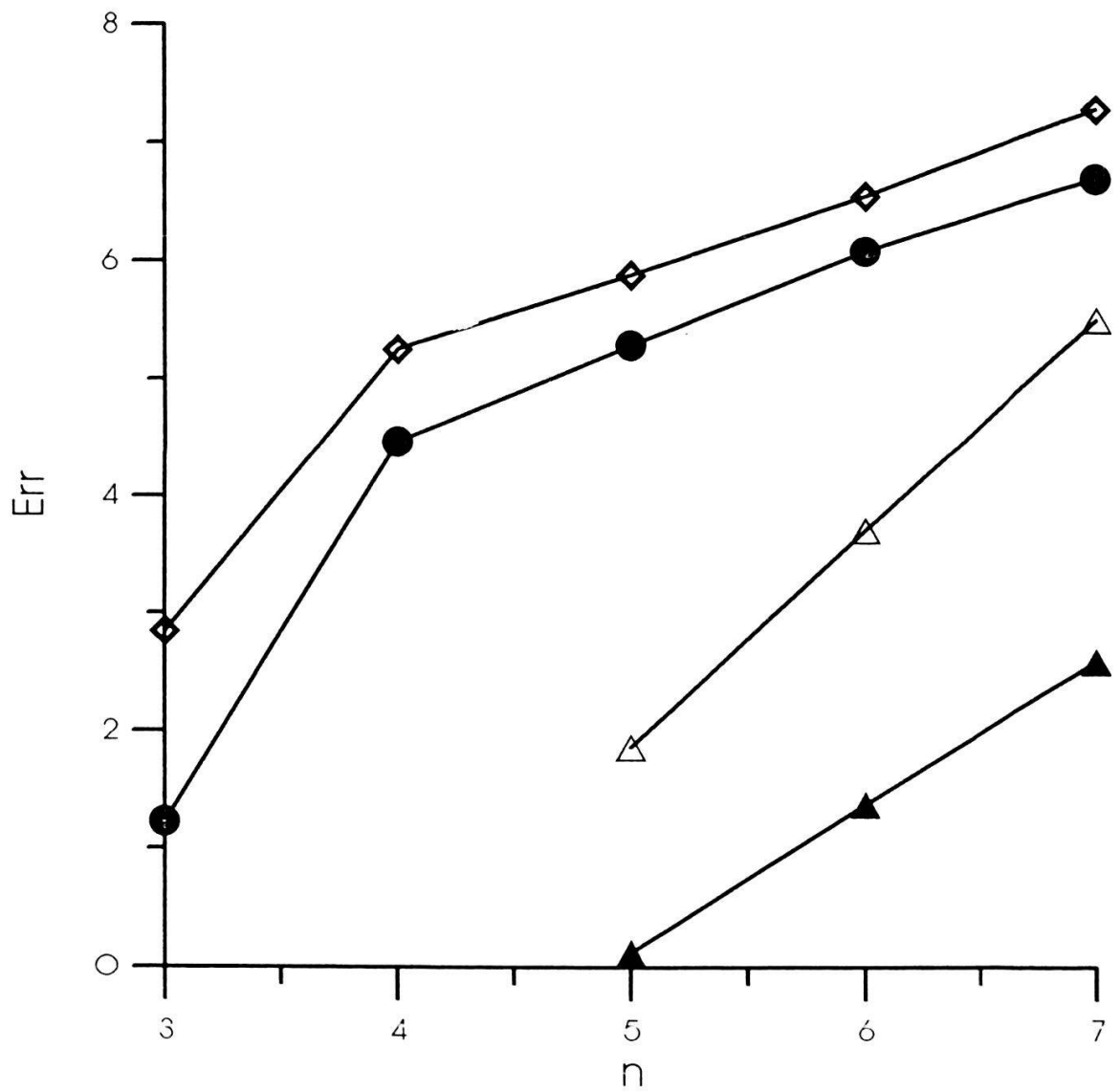


Figure 4: Values of Err for several values of n for the resonance $E=989.701916$
The non-existence of a value for a method indicates that Err is negative.

- ▲— Method MI
- △— Method MII
- Method MIII
- ◇— Method MIV

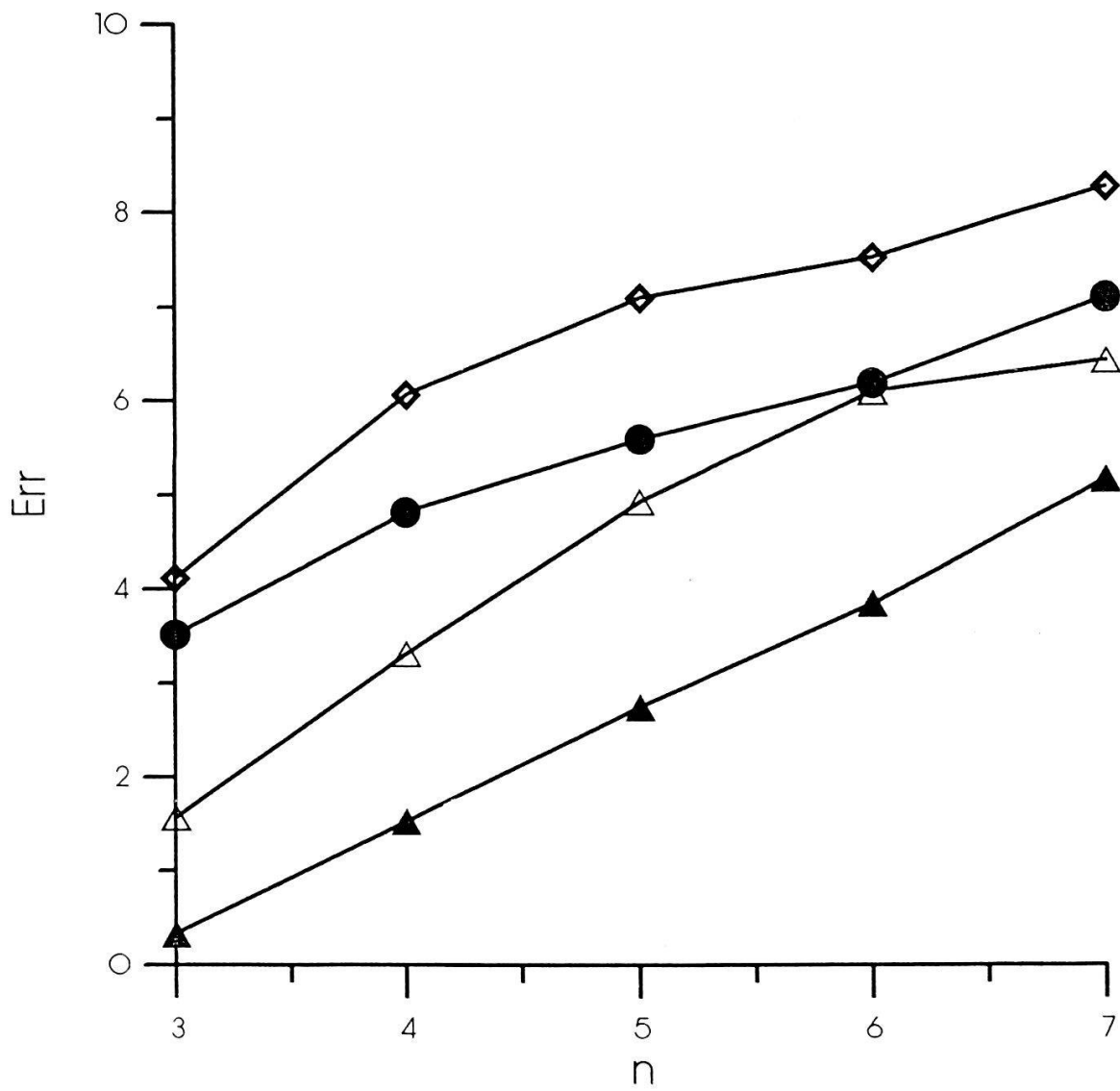


Figure 5: Values of Err for several values of n for the resonance $E=61.482588$

- ▲— Method MI
- △— Method MII
- Method MIII
- ◇— Method MIV

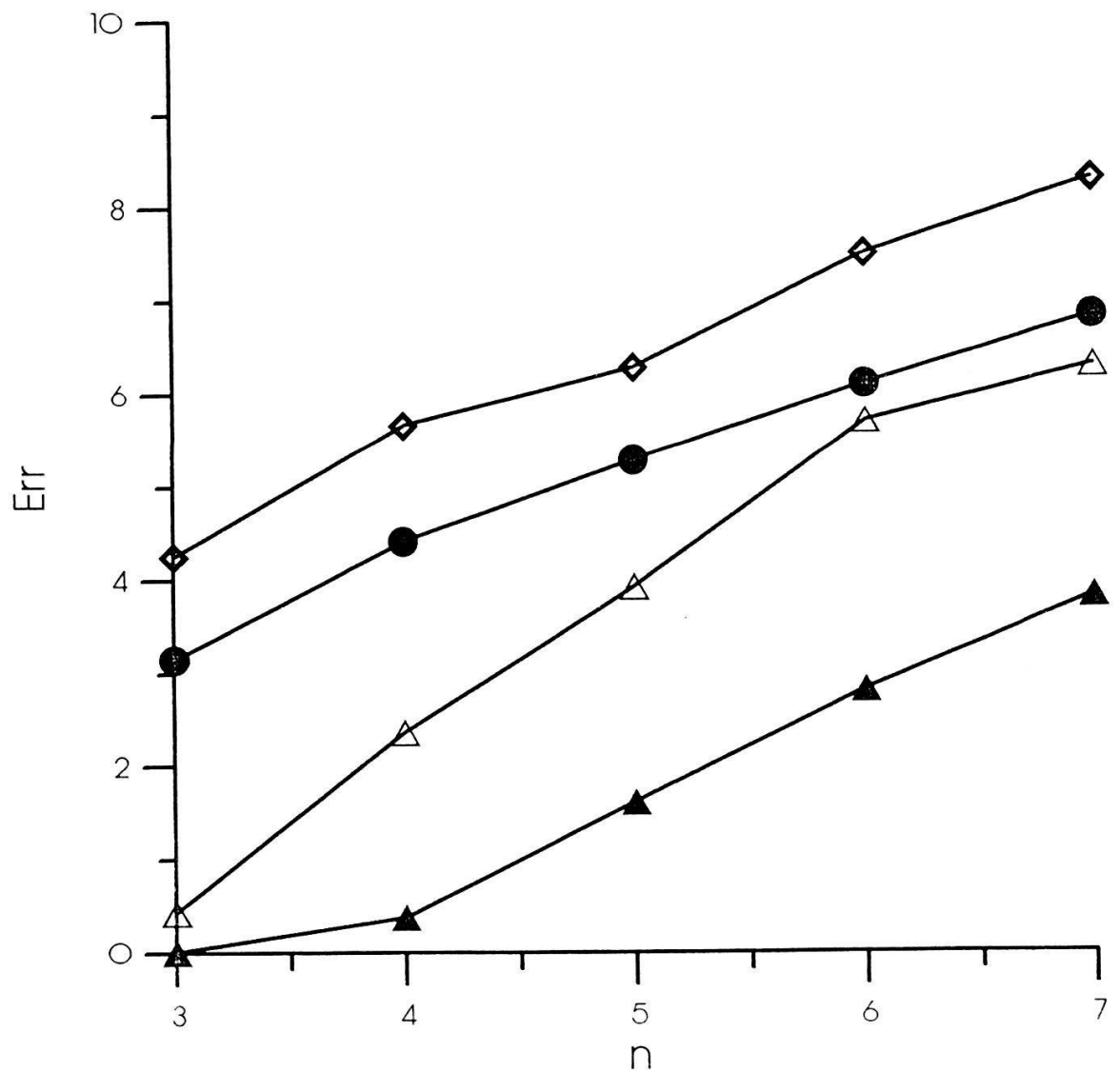


Figure 6: Values of Err for several values of n for the resonance $E=173.075711$

- ▲ Method MI
- △ Method MII
- Method MIII
- ◆ Method MIV

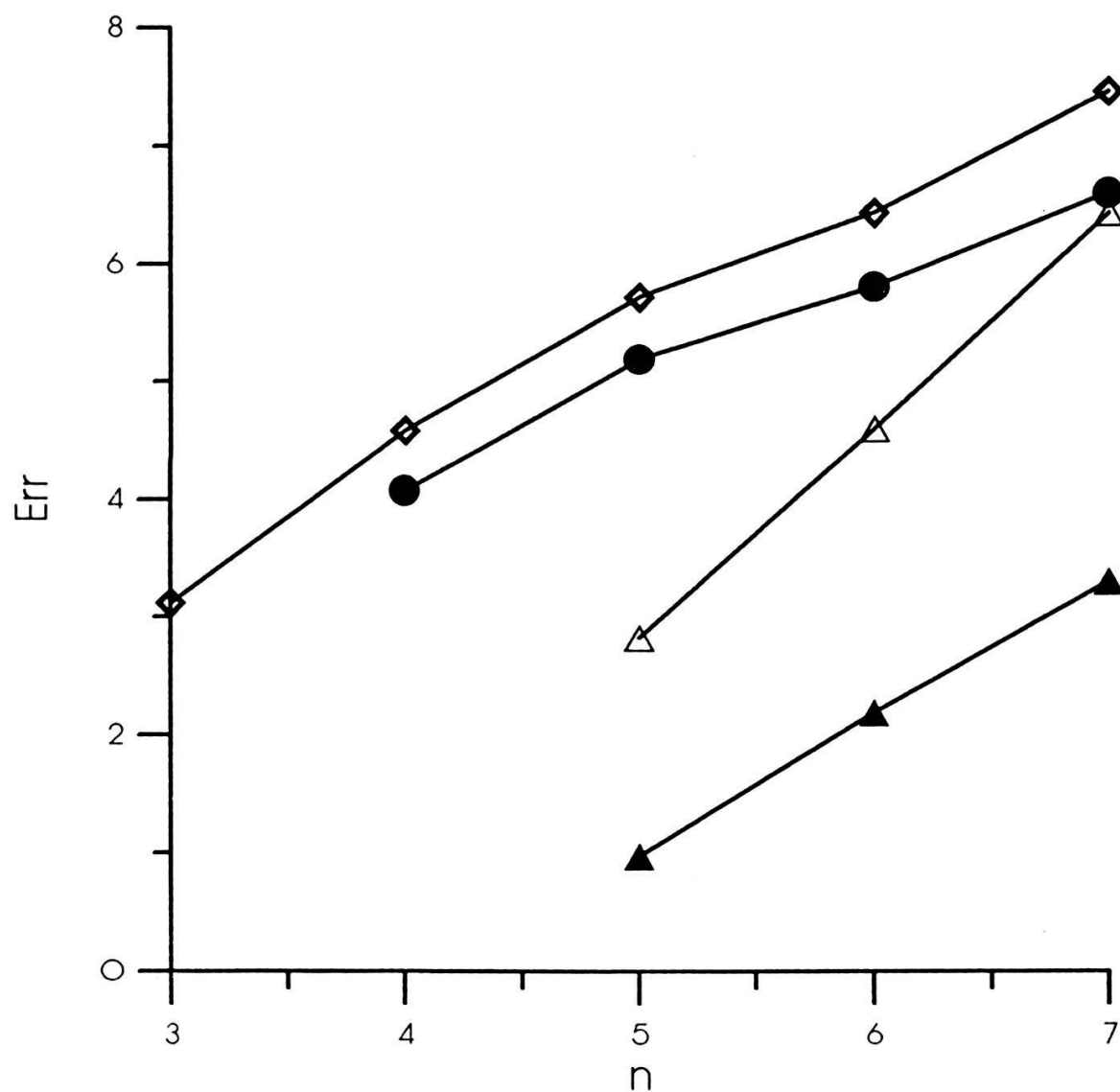


Figure 7: Values of Err for several values of n for the resonance $E=352.682070$
The non-existence of a value for a method indicates that Err is negative.

- ▲— Method MI
- △— Method MII
- Method MIII
- ◇— Method MIV

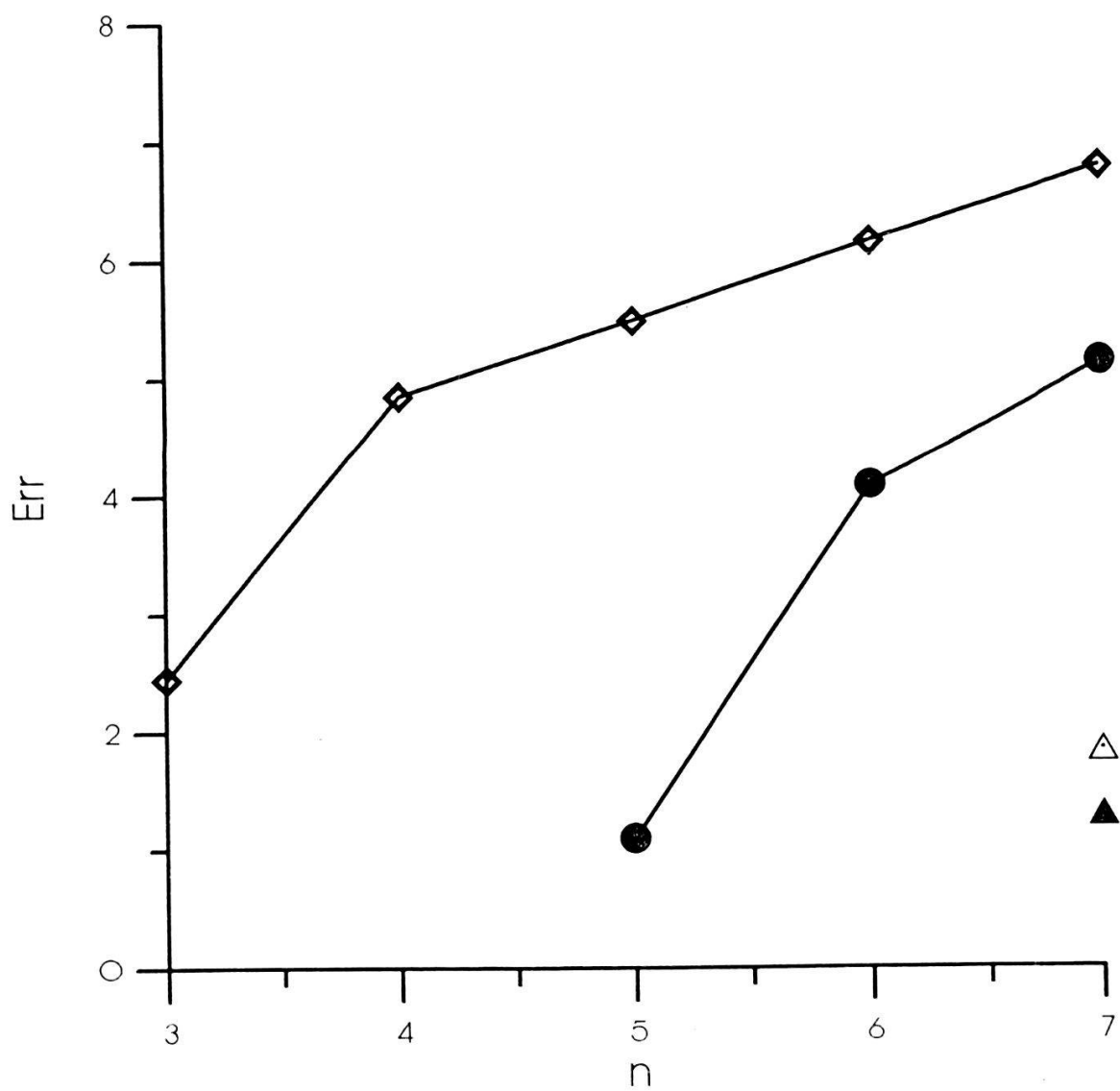


Figure 8: Values of Err for several values of n
for the resonance $E=1002.768393$
The non-existence of a value for a
method indicates that Err is negative.

- ▲— Method MI
- △— Method MII
- Method MIII
- ◇— Method MIV