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Special Issue to celebrate 125th Birth Anniversary of Prof. K. C. Kar

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[Founder President: Late Prof. K. C. Kar, D. Sc.]

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PREFACE

The Calcutta Institute of Theoretical Physics (CITP) is celebrating the 125th birth anniversary of its founder Prof. Kulesh Chandra Kar this year. This institute was set up by Prof. Kar in his residence in 1953 to hold meetings and discussions on a regular basis on new and emerging topics in physics. These meetings enabled young and aspiring physicists to have a forum beyond the daily grind of the regular learning and teaching process which are obviously essential for survival. While the disciplined learning process is absolutely necessary, Prof. Kar recognized, a century ago, that it is equally vital, equally demanding and in many ways immensely fulfilling to have an education beyond the daily grind. Hence the emergence of CITP. To celebrate the 125th birth anniversary of its founder, the institute organized a two-day event covering essentially all aspects of theoretical physics. The vital role of symmetry in the study of almost all physics related issues, the fundamental constituents of matter as envisaged by high energy physicists, the intriguing coming together of quantum physics and the classical world of gravity, the emergence of quantum computation, the contribution of S N Bose to a prediction that had to wait seventy years for experimental confirmation, the ever-fascinating world of astrophysics and the incredible mixing of biology with physics and mathematics formed the framework of a two day celebration. We do hope that the publication of the write-ups of the discussion will be enjoyed by those who were not actually present at the event.

Prof. Jayanta Kumar Bhattacharjee,

Director, CITP, Kolkata

SECRETARY'S REPORT ON THE CONFERENCE

I am very proud to present the outcome and results of 2- Day National Conference on "Recent Trends in Physics and Mathematics" held during October 22-23, 2024 at Presidency University,Kolkata to celebrate 125th Birth Anniversary of Professor Kulesh Chandra Kar, an outstanding theoretical physicist and an eminent and dedicated educationist, who spent most of his formal working period as a teacher in Presidency College (now known as Presidency University), Kolkata, with some short stints at Scottish Church College, Kolkata and Serampore College and Rajshahi College. In the inaugural session following dignitaries were present:

Prof. N N Chakraborty, Vice-Chancellor, Presidency University, Prof. Ashoke Nath Basu, Former Vice-Chancellor, JU, Prof. J K Bhattacharjee, Director, CITP, Dr. P R Ghosh, Vice-President, CITP, Prof. Arunava Chakraborty, HOD, Physics, Presidency University. This event has attracted 76 student and teacher participants from different Colleges and Universities of India.

The main aim of this conference was to bring together leading academicians, researchers, teachers and students to exchange and share their experiences. It was also meant to provide the participants with an in-depth understanding of some modern topics of Physics and Mathematics.Distinguished scientists of different research institutions of India were invited to focus the following modern topics.

1. Quantum Gravity - Prof.Soumitra Sengupta, IACS,Kolkta
2. Quantum Statistics - Prof.J K Bhattacharjee, IIT, Kanpur
3. Foundation of Quantum Mechanics - Prof. Guruprasad Kar, ISI, Kolkata
4. High Energy Physics (LHC) - Prof. Satyaki Bhattacharya, SINP, Kolkata
5. Solar Magneto-Hydrodynamics - Prof. Arnab Rai Choudhuri, IISc, Bangalore
6. Biological Physics - Prof. Indrani Bose, Bose Institute, Kolkata
7. Introduction to Divergence Series and its Applications to Physical Problems- Prof. Dhiranjan Roy, Ex-Professor, JU, Kolkata

Keynote lecture was presented by Prof. Parthasarathi Mitra, Ex-Professor, SINP, Kolkta, an eminent personality in Particle Physics. Each technical session had a chair, who was expert in the domain. Each speaker was given 50 minutes for the presentation, which

was followed by question and answer session for 5 minutes. The resource persons were felicitated with mementos.

Two-day Conference ended with a valedictory session where renowned teachers, Mr. Partha Pratim Roy of South Point High School, Kolkata and Dr. Abhijit Kar Gupta of Panshkura Banamali College were invited to discuss " Science Education: past and present". Prof. Arunava Chakraborty, HOD, Physics of Presidency University chaired this session. Active participation of the audience, particularly students in the interactive session was remarkable.

It was announced that lectures presented in the conference and seminar organised by CITP this year would be published in a special Volume of Indian Journal of Theoretical Physics (Free access). This volume will be uploaded to our website: www.citphy.org. In the first issue of this we have planned to publish two articles:

1. Introduction to Divergent Series: Application to Some Physical Problems by Prof. Dhiranjan Roy, Ex-Professor, JU.
2. Modeling of Blood Flow Through a Deformable Artery by Prof. G C Shit, JU

Prof. D. Roy started his research work on Lattice Dynamics and Defects in Crystals and subsequently switched to Computational Physics and Interdisciplinary Applications.Prof. Roy has published about 75 papers in different Journals of International repute and a number of articles in teaching Journals.After serving New alipore College as a lecturer in Physics for about 15 years he joined Jadavpur University and retired in 2007.His long experience in teaching Mathematical Physics has served the interest of UG, PG students and researchers.He has proved himself as a brilliant teacher in the true sense of the term. Hope his review article of 69 pages will be very helpful to advanced learners and teachers.

Prof. Gopal Chandra Shit is presenty a Professor in Applied Mathematics,J U.His research interest includes Biofluid Mechanics,Microfluidics and Bioheat Transfer in living tissues.He has already published more than 110 research papers in reputed international Journals. He is also recipient of several prestigious Awards and Honours.

Calcutta Institute of Theoretical Physics is particularly grateful to the department of Physics, Presidency University for providing the premises, technical equipments and ever-helpful staff. And last, but certainly not the least, CITP wishes to thank wholeheartedly all the contributors and participants of this event for making it an informative as well as enjoyable two days!

Susil Kumar Sarkar,
Secretary, CITP, Kolkata

C O N T E N T S

Introduction to Divergent Series : Application to Some Physical Problems

Dhiranjan Roy

Retired Professor, Department of Physics, Jadavpur University, Kolkata

(This papaer was presented in the 2-day National Seminar organized by CITP during October 22-23 ,2024)

Abstract

The mathematical analysis of many scientific problems involves infinite series at some stage which may be convergent or divergent. Evaluating the sum of an infinite series is the same as finding the limit of the associated sequence. For a divergent series we introduce the concept of *anti-limit* (from where the sum diverges). Nonlinear sequence transforms are efficient in evaluating the sum of slowly convergent series as well as in finding the *sum* of a divergent series. In the present article, I shall briefly present the different nonlinear transforms like the Padé approximants and Levin-like transforms and consider some applications in the different fields of physics.

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I Introduction

The mathematical analysis of many scientific problems involves infinite series at some stage. An infinite series S and its n-th partial sum S_n are defined as

$$S = \sum_{i=0}^{\infty} t_i, \quad S_n = \sum_{i=0}^{n-1} t_i. \tag{1}$$

where the t_i's are complex numbers in general. It is evident that the sum of an infinite series $S = \lim_{n\to\infty} S_n$. The sum S of the infinite series is defined as the limit of this infinite sequence, where this limit exists, *i.e.,* series and sequence, can sometimes be used interchangeably. If the limit exists for an infinite series or sequence, then it is said to be convergent and when this limit is not finite, it is said to be divergent.

An example of a slowly convergent series is the well known power series for $\ln(1+z)$, which converges only for $|z| < 1$. For $z = 1$ we have

$$\ln 2 = \sum_{i=0}^{\infty} \frac{(-1)^i}{i+1} = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + ... \tag{2}$$

so that it is barely convergent, in fact conditionally so. One comes across this series very often, for instance in evaluating the Coulomb energy of an infinite one dimensional ionic lattice. To evaluate $\ln 2$ to an accuracy of n decimal digits from equation - 2, one would need at least 10^n terms. Hence to obtain $\ln 2$ by the direct method correctly up to 16 decimal places one has to sum at least 10^{16} terms. A computer which sums 10^6 terms a second will need at least 300 years to compute it!

Another mathematical example is provided by the series representation of the Riemann zeta function

$$\zeta(s) = \sum_{n=0}^{\infty} (n+1)^{-s}. \tag{3}$$

The infinite series diverges for negative negative s. Though this infinite series for $\zeta(s)$ converges when $s > 1$, yet the rate of convergence is not very good unless the value of s is moderately large. If s is only slightly greater than unity, the rate of convergence is extremely slow. For example, to evaluate $\zeta(1.001)$ to an accuracy of one in hundred one would require about 10^{20} terms!

Consider the simple differential equation

$$(1+x)\frac{dy}{dx} = -2y, \quad y(0) = 1. \qquad \text{Solution} \Rightarrow y(x) = \frac{1}{(1+x)^2};$$

Normally we attempt series solution for a differential equation when it cannot be solved analytically. However, there is no harm to attempt a series solution for the above problem . Assuming $y(x) = \sum_{n=0}^{\infty} a_n x^n$, we get the recurrence relation $a_{n+1} = -\frac{n+2}{n+1} a_n$ with $a_0 = 1$ and hence

$$y(x) = 1 - 2x + 3x^2 - 4x^4 + \cdots .$$

For $x = 1$, we get the series $y(1) = 1 - 2 + 3 - 4 + \cdots$ which is divergent. Can I conclude that the sum of this divergent series is $y(1) = \frac{1}{2^2} = \frac{1}{4}$?

Different sequence transforms can be used to obtain different approximants of the same function. There is also the possibility of applying these transforms on series whose terms are not monomials, a Fourier series being an example. Thus convergence accelerating sequence transforms are interesting on their own as well as in their application in various fields where one has to deal with infinite series and sequences which may be divergent. I shall try to convince the reader that most of the divergent series the *sum* , we encounter in physical problems, has a meaning. Some of these transforms and their applications in various situations form the contents of this article.

2 Sequence Transform

Let $\{S_n\}$ be an infinite sequence with limit S. A sequence transform turns $\{S_n\}$ into another sequence $\{S'_n\}$. Each member of the derived sequence is a function of $(k+1)$ terms, say, of the original sequence. Formally we can write

$$\{S'_n\} = T_{kn}\{S_n\}.$$

The index k is a measure of the number of terms of the sequence required to define the corresponding transform. In particular, the original sequence can be written as $T_{0n}(\{S_n\}) \equiv \{S_n\}$and for obvious reasons is also called the zeroth sequence. Therefore, a sequence transform converts an infinite sequence into another, unless it exactly evaluates the limit of the latter. If this limit is an irrational number, there is no possibility of the derived sequence being finite.

Let us consider the forward difference operator Δ , defined by

$$\Delta^{k+1}S_n = \Delta^k S_{n+1} - \Delta^k S_n, \quad \Delta^0 S_n = S_n.$$

The individual terms of a series and its partial sums are thus simply related. The terms series and sequence can therefore be applied interchangeably in that a sequence transform may very well be called a series transformation.

Both contexts are useful, but a word of note here. A convergent sequence need not always be associated with the partial sums of a series. Such sequences may arise in many different ways as, for example, when the sequence is defined by successive partial products,

$$S_n \equiv \Pi_{i=0}^{n-1} t_i$$

so that $S = \Pi_{i=0}^{\infty} t_i$.

If both the sequences $\{S_n\}$ and $T(\{S_n\})$ converge to the same limit, the transform T is said to be *regular*. Thereby, a regular sequence transform provides an operational definition of the limit of an infinite sequence, consistent with the usual definition. For a regular sequence transform it may so happen that

$$|S - T_{kn}\{S_n\}| < |S - S_n|.$$

Then T is a convergence accelerating sequence transform. This means that $T_{kn}\{S_n\}$ is closer to S than S_n itself.

Sequence transforms belong to two broad classes, linear and nonlinear. The transform T is said to be linear if

- (i) $T\{cS_n\} = cT\{S_n\}$ where c is a constant, in general complex.

- $(ii)\ \ T\{S_n + S_n^{'}\} = T\{S_n\} + T\{S_n^{'}\}$

Otherwise the transform is said to be nonlinear.

The nonlinear methods are more powerful in general than the linear ones. A linear method may, however, be comparable in effectiveness in special circumstances as, for example, when the parameters of the sequence transform are suitably chosen for specific sequences or when the method is exact on a certain class of sequences. Many transforms are very effective on different classes of sequences and Delahaye and Germain-Bonne have proved that a universal transformation which accelerates the convergence of all types of logarithmic sequences cannot exist [1].

2.1 Types of Convergence

Let $\{S_n\}$ be a sequence which converges to the limit S. Define the remainder r_n after n terms as $r_n \equiv S - S_n$. For a converging sequence $\lim_{n\to\infty} r_n = 0$. The ratio

$$\rho \equiv \lim_{n\to\infty} \frac{r_{n+1}}{r_n} = \lim_{n\to\infty} \frac{S - S_{n+1}}{S - S_n} \tag{4}$$

can be used to classify sequences by the nature of their convergence. If $|\rho| > 1$, the sequence diverges and if $|\rho| \leq 1$, it converges. If $|\rho| < 1$, the convergence is said to be linear and if $|\rho| = 1$, the convergence is said to be logarithmic. If, however, $|\rho| = 0$, the convergence is said to be hyperlinear.

The most common example of a linearly convergent series is the geometric series for which $t_n = z^{n-1}$ and $S = (1-z)^{-1}$ so that

$$S_n = \sum_{i=0}^{n-1} z^i = S - \frac{z^n}{1-z}, \quad 0 < |z| < 1. \tag{5}$$

Here $\rho = z$.

2.2 Divergent Sequences

In the following, divergent series will be taken up quite often. Hence it is convenient to include a short discussion at this point. Divergent series have been discussed widely and in depth in many places [2-4]. Here we adopt a somewhat unusual approach, that of introducing the *anti limit* [5]. There is no pretense to either exactness or rigour. Also, this seems to be as good a place as any, to introduce a pictorial representation of convergence acceleration, which provides some insight. In this, the partial sums are plotted against the sequence index and the limit is shown by a straight line parallel to the abscissa as in figure 1.1.

The limit of a convergent sequence is now seen from figure -1 to be the point at which the variations level out for a monotone sequence and the point where the oscillations of an alternating sequence die out. For a divergent sequence, the anti limit can be thought of as the point from which the sequence moves away

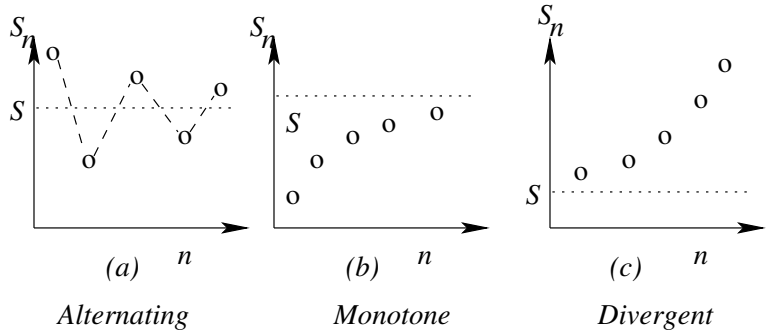


Figure 1: Partial sums S_n of (a) an alternating convergent sequence, (b) a monotone convergent sequence and (c) a monotone divergent sequence.

steadily and, for oscillatory divergence, the point from which the oscillations begin. This picture will be invoked frequently in order to introduce or clarify a point.

The existence of the anti limit can be illustrated by examples if one is prepared to forsake analytical caution for the time being, and believe the assurance that formal and rigorous justifications for the *results* thus obtained exist in spite of the apparent liberties taken.

The sum of the infinite geometrical series is

$$\sum_{i=0}^{\infty} z^i = \frac{1}{1-z}, \qquad |z| < 1.$$

Differentiating successively we have,

$$\left(z\frac{d}{dz}\right)^{\nu}\left(\sum_{k=0}^{\infty} z^i\right) = \sum_{i=0}^{\infty} i^{\nu} z^i.$$

Within the domain of convergence of the geometric series we have formally

$$S(\nu) \equiv \sum_{i=0}^{\infty} i^{\nu} z^i = \left(z\frac{d}{dz}\right)^{\nu} \frac{1}{1-z}, \qquad |z| < 1. \tag{6}$$

Now the right hand side of the above identity is easily evaluated even for values of z for which $|z| > 1$ (except for the point $z = 1$). But the series on the left hand side becomes a divergent series for any such value of z. Thus finite numbers may be associated with such divergent series and may be defined as their *sums*. We reserve a somewhat more elaborate discussion of divergent series and their summability for a later section. Here we demonstrate a summability method only for series defined by the left hand side of equation -6. Specifically,

$$\sum_{i=0}^{\infty} z^i = \frac{1}{1-z}.$$

For $z = -1$, the left hand side gives the divergent series

$$1 - 1 + 1 - 1 + \cdots,$$

whereas the right hand side gives the value $\frac{1}{2}$. Similarly, using $\nu = 1$ and 3 in equation 6 we have

$$\begin{aligned} \sum_{i=0}^{\infty} iz^i &= \frac{z}{(1-z)^2}. \\ \sum_{i=0}^{\infty} i^3 z^i &= \frac{z\left(z^2 + 4z + 1\right)}{(1-z)^4}. \end{aligned}$$

Using the value $z = -1$ on both sides we *sum* the resulting divergent series as

$$\begin{aligned} 1 - 2 + 3 - 4 + \cdots &= \frac{1}{4} \\ 1^3 - 2^3 + 3^3 - 4^3 + \cdots &= \frac{1}{8}. \end{aligned}$$

Thus finite values can be obtained for sums of series which formally diverge. The values thus obtained can be justified by more sophisticated analysis [2, 6]. Interestingly, summability methods work mostly for divergent series which are alternating in nature. A monotone divergent series can usually be summed if it can be related to a corresponding alternating counterpart. For example, the series

$$1 + 2 + 3 + 4 + \cdots,$$

which is basically $\zeta(-1)$ [6] has the value $-\frac{1}{12}$ and can be *summed* by using the result

$$1 + 2 + 3 + 4 + \cdots = 1 - 2 + 3 - 4 + \cdots + 2(2 + 4 + 6 + \cdots)$$

or

$$3(1 + 2 + 3 + 4 + \cdots) = -(1 - 2 + 3 - 4 + \cdots)$$

and

$$1 + 2 + 3 + 4 + \cdots = -\frac{1}{12}.$$

We mention here Hardy's treatise on divergent series [2] as well as the fact that a large part of the analytical treatment of divergence concerns itself only with linear sequence transforms.

2.3 Linear Transforms

2.3.1 Hutton Transform

A glance at the graphical representation (figure - 2) of a convergent alternating sequence suggests what happens to be the simplest convergence accelerating

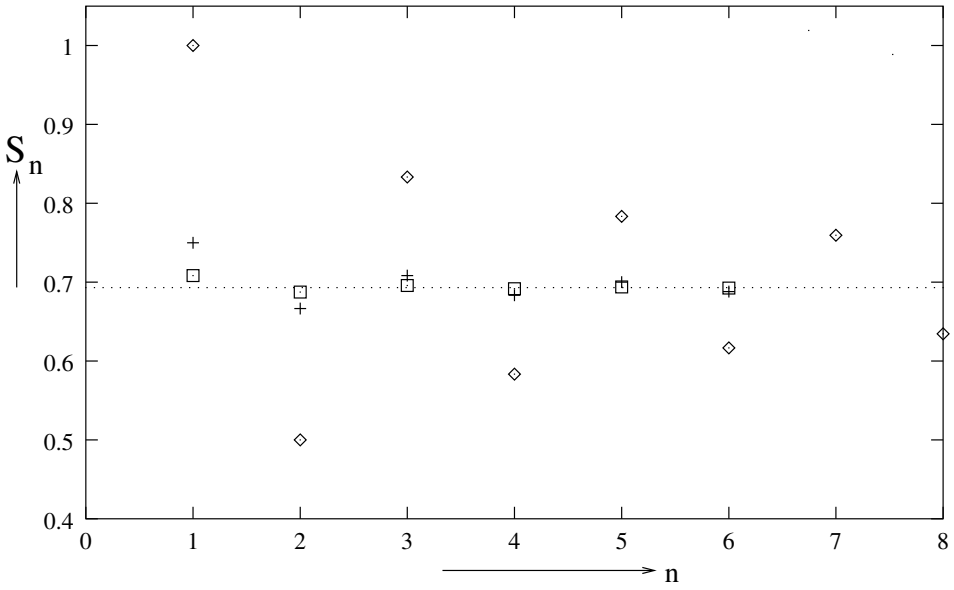


Figure 2: Iterations of Hutton transform on the sequence for $\ln 2$ (equation - 2). The circles represent the zeroth sequence; + represents the first application of the Hutton transform; the squares represent the next application of the transform.

sequence transform, *viz.*, the Hutton transform and simultaneously indicates some of its possible properties. For general matrix transformation one is referred to the book by Petersen [7].

Clearly the mean of any two successive terms of $\{S_n\}$ is much nearer to the limit S than either of them and has the sign of the earlier term. Thus

$$S'_n = T_{1n} \equiv \frac{1}{2}\left(S_n + S_{n+1}\right)$$

defines a sequence transformation. Both sequences S_n and S'_n tend to the same limit S. and the remainder r'_n in the transformed sequence is the mean of r_n and r_{n+1}, and is smaller in magnitude than either of them since the magnitude of r_n decreases steadily while alternating in sign. Therefore r'_n converges to zero faster than r_n so that S'_n converges to S faster than S_n. The convergence of S_n has thus thus been accelerated by means of a simple sequence transform.

For a zeroth sequence which is alternating, the derived sequence is also alternating. However, the oscillation of the derived sequence about the limit is much smaller in magnitude as can be seen from the figure- 2. The process can be applied iteratively to get better results. The results of two iterations are also indicated in figure - 2.

If both S_n and S_{n+1} are of the same sign then S_{n+1} is already closer to S than $\left(S_n + S_{n+1}\right)/2$, so that it is apparent that the Hutton transform is not

capable of accelerating the convergence of a monotone sequence.

2.3.2 Euler Transform

In 1755 Euler published the series transform which bears his name and is useful device for accelerating the convergence of an alternating series. Let

$$S = a_1 - a_2 + a_3 - a_4 + \cdots + (-1)^{n+1}\, a_n + \cdots$$

with all $a_n > 0$. Then

$$\begin{aligned} S &= \frac{1}{2}a_1 - \frac{1}{2}\,(a_2 - a_1) + \frac{1}{2}\,(a_3 - a_2) + \cdots \\ &= \frac{1}{2}a_1 - \frac{1}{2}\Delta a_1 + \frac{1}{2}\Delta a_2 - \frac{1}{2}\Delta a_3 + \cdots \\ &= \frac{1}{2}a_1 - \frac{\Delta}{2}\,(a_1 - a_2 + \cdots) \\ &= \frac{1}{2}a_1 - \frac{1}{2}\Delta S. \end{aligned}$$

so that

$$S = \frac{1}{2}\left(1 + \frac{\Delta}{2}\right)^{-1} a_1$$

whence, by means of a formal binomial expansion,

$$S = \sum_{j=0}^{\infty} (-1)^j \frac{1}{2^{j+1}} \Delta^j a_1. \tag{7}$$

In order to apply the Euler transform we must first make a difference table for the terms of the series. The application of the Euler transform on the series given in equation-2 does not need much numerical work since $a_n = \frac{1}{n}$. For then,

$$\Delta^k a_n = \frac{(-1)^k k!}{(n)_{k+1}}, \quad \text{so that} \quad \Delta^k a_1 = \frac{(-1)^k}{k+1}.$$

Therefore

$$\ln 2 = \sum_{j=1}^{\infty} \frac{1}{j\, 2^j}. \tag{8}$$

One can make a difference table and evaluate $\ln 2$ from equation-7 by using the difference table or directly from equation-8.

The sum over the first ten terms is

$$S = \frac{1}{2} + \frac{1}{2^2}\frac{1}{2} + \frac{1}{2^3}\frac{1}{3} + \frac{1}{2^4}\frac{1}{4} + \frac{1}{2^5}\frac{1}{5} + \frac{1}{2^6}\frac{1}{6} + \frac{1}{2^7}\frac{1}{7} + \frac{1}{2^8}\frac{1}{8} + \frac{1}{2^9}\frac{1}{9} + \frac{1}{2^{10}}\frac{1}{10}$$

$$= 0.693065.$$

Thus with only ten terms of the derived series we obtain an accuracy of three decimal places.

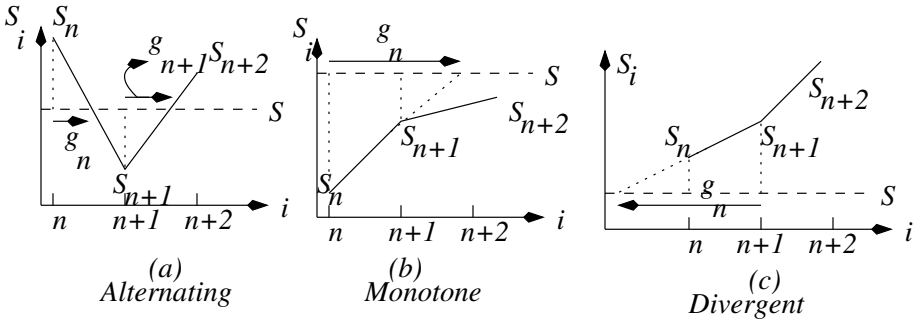


Figure 3: Graphical representations of the relation given by equation-11; (a) for an alternating convergent sequence; (b) for a monotone convergent sequence and (c) for a monotone divergent sequence.

2.4 Nonlinear Convergence Accelerating Transforms

Nonlinear sequence transforms are fundamentally different from linear sequence transforms in that the derived sequence is a nonlinear function of the original sequence. Let $\{S_n\}$ be an infinite sequence with limit S. Let us define a sequence $\{g_n\}$ related to the sequence $\{S_n\}$ as follows:

$$S - S_n = r_n = g_n \Delta S_n, \tag{9}$$

where $\{r_n\}$ is the sequence of remainders. For a graphical representation of the relation refer to the schematic plots of the partial sums of a convergent alternating series, a convergent monotone series and a monotone divergent series, shown in figure-3. The horizontal dotted lines are the limits of the sequences in cases of convergent series and the anti-limit for the divergent series. Let g_n denote the distance between the points (n, S) and the point at which the straight line joining S_n and S_{n+1} intersects the straight line $S_i = S$. Then from the dotted similar triangles one obtains the following relation for all the cases:

$$\frac{S - S_n}{g_n} = \frac{S_{n+1} - S}{1 - g_n} = S_{n+1} - S_n \tag{10}$$

whence

$$S = S_n + g_n \Delta S_n. \tag{11}$$

It can be seen from the illustration that in the limit $n \to \infty$, g_n approaches the value $\frac{1}{2}$ for an alternating series. But for a monotone series g_n goes to infinity. When this relation is written in the form

$$S = (1 - g_n)\, S_n + g_n S_{n+1},$$

it is obvious that the transform defines a mean on $\{S_n\}$ with respective weights $\{g_n\}$.

The nature of the approach of S_n to the limit S is reflected in the nature of variation of g_n with n. If the dependence of g_n on n can be guessed from the original sequence, then this information can be used to derive an expression for the limit.

Equation-11 can be written in a more general form

$$S = S_n + g_n \omega_n, \tag{12}$$

where $\omega_n = \Delta S_n$ or ΔS_{n-1} and both forms are useful.

Thus, an approximation for g_n provides a corresponding approximation for S. The technique of accelerating the convergence of a sequence consists in approximating the limit from the information contained in the sequence itself. If each term in $\{g_n\}$ is assumed to be a known function of $(k+1)$ arguments, *i.e.,* if

$$g_{kn} = g_{kn}\left(S_n, \rho_{n+1}, \rho_{n+2}, \ldots, \rho_{n+k}\right) \tag{13}$$

with

$$\rho_n \equiv \frac{t_{n+1}}{t_n} = \frac{\Delta S_n}{\Delta S_{n-1}},$$

then g_{kn} can be taken as an approximation to g_n.

With this approximation for g_{kn}, a corresponding approximation for S may be obtained by the sequence transformation

$$T_{kn}\{S_n\} = S_n + g_{kn} \Delta S_n. \tag{14}$$

In the double-indexed infinite table of transformed values T_{kn}, each element approximates the limit of the original infinite sequence. Improvement in the approximation is expected along the rows, the columns and the diagonals.

To be useful a sequence transform which accelerates convergence has necessarily to be regular. Hence the convergence of the derived sequence may again be accelerated by using the same transform and this bears further repetition. Such iteration is expected to improve the estimation of the limit. The iterative scheme for the approximation may thus be written as

$$T_{kn}^{(\mu+1)} = T_{kn}^{(\mu)} + g_{kn}^{(\mu)} \Delta T_{kn}^{(\mu)} \tag{15}$$

with

$$T_{kn}^{(0)} = S_n$$

and

$$g_{kn}^{(\mu)} = g_{kn}\left(\{T_{kn}^{(\mu)}\}\right)$$

where μ is the order of iteration. The n-th term in the μ-*th* iteration of the k-th order transform thus requires $n + \mu(k+1)$ terms of the original series. In most applications $n = 1$.

We shall discuss the different transforms and their iterations in the subsequent sections.

2.4.1 The Aitken's Δ^2-transform

Perhaps the simplest and the oldest nonlinear transform is Aitken's Δ^2-transform [8] and has been amply discussed in the literature. As we have discussed in the previous section, an approximation for g_n in equation-11 gives an approximation for S. The simplest assumption for g_n is that g_n is independent of n, *i.e.,* g_n is a constant, which implies that $\Delta g_n = 0$. With this assumption we get from equation -11

$$\Delta g_n = \Delta \left(\frac{S - S_n}{\Delta S_n} \right) = 0. \tag{16}$$

As S is the limit of the sequence and consequently independent of n, we can take S outside the Δ-operator and solve for S. This gives

$$S \simeq A_{2n} = \frac{\Delta\left(\dfrac{S_n}{\Delta S_n} \right)}{\Delta\left(\dfrac{1}{\Delta S_n} \right)}. \tag{17}$$

T_{2n} or T_n is the symbol for a general transform and to distinguish between the different transforms we use the symbol A_n for the above transformation. Henceforth we shall omit the index k when there is no scope of confusion and write A_n for A_{2n}.

This is the famous Δ^2-transform of Aitken, which we can recast into other equivalent forms such as

$$A_n = \frac{\dfrac{S_{n+1}}{\Delta S_{n+1}} - \dfrac{S_n}{\Delta S_n}}{\dfrac{1}{\Delta S_{n+1}} - \dfrac{1}{\Delta S_n}}, \tag{18}$$

$$A_n = \frac{S_n S_{n+2} - S_{n+1}^2}{S_{n+2} - 2S_{n+1} + S_n}., \tag{19}$$

$$A_n = S_{n+1} - \frac{\Delta S_{n+1} \Delta S_n}{\Delta^2 S_n}, \tag{20}$$

$$A_n = S_n - \frac{(\Delta S_n)^2}{\Delta^2 S_n}. \tag{21}$$

Though the above forms are formally equivalent, yet they may differ from the point of view of numerical computation.

For a geometric series g_n =constant and $\Delta g_n = 0$. This implies that the Δ^2-transform will be exact on a geometric series.

The properties of the Δ^2-transform are discussed in the books by Wimp [9] and Brezinski and Zaglia [10] and in the review article by Weniger [11].

One can use the iterated version of the Aitken transform can be written as

$$A_n^{(\mu+1)} = A_n\{A_n^{(\mu)}\}, \text{ with } A_n^0\{S_n\} = S_n \tag{22}$$

Table 1: Iteration of Δ^2-transform on the series for $\ln 2$ given in equation 2.

n	$A_n^{(0)}$	$A_n^{(1)}$	$A_n^{(2)}$	$A_n^{(3)}$
1	1.0	0.7	0.69327731	0.6931488
2	0.5	0.69047619	0.69310576	
3	0.83333333	0.69444444	0.693163341	
4	0.58333333	0.69242424		
5	0.78333333	0.69358974		
6	0.61666667			
7	0.75952381			

Table 2: Iteration of Δ^2-transform on the series for $\zeta(2)$ given in equation 3.

n	$A_n^{(0)}$	$A_n^{(1)}$	$A_n^{(2)}$	$A_n^{(3)}$	$A_n^{(4)}$	$A_n^{(5)}$
1	1.0	1.45	1.5755	1.6182	1.6345	1.6432
2	1.25	1.5040	1.5903	1.6228	1.6358	
3	1.3611	1.5347	1.6000	1.6260	1.6369	
4	1.4236	1.5545	1.6068	1.6285		
5	1.4636	1.5683	1.6118	1.6304		
6	1.4914	1.5785	1.6157			
7	1.5118	1.5862	1.6187			
8	1.5274	1.5924				
9	1.5398	1.5974				
10	1.5498					
11	1.5580					

For implementing the Δ^2-transform one requires at least three terms in the original series and for finding $A_n^{(\mu)}$ one requires $(2\mu + n)$ terms of the original series.

The performance of the iteration of Δ^2-transform on the sequence for $\ln 2$ and $\zeta\,(2)$ are shown in the table-1 and table-2 respectively.

●▷

Finding Euler Constant

Let us consider another sequence defined by

$$S_n = \sum_{i=1}^{n} \frac{1}{i} - \ln n. \tag{23}$$

Both the individual terms on the right hand side, i.e, $\sum_{i=1}^{n} \frac{1}{i}$ and $\ln n$, diverge to infinity as n tends to infinity. However, $\lim_{n\to\infty} \; S_n$ remains finite. The limit is known as the Euler constant γ. Its value is $0.577215664901533\cdots$.

The convergence of the sequence given by equation-23 is very slow. With 10^3 terms one gets only 0.57771558 from the direct sum. The iteration of Δ^2-

Table 3: Iteration of Δ^2-transform on the sequence given by equation-24.

n	$m = 2^{n-1}$	$A_n^{(0)}$	$A_n^{(1)}$	$A_n^{(2)}$	$A_n^{(3)}$
1	1	1.0	0.552329		0.577221
2	2	0.806853	0.571282		
3	4	0.697039	0.575804		
4	8	0.638416			
5	16	0.608140			

transform accelerates the convergence of this sequence. However, there is a significant gain on redefining the zeroth sequence as

$$S_n = \sum_{1}^{2^{n-1}} \frac{1}{i} - \ln\left(2^{n-1}\right). \tag{24}$$

In other words, from a sequence $\{S_n,\, n = 0,\, 1, \ldots\}$, the sub-sequence $\{S_{2^{n-1}}, n = 0, 1, \ldots\}$ is taken as the zeroth sequence. Such redefinition of a sequence is often helpful. Table-3 displays the result obtained by applying the Δ^2-transform on the above redefined sequence. ◁●

2.5 The Levin-Weniger Transforms

It has been shown that imposing a structure on g_n leads to a specific sequence transform. With $\omega_n = \Delta S_n$, the condition $\Delta g_n = 0$ leads to the Δ^2-transform. It is tempting to continue the generalization according to the scheme

$$\Delta^k g_n = 0, \quad k = 1, 2, 3, \ldots \tag{25}$$

which gives rise to the sequence transform in following form:

$$\Delta^k \left(\frac{S - S_n}{\Delta S_n} \right) = 0$$

or

$$S \approx d_k^{(n)} = \frac{\Delta^k \left(S_n/\Delta S_n\right)}{\Delta^k \left(1/\Delta S_n\right)} \tag{26}$$

This sequence transform was devised by Drummond [13] and bears his name. For positive series, however, the scheme does not improve convergence beyond $k = 2$.

As stated earlier, g_n to increase monotonically with n for a positive series. A monotone sequence $\{S_n\}$ converges marginally when $\Delta S_n \sim \frac{1}{n}$, implying that g_n cannot increase faster than, or even as fast as n^2. This gives some understanding of why $d_k^{(n)}$ does not work well on a monotone sequence for $k > 2$.

It can be argued that g_n increases faster than n but slower than n^2[18] . Further refinements in the functional form can be achieved by adding terms in

$\frac{1}{n}$ and its higher powers. Accordingly, a generally valid form for g_n would be

$$g_n = \alpha n + \sum_{i=0}^{\infty} \frac{\alpha_i}{n^i} \tag{27}$$

where α and α_i's are constant. When these constants are known for a sequence, thereby its limit is also known.

To obtain the Levin transforms, we start from the more general *ansatz*

$$S = S_n + g_{kn}\omega_n \tag{28}$$

where ω_n is either ΔS_n or ΔS_{n-1}. Let us now approximate g_{kn} by terminating the series in equation -27, so that

$$g_{kn} = \alpha n + \sum_{i=0}^{k-2} \frac{\alpha_i}{n^i} = \frac{P_{k-1}}{n^{k-2}} \tag{29}$$

or

$$S = S_n + \frac{P_{k-1}}{n^{k-2}}\omega_n \tag{30}$$

where P_{k-1} is a polynomial in n of degree $k-1$ involving k constants. As Δ^k will annihilate a polynomial of degree $k-1$, we have

$$\Delta^k P_{k-1} = \Delta^k \left(n^{k-2} g_{kn}\right) = 0 \tag{31}$$

The corresponding transform is

$$S \approx u_k^{(n)} = \frac{\Delta^k \left(n^{k-2} S_n/\omega_n\right)}{\Delta^k \left(n^{k-2}/\omega_n\right)}. \tag{32}$$

and is referred to as the u-transform of Levin [14].

A generalization of this transform can be obtained by assuming

$$g_{kn} = \alpha \left(n+\beta\right) + \sum_{i=0}^{k-2} \frac{\alpha_i}{\left(n+\beta\right)^i} = \frac{P_{k-1}}{\left(n+\beta\right)^{k-2}} \tag{33}$$

β being an arbitrary constant. This leads to

$$T_{kn} = u_k^{(n)} = \frac{\Delta^k \left[\left(n+\beta\right)^{k-2} S_n/\omega_n\right]}{\Delta^k \left[\left(n+\beta\right)^{k-2}/\omega_n\right]} \tag{34}$$

The expansion of the Δ-operator in the terms of a sequence,

$$\Delta^k f_n = \sum_{j=0}^{k} (-)^j \binom{k}{j} f_{n+j},$$

Table 4: Performance of u and t transforms ($\beta = 0$) on the series for $\ln 2$ given by equation-2. S is the limit of the sum obtained by the transform used

transform used	S	absolute relative error	transform used	S	absolute relative error
u_2	0.6875	$8.1\,10^{-3}$	t_2	0.6944	$1.9\,10^{-3}$
u_3	0.69345	$4.4\,10^{-4}$	t_3	0.6931372	$1.4\,10^{-5}$
u_4	0.6931423	$7.0\,10^{-6}$	t_4	0.6931439	$4.7\,10^{-6}$
u_5	0.6931465	$8.4\,10^{-7}$	t_5	0.693147401	$3.2\,10^{-7}$
u_6	0.69314722	$7.1\,10^{-8}$	t_6	0.69314717779	$4.0\,10^{-9}$
u_7	0.6931471795	$1.5\,10^{-9}$	t_7	0.693147180015	$7.9\,10^{-10}$
u_8	0.69314718046	$1.3\,10^{-10}$	t_8	0.6931471806012	$6.0\,10^{-11}$
u_9	0.6931471805678	$1.3\,10^{-11}$	t_9	0.69314718055924	$1.0\,10^{-12}$

gives a corresponding explicit form for the transform (with $\omega_n = \Delta S_{n-1}$) as

$$u_k^{(n)} = \frac{\sum_{j=0}^{k} (-)^j \binom{k}{j} (\beta + n + j)^{k-2} \frac{S_{n+j}}{\Delta S_{n+j-1}}}{\sum_{j=0}^{k} (-)^j \binom{k}{j} (\beta + n + j)^{k-2} \frac{1}{\Delta S_{n+j-1}}}. \tag{35}$$

and one gets the u-transform of Levin [14]. Very often in numerical work, overflow may occur for large values of k. Hence both the numerator and the denominator are divided by the common factor $(\beta + n + k)^{k-2}$ in order to decrease the magnitude of the respective terms. This gives

$$u_k^{(n)} = \frac{\sum_{j=0}^{k} (-)^j \binom{k}{j} \frac{(\beta + n + j)^{k-2}}{(\beta + n + k)^{k-2}} \left(\frac{S_{n+j}}{\Delta S_{n+j-1}} \right)}{\sum_{j=0}^{k} (-)^j \binom{k}{j} \frac{(\beta + n + j)^{k-2}}{(\beta + n + k)^{k-2}} \left(\frac{1}{\Delta S_{n+j-1}} \right)} \tag{36}$$

Though it has been proved that the u-transform is regular and accelerative on linearly convergent series [19] and also that it is regular on alternating series [14,19], there exists no analysis in the literature which throws any light on the problem of regularity of the u-transform on logarithmically convergent monotone sequences. From a numerical study on a number of test sequences it appears that the instability of the u-transform is not intrinsic to the algorithm, but is caused by the truncation errors inevitably incurred in a finite precision real arithmetic [20,21].

For an alternating sequence, g_n does not diverge but tends to a finite value, so instead of equation-33 one can assume

$$g_n = \sum_{i=0}^{\infty} \frac{\alpha_i}{(n + \beta)^i} \tag{37}$$

and write the truncated series as

$$g_{kn} = \sum_{i=0}^{k-1} \frac{\alpha_i}{(n+\beta)^i} = \frac{P_{k-1}}{(n+\beta)^{k-1}}. \tag{38}$$

For $\omega_n = \Delta S_{n-1}$, one gets in a similar way the t-transform of Levin,

$$t_k^{(n)} = \frac{\sum_{j=0}^{k}(-)^j \binom{k}{j} \frac{(\beta+n+j)^{k-1}}{(\beta+n+k)^{k-1}} \left(\frac{S_{n+j}}{\Delta S_{n+j-1}}\right)}{\sum_{j=0}^{k}(-)^j \binom{k}{j} \frac{(\beta+n+j)^{k-1}}{(\beta+n+k)^{k-1}} \left(\frac{1}{\Delta S_{n+j-1}}\right)} \tag{39}$$

This transformation was proposed by Levin [14] for an alternating series. Here also, for convenience we have divided both the numerator and denominator by the common factor $(n+\beta+k)^{k-1}$. Smith and Ford [15] remarked that this transform gives the best simple remainder estimate for a convergent series with strictly alternating terms. It may be remarked that, with $\omega_n = \Delta S_n$, one can obtain a similar set of transforms. As these transforms will need one extra term for their implementation, we do not consider these transforms. The parameter β can be properly exploited in many situations. However, in the subsequent applications we shall choose $\beta = 0$. In constructing a transform of any order, one would encounter a term $\Delta S_0 = S_1 - S_0$, and S_0 should be chosen to be zero. In most applications we shall start with $n = 1$ and designate the transforms as u_k and t_k respectively.

It is found that the t-transform fails to accelerate the convergence of the series for $\zeta(2)$. Though the t-transform works somewhat better on an alternating series, the u-transform performs reasonably well for both alternating and monotone sequences.

•◁

A different class of transform can be obtained by writing the truncated expression for g_{kn} in the form

$$g_{kn} = \sum_{i=0}^{k-1} \frac{\alpha_i}{(n+\beta)_i} = \frac{P_{k-1}(n)}{(n+\beta)_{k-1}}, \tag{40}$$

where $(z)_\nu$ is the usual Pochhammer symbol

$$(z)_\nu = \frac{\Gamma(z+\nu)}{\Gamma(z)} = z(z+1)(z+2)\cdots(z+\nu-1).$$

Proceeding exactly as before ($\omega_n = \Delta S_{n-1}$)one obtains the τ -transform and is given by

$$\tau_k^{(n)} = \frac{\sum_{j=0}^{k}(-)^j \binom{k}{j} (\beta+n+j)_{k-1} \frac{S_{n+j}}{\Delta S_{n+j-1}}}{\sum_{j=0}^{k}(-)^j \binom{k}{j} (\beta+n+j)_{k-1} \frac{1}{\Delta S_{n+j-1}}}. \tag{41}$$

Table 5: Performance of τ and y transforms ($\beta = 0$) on the series for $\ln 2$ given by equation-2. S is the limit of the sum obtained by the transform used.

transform used	S	absolute relative error	transform used	S	absolute relative error
τ_2	0.6944	$1.9\,10^{-3}$	y_2	0.6875	$8.1\,10^{-3}$
τ_3	0.69321	$9.8\,10^{-5}$	y_3	0.69345	$4.4\,10^{-4}$
τ_4	0.6931497	$3.7\,10^{-6}$	y_4	0.693161	$2.0\,10^{-5}$
τ_5	0.69314726	$1.2\,10^{-7}$	y_5	0.6931476	$7.1\,10^{-7}$
τ_6	0.693147183	$3.9\,10^{-9}$	y_6	0.693147196	$2.3\,10^{-8}$
τ_7	0.69314718064	$1.2\,10^{-10}$	y_7	0.69314718106	$7.3\,10^{-10}$
τ_8	0.693147180562	$3.8\,10^{-12}$	y_8	0.69314718057	$2.3\,10^{-11}$
τ_9	0.6931471805600	$1.2\,10^{-13}$	y_9	0.6931471805604	$1.0\,10^{-13}$

This is similar to the t-transform of Levin with the power replaced by the Pochhammer symbol. The transform was introduced by Sidi [16,17]. Weniger [11] independently discovered it and fruitfully demonstrated that this can be an extremely useful computational tool [22, 23]. With

$$g_{kn} = \alpha\,(n+\beta) + \sum_{i=0}^{k-2} \frac{\alpha_i}{(n+\beta)_i} = \frac{P_{k-1}\,(n)}{(n+\beta)^{k-2}} \tag{42}$$

and proceeding in a similar way one obtains

$$y_k^{(n)} = \frac{\sum_{j=0}^{k}(-)^j \binom{k}{j} (\beta+n+j)_{k-2}\, \frac{S_{n+j}}{\Delta S_{n+j-1}}}{\sum_{j=0}^{k}(-)^j \binom{k}{j} (\beta+n+j)_{k-2}\, \frac{1}{\Delta S_{n+j-1}}}. \tag{43}$$

In most of the applications, one uses the transforms with $n = 1$. Very often in numerical work, overflow may occur for large k. Hence, both the numerator and denominator $\tau_k^{(n)}$and $y_k^{(n)}$ are divided by the common factor $(\beta+n+j)_{k-1}$ and $(\beta+n+j)_{k-2}$ respectively. As before, if we start with $n = 1$we shall designate the transforms as τ_k and y_k respectively. In these cases, as well, we encounter a term $\Delta S_0 = S_1 - S_0$ in the sum and we must choose $S_0 = 0$. A new class of similar transforms can be obtained with $\omega_n = \Delta S_n$ [11].

Subsequently, Chaterjee and Roy extended these transforms which are tailored to sum the hyper-geometric series [35]

2.6 PadéApproximants

. Let $f\,(z)$ be a function of a complex variable z and let its power series expansion is known, then the Padé approximant express it in the form of a ratio of two polynomials. The $[N/M]$ Padé approximant of $f\,(z)$ is the uniquely determined

irreducible rational polynomial defined by

$$[N/M] = \frac{A_N(z)}{B_M(z)} \tag{44}$$

where $A_N(z)$ and $B_M(z)$ are polynomials in z of degree N and M respectively, such that for any pair of integers (N, M),

$$f((z) - [N/M] = \mathcal{O}\left(z^{M+N+1}\right), \qquad z \to 0. \tag{45}$$

The basic idea of Padé approximation is to choose an approximating function in such a way that the value of the function at $z = 0$ and its first $N+M$ derivatives there agree with those of the given function and this is done by matching the first $N + M + 1$ terms of the original power series. Thus this approximation is an extreme case of one point interpolation, higher accuracy being achieved by matching higher derivatives at that point.

As the value of a rational function remains unchanged if both the numerator and denominator are divided by the same constant, the constant term in denominator can be set to unity, so that the structure of the Padé approximant $[N/M]$ is,

$$[N/M] = \frac{p_0 + p_1 z + p_2 z^2 + \ldots + p_N z^N}{1 + q_1 z + q_2 z^2 + \ldots + q_M z^M}. \tag{46}$$

where the p_i's and the q_i's are constant coefficients. The assumption that $q_0 = 1$ is quite general. If $q_0 = 0$, the rational function does not exist at $z = 0$, unless $p_0 = 0$, in which case there is a common factor between $A_N(z)$ and $B_M(z)$ and the approximant is really $[N - 1/M - 1]$. Hence in the subsequent discussion we shall always assume $q_0 = 1$.

Let us now consider the difference

$$f(z) - [N/M] = \frac{\left(\sum_{k=0}^{\infty} a_k z^k\right)\left(\sum_{i=0}^{M} q_i z^i\right) - \sum_{j=0}^{N} p_j z^j}{\sum_{j=0}^{M} q_j z^j}$$

In order to conform to equation- 45, the coefficients of z^j in the numerator should vanish for $j = 0, 1, 2, \ldots, N + M$, which gives

$$\sum_{i=0}^{j} a_{j-i} q_i = p_j, \qquad j = 0, 1, 2...N$$

with $p_j = 0$ if $j > N$ and

$$\sum_{i=0}^{j} a_{j-i} q_i = 0 \qquad j = N + 1, N + 2...N + M \tag{47}$$

with $q_j = 0$ if $j > M$ and $a_i = 0$ for $i < 0$. The equation-47 represents a set of $N + M + 1$ linear equations in $N + M + 1$ unknowns. This can be solved to get the coefficients $\{p_i\}$ and $\{q_i\}$ provided the coefficient matrix is non singular.

It is customary to arrange the Padé approximants [24 ,25,26] in the form of a two dimensional array shown below and referred to as the Padé table.

$$\begin{array}{ccccc} [0/0] & [0/1] & [0/2] & [0/3] & \cdots \\ [1/0] & [1/1] & [1/2] & [1/3] & \cdots \\ [2/0] & [2/1] & [2/2] & [2/3] & \cdots \\ [3/0] & [3/1] & [3/2] & [3/3] & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{array}$$

The first column of the Padé table consists of the partial sums of the Taylor series. The elements running parallel to the main diagonal have a constant difference in the degree of the numerator and the denominator. The anti diagonal sequences all involve the same number of coefficients. The elements in the diagonal and above it are proper fractions, while those below are not. In general, if the order of the polynomials in the numerator and denominator of a rational function be n and m respectively, then the $[N/M]$ Padé approximant reproduces this function exactly for $N \geq n$ and $M \geq m$.

As an example, the [0/1], [1/1] and [1/, 2] Padé approximants for the function $\ln(1+z)/z$ are respectively given by $\frac{1}{1+\frac{z}{2}}$, $\frac{1+\frac{z}{6}}{1+\frac{2z}{3}}$ and $\frac{1+\frac{z}{2}}{1+z+\frac{z^2}{6}}$.

2.7 Summing Divergent Series

2.7.1 Analytic Continuation

If a function $f(z)$ be analytic near every point $P(z_0)$ on the complex plane, then we can expand the function in a power series of $(z - z_0)$, the coefficients being the successive derivatives of the function at z_0. The function may be singular at one or more than one point. If A be a singularity of $f(z)$ nearest to P, then the circle within which this expansion is valid is the one with the centre at P and radius of convergence equal to PA (figure-4). For example, for the function $f(z) = \dfrac{1}{(1-z)}$ and $z_0 = 0$, the circle of convergence is a circle of radius 1 with the centre at the origin. The question one now faces is - given a power series which converges and represents a function for values of z within the circle of convergence, can we find by means of it the value of the function for values of z outside the circle of convergence? The answer to this is yes and for this purpose let us choose a point P_1 within the circle of convergence which does not lie in between P and A on the line PA. From the given series we can find the value of the function and all its derivatives at P_1 and consequently build a Taylor series with P_1 as the origin. This new series will now define a function analytic within some other circle with P_1 as centre. This circle will extend to the singularity which is nearest to P_1 and this may or may not be A. In either of the cases, this new circle will have some region which lie partly outside the old

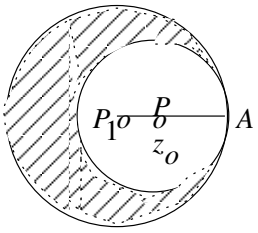


Figure 4: Pictorial representation of analytic continuation of a function. The unshaded portion is the region of the complex plane within which the function is analytic. The shaded portion is the region where the function is analytically continued.

circle of convergence. For points within this region the new series may be used to define the value of the function, although the old series could not be used to do so. This process can be continued and the process is known as *analytic continuation.*

To illustrate the process of analytic continuation let us consider the expansion of $f(z) = \dfrac{1}{(1-z)}$ about $z_0 = 0$, which can be written as

$$f(z) = \frac{1}{(1-z)} = 1 + z + z^2 + z^3 + \cdots \tag{48}$$

The function has a singularity at $z = 1$ and hence the radius of convergence of the series is 1 and the function is analytic for $|z| < 1$. The above series cannot be used to find the value of the function for $z = -\frac{5}{4}$. But, using this series we can evaluate the function and all its derivatives for, say, $z = -\frac{3}{4}$ and find the Taylor series expansion about $z = -\frac{3}{4}$ which can be written as

$$\frac{4}{7}\left[1 + \frac{4}{7}\left(z + \frac{3}{4}\right) + \left(\frac{4}{7}\right)^2\left(z + \frac{3}{4}\right)^2 + \left(\frac{4}{7}\right)^3\left(z + \frac{3}{4}\right)^3 + \cdots\right]$$

and the radius of convergence of this series is $\frac{7}{4}$ and its center is at $z = -\frac{3}{4}$. The point $z = -\frac{5}{4}$ lie within this circle and we can use the above series for finding the value of the function at $z = -\frac{5}{4}$ and this is given by

$$\frac{4}{7}\left[1 + -\frac{2}{7} + \left(\frac{2}{7}\right)^2 - \left(\frac{2}{7}\right)^3 + \cdots\right] = \frac{4}{7}\,\frac{1}{1+\frac{2}{7}} = \frac{4}{9}$$

and agrees with the value of the function $\frac{1}{(1-z)}$ at $z = -\frac{5}{4}$. Though the original series could be used to find the value of the function for $z = -\frac{5}{4}$, we can use the series subsequently obtained, to find the value by the process of analytic continuation. There are various ways by which the *sum* of a divergent series can be evaluated. We consider a few of them in the subsequent sections.

2.7.2 Borel's Method of Summatiom

Let

$$f(z) = \sum_0^\infty a_n z^n$$

be analytic for $|z| \leq r$.

Let us define

$$\phi(z) = \sum_0^\infty \frac{a_n}{n!} z^n$$

and consider the function

$$f_1(z) = \int_0^\infty e^{-t} \phi(zt)\, dt$$

This integral is an analytic function for $|z| < r$. Integrating by parts we get

$$\begin{aligned} f_1(z) &= \left[-e^{-t}\phi(zt)\right]_0^\infty + z\int_0^\infty e^{-t}\phi'(zt)\, dt \\ &= \left[-e^{-t}\phi(zt)\right]_0^\infty + \left[-ze^{-t}\phi'(zt)\right]_0^\infty + z^2\int_0^\infty e^{-t}\phi''(zt)\, dt \\ &= \sum_{n=0}^m \left[-z^n e^{-t}\phi^{(n)}(zt))\right]_0^\infty + z^{m+1}\int_0^\infty e^{-t}\phi^{(m+1)}(zt)\, dt \\ &= \sum_0^\infty a_n z^n = f(z), \end{aligned} \tag{49}$$

as

$$Lt_{t\to 0} e^{-t}\phi^{(n)}(zt) = a_n$$

and

$$Lt_{t\to\infty} e^{-t}\phi^{(n)}(zt)) = 0 \quad \text{for } |z| < r$$

Consequently

$$f(z) = \int_0^\infty e^{-t}\phi(zt)\, dt \tag{50}$$

where $\phi(z) = \sum_0^\infty \frac{a_n}{n!} z^n$ is called the *Borel function* [6] associated with $\sum_0^\infty a_n z^n$.

Thus if

$$S = \sum_0^\infty a_n z^n \quad \text{and} \quad \phi(z) = \sum_0^\infty \frac{a_n}{n!} z^n,$$

we can demonstrate that

$$S = \int_0^\infty e^{-t}\phi(zt)\, dt \tag{51}$$

and the series is said to be *Borel summable*. It may be mentioned that the integral represents an analytic function in a more extended region than the interior of the circle $|z| = r$ and gives the analytic continuation of the function.

To illustrate this, let us consider once more the series

$$S = 1 + z + z^2 + z^3 + \cdots = \sum_{i=0}^{\infty} z^i. \tag{52}$$

The Borel function associated with the series is given by

$$\phi(z) = \sum_{0}^{\infty} \frac{z^n}{n!} = e^z$$

and hence the Borel sum of the series can be written as

$$f(z) = \int_0^{\infty} e^{-t}\phi(zt)\, dt = \int_0^{\infty} e^{-t(1-z)} dt = \frac{1}{1-z} \tag{53}$$

2.7.3 Application of NonlinearTransforms on Divergent Series

Let us consider the divergent geometric series

$$S = 1 + 2 + 4 + 8 + 16 + \cdots$$

which is *Borel summable*, the sum being -1.

The simplest nonlinear transform is the Aitken's Δ^2-transformation. To apply the Δ^2-transform on it we note that the first three terms of the sequence of partial sums are

$$S_1 = 1; \;\; S_2 = 3; \;\; S_3 = 7.$$

The Δ^2-transform , when applied to this sequence, gives for the limit

$$S = \frac{\frac{1}{2} - \frac{3}{4}}{\frac{1}{2} - \frac{1}{4}} = -1$$

This is not surprising as we have already noted that the Δ^2-transform *sums* a geometric series exactly. •◁

Finding $\zeta(s)$ for arbitrary s

We consider the series for $\zeta(2)$ as a prototype example. The power of these nonlinear transforms is better demonstrated by considering the series $\zeta(s)$ in general. Using these transforms it is possible to obtain an expression for $\zeta(s)$ which is valid for a wide range of s. The series for $\zeta(s)$, as given by equation-3, when written explicitly is as follows:

$$\zeta(s) = 1 + \frac{1}{2^s} + \frac{1}{3^s} + \frac{1}{4^s} + \frac{1}{5^s} + \cdots$$

This series is of interest because of the fact that for $s > 1$ it is convergent and for $s < 1$ it is a divergent one and is *summable*. For $s = 1$, it is divergent and is not *summable*. In fact,

$$\zeta(-2m) = 0; \qquad \zeta(1-2m) = -\frac{B_{2m}}{2m},$$

and

$$\zeta(2m) = (-1)^{m+1} 2^{2m-1} \pi^{2m} \frac{B_{2m}}{(2m)!} \qquad m = 1, 2, 3 \cdots,$$

where B_m's are the Bernoulli numbers which are defined as $\frac{x}{e^x-1} = \sum_{n=0}^{\infty} B_n \frac{x^n}{n!}$. It can be shown that except B_1all other odd B_n's are zero. The first few of the even Bernoulli numbers are as follows:

$B_0 = 1$,$B_1 = -\frac{1}{2}$, $B_2 = \frac{1}{6}$, $B_4 = -\frac{1}{30}$, $B_6 = \frac{1}{42}$, $B_8 = -\frac{1}{30}$, $B_{10} = \frac{5}{66}$, $\cdots$.

To obtain an expression for $\zeta(s)$ we start with the series for $\eta(s)$, which is given by

$$\eta(s) = 1 - \frac{1}{2^s} + \frac{1}{3^s} - \frac{1}{4^s} + \frac{1}{5^s} - \cdots$$

and use the relation between $\zeta(s)$ and $\eta(s)$, which can be written as

$$\eta(s) = \left(1 - \frac{1}{2^{s-1}}\right) \zeta(s).$$

Using the τ-transform of order 4, which requires only five terms of the series, one can build an approximate expression for $\eta(s)$, which is given by

$$\eta(s) \simeq \tau_4 = \frac{1 + 16\ 2^s\ S_2 + 60\ 3^s\ S_3 + 80\ 4^s\ S_4 + 35\ 5^s\ S_5}{1 + 16\ 2^s + 60\ 3^s + 80\ 4^s + 35\ 5^s}. \tag{54}$$

In the above expression S_n's are the partial sums of the series for $\eta(s)$, *i.e.,*

$$S_1 = 1, \quad S_2 = 1 - 2^{-s}, \quad S_3 = 1 - 2^{-s} + 3^{-s}, \quad \cdots$$

The coefficients in the expression given by equation-54 are the product of $\binom{k}{j}$ and $(j+1)_{k-1}$ with j running from 0 to k, where k is the order of the transform.

The expression for $\zeta(s)$ can thus be written as

$$\begin{aligned} \zeta(s) \quad \simeq \quad & \left(\frac{2^{s-1}}{2^{s-1}-1}\right) \times \\ & \frac{1 + 16\ 2^s\ S_2 + 60\ 3^s\ S_3 + 80\ 4^s\ S_4 + 35\ 5^s\ S_5}{1 + 16\ 2^s + 60\ 3^s + 80\ 4^s + 35\ 5^s}. \end{aligned} \tag{55}$$

It can be easily verified that for $s = 0, -1, -2$ the above expression reduces respectively to $-\frac{1}{2}$, $-\frac{1}{12}$ and 0, which are exact values of $\zeta(s)$ for the above values of s, though the series is formally divergent for these values of s. For other values of s, the expression reproduces the function approximately. For example,

the values of $\zeta(2)$ and $\zeta(4)$ obtained from the expression are respectively are 1.64493257 and 1.08232256, the exact values being $1.644934066848227\cdots$ and $1.082323233711138\cdots$. The accuracy of the values obtained from the expression increases as one considers large positive values of s. The expression reproduces the function with sufficient accuracy even for s close to 1. For example, with $s = 1.001$ the expression gives the value 1000.5809, the correct value being 1000.5773. However, for large negative values of s the function is not well reproduced by the expression. The same expression can, however, be used to evaluate $\zeta(s)$ for large negative s, if one agrees to use the remarkable result due to Riemann [6]

$$\zeta(1-s) = \pi^{-s} 2^{1-s} \Gamma(s) cos\left(\frac{s\pi}{2}\right) \zeta(s) \tag{56}$$

Thus, if one evaluates $\zeta(-19)$ from the above expression using the value of $\zeta(20)$ calculated from equation- 55 one obtains the value 26.45621212121212243, which is correct to eighteen digits! If one needs higher accuracy one can build a higher order transform which is easy to build. Again, one can use equation- 55 to find $\zeta'(0)$and this gives -0.918950, the exact value being $-\frac{1}{2}\ln(2\pi) = -0.918939$.

3 Global Approximations for Functions

3.1 Global Padé Approximants

In this section we focus our attention to the approximation of functions for which asymptotic expansions are available and illustrate that good approximants for the functions can be constructed which are valid for the entire range of the variable even when the body of apriori information appears at the out set to be quite small and refer these as global approximants. An early review of global Padé approximation is given by Frost and Harper [27]. Some recent works on two-point and multi-point approximants can be found in references [28-31] and references cited therein.

If the power series expansion of a function $f(z)$ s known, one can construct the $[n/m]$ Padé approximant for the function..

In the usual Padé approximants n and m can have any value. However, for a global Padé approximant and this is restricted and n and m are related and nature of the relation depends on the nature of the asymptotic expansion of the function.

Let us now assume that we have, in addition, an asymptotic expansion for $f(z)$ in the form

$$f(z) \sim b_0 + b_1 y + b_2 y^2 + \cdots, \tag{57}$$

where $y = 1/z$. This suggests that the degree of the polynomials of the numerator and denominator of the $[n/m]$ Padé approximant should be the same, *i.e.*, $n = m$. Thus the global approximant for the function should be of the following form:

$$f(z) \simeq [n/n] = \frac{P_n(z)}{Q_n(z)} = \frac{p_0 + p_1 z + \cdots + p_n z^n}{1 + q_1 z + \cdots q_n z^n}. \tag{58}$$

The problem is to determine the $(2n+1)$ unknown constants. We want to fix the constants in such a way that the first few terms of both the expansions agree. The total coefficients that can be made to agree is obviously $(2n+1)$. If we impose that the first r $(r < n)$ coefficients of the expansion of $[N/N]$ should agree with those of the series expansion of $f(z)$, then the set of r equations are given by

$$\sum_{i=0}^{j} a_{j-i}\, q_i = p_j, \qquad j = 0,\ 1,\ 2, \cdots, r-1. \tag{59}$$

To obtain the rest set of unknown coefficients, we recast equation-58 in the following form by dividing both the numerator and denominator by z^n and is given by

$$[n/n] = \frac{p_n + p_{n-1} y + \cdots + p_0 y^n}{q_n + q_{n-1} y + \cdots + y^n} \tag{60}$$

and the rest set of equations now reduce to

$$\begin{aligned}
\sum_{i=0}^{j} b_{j-i} q_{n-i} &= p_{n-j}, \qquad j = 0,\ 1,\ 2, \cdots, n \\
\sum_{i=0}^{j} b_{j-i} q_{n-i} &= 0, \qquad j = n+1,\ n+2, \cdots, n-r\,.
\end{aligned} \tag{61}$$

Equations-59 and 61 together constitute a set of $(2n+1)$ linear equations which can be solved for the set $\{p_i\}$ and $\{q_i\}$. With these values for the coefficients, equation-58 represents a global Padé approximant for the function.

If $r > n$, then the set of equations from which the unknown coefficients are to be determined are given by

$$\begin{aligned}
\sum_{i=0}^{j} a_{j-i}\, q_i &= p_j, \qquad j = 0,\ 1,\ 2, \cdots, n \\
\sum_{i=0}^{j} a_{j-i}\, q_i &= 0, \qquad j = n+1,\ n+2, \cdots, r \\
\sum_{i=0}^{j} b_{j-i}\, q_i &= p_{n-i}, \qquad j = 0,\ 1,\ 2, \cdots, 2n+1-r.
\end{aligned} \tag{62}$$

It may be mentioned here that for different choice of r one obtains different global approximants. The value of r for which a global approximant will reproduce the function over the entire range with maximum accuracy depends, in general, on the function to be approximated.

If it happens that b_0 in the asymptotic expansion given by equation-57 is zero, so that the first term in the asymptotic expansion is $y\left(\frac{1}{z}\right)$, then in the global Padé approximant the order of the polynomial in the denominator should be higher by one than that of the numerator and the approximant will be $[N/N+1]$ Padé approximant. The $(2n+2)$ unknown coefficients can be determined in a way similar to that outlined above.

In some situations, as we shall encounter frequently, the asymptotic expansion is given by

$$\begin{aligned} f(z) &\sim b_{-1}z + b_0 + b_1\frac{1}{z} + b_2\frac{1}{z^2} + \cdots \\ &= b_1\frac{1}{y} + b_0 + b_1 y + b_2 y^2 + \cdots . \end{aligned} \tag{63}$$

In such a situation, the global approximant will be a $[N/N-1]$ Padé approximant.

The large-z expansion of a function $f(z)$ is not necessarily in the form of a series in $1/z$ as we shall encounter later. The method of obtaining global approximants in such situations will be explained in specific cases subsequently.

Consider the function $f(z) = \sqrt{(1+z^2)}$. For small z, one can make the series expansion

$$f(z) == 1 + \sum_{n=1}^{\infty} (-)^{n+1} \frac{(2n-2)!}{n!\,(n-1)!\,2^{2n-1}} z^{2n} = 1 + \frac{z^2}{2} - \frac{z^4}{8} + \cdots .$$

Alternatively, we can write

$$f(z) = z\sqrt{1+\frac{1}{z^2}} = z\left(1 + \frac{1}{2z^2} - \frac{1}{8z^4} + \cdots\right) = \frac{1}{y} + \frac{y}{2} - \frac{y^3}{8} + \cdots .$$

A very similar set of expansion can be obtained with a simple quantum mechanical two state system [32] with the Hamiltonian $H = \sigma_x + \lambda\sigma_z$, where σ's are the Pauli matrices and λ is the coupling constant, For small λ ($\lambda << 1$), the σ_z term may be treated by perturbation. Alternatively, for large λ ($\lambda >> 1$), the Hamiltonian can be written as $H = \lambda(\sigma_z + 1/\lambda\,\sigma_x)$, and the σ_x term can be treated by perturbation. Considering perturbation up to second order, the eigenvalues are respectively given by $1+\frac{\lambda^2}{2}$ and $\lambda+\frac{1}{2\lambda}$ and has the same structure as that of the series considered above.

The global Padé approximant will be of the form $[N/N-1]$. It is found that global approximants, which uses almost equal number of terms of both the series, better reproduces the function. Two such global Padé approximants for the function are as follows:

$$
\begin{aligned}
g[4/3] &= \frac{1+2z+\dfrac{5z^2}{2}+2z^3+z^4}{1+2z+2z^2+z^3}, \\
g[5/4] &= \frac{1+\dfrac{5z}{2}+\dfrac{15z^2}{4}+\dfrac{15z^3}{4}+\dfrac{5z^4}{2}+z^5}{1+\dfrac{5z}{2}+\dfrac{13z^2}{4}+\dfrac{5z^3}{2}+z^4}.
\end{aligned}
$$

The maximum error for $g[4/3]$ is about 0.17% and that for $g[5/4]$ is 0.03%.

The large-z expansion of a function $f(z)$ is not necessarily in the form of a series in $1/z$. For example,

$$
\int_0^x e^{t^2} dt \sim \frac{1}{2x} e^{x^2} \left[1 + \frac{1}{2x^2} + \frac{1.3}{(2x^2)^2} + \cdots \right], \qquad x \to +\infty
$$

$$
\int_0^\infty \frac{1}{1+xt} dt \sim \frac{\ln x}{x}, \qquad x \to +\infty
$$

The method of obtaining a two-point approximants in such situations will depend on the specific case.

The elliptic integral of the second kind is given by

$$
E(m) = \int_0^{\pi/2} \left(1 - m \sin^2 \theta\right)^{1/2} d\theta. \tag{64}
$$

Expanding the integrand, the above integral can be expanded in a power series in m and is given by

$$
s = \frac{\pi}{2} \left(1 - \left(\frac{1}{2}\right)^2 \frac{m}{1} - \left(\frac{1.3}{2.4}\right)^2 \frac{m^2}{3} - \left(\frac{1.3.5}{2.4.6}\right)^2 \frac{m^3}{5} - \cdots \right). \tag{65}
$$

A global approximant for $E(m)$ can be obtained by noting that $E(m)$ goes to zero at $m = 1$ like $(1-m)^\gamma$, where γ is close to 1. If we choose $\gamma = \frac{9}{10}$, then the series for $(1-m)^{9/10}$ is

$$
s_1 = 1 - \frac{9m}{10} - \frac{9m^2}{200} - \frac{33m^3}{2000} - \frac{693m^4}{4000000} - \cdots
$$

We form the approximants $g[2/2]$ and $g[3/3]$ with the series $s - s_1$and these are as follows:

$$
g[2/2] = \frac{0.57079633 + 0.18511797m - 0.31720338m^2}{1 - 0.56444468m - 0.0039050662m^2}.
$$

$$g[3/3] = \frac{0.57079633 - 0.13162639m - 0.44028279m^2 + 0.15678251m^2}{1 - 1.11936129m + 0.27365505m^2 + 0.00015442699n^3}$$

The sums of the approximants and $(1-m)^{9/10}$ will be representations of the function. The approximants reproduce the function over the entire range fairly accurately. $\bullet\triangleleft$

3.2 Global Approximants with Levin-like Transforms

To construct a Levin-like transform of order k, one needs $k+1$ terms of the original series. In these transforms β is a free parameter and the first $(k+1)$ terms of the series expansion of any of the above transforms of order k agree with the first $(k+1)$ terms of the series which are used as input for any value of β. Thus one can choose the value of β conveniently in different situations so as to obtain a better representation of the function.

In the global Padé approximant, the order of the polynomial in the numerator may be equal, less than or greater than that of the denominator, depending on the nature of the asymptotic series. A Levin-like transform of order k gives an approximant in the form of a rational function of which the orders of the polynomials in the numerator and denominator are respectively $k-1$ and k. It thus seems that one can construct a global approximant with a Levin-like transform only for those functions for which the asymptotic expansion starts with $y = 1/z$. Another problem with these transforms is that the coefficients of the polynomials in the numerator and the denominator of the approximants are nonlinear functions of the coefficients of the series expansion of the function. With this in mind, we now demonstrate how one can obtain global approximants for different functions.

If the series is given by equation $f(z) = \sum_{n=0}^{\infty} a_n z^n$ and the asymptotic expansion of the function starts with $y = 1/z$, then to obtain a global approximant of order k we start with the series

$$a_0 + a_1 z + a_2 z^2 + \cdots + a'_{k-n} z^{k-n} + \cdots + a'_k z^k.$$

Out of the $k+1$ terms, needed to construct a transform of order k, the first $k-n$ terms correspond to the first $k-n$ terms of the usual series expansion of the function and the primed coefficients of the subsequent terms are still to be determined from the asymptotic expansion of the function. We now construct an approximant of order k with the above series, replace z by $1/y$ and make a series expansion of the resulting expression about $y = 0$. The coefficients of y in this expansion will involve a''s and equating the first $n+1$ coefficients with those of the asymptotic expansion of the function one can determine the $n+1$ unknown coefficients. These equations are, in general, nonlinear and can have more than one set of solution. When one substitutes the values of the a''s in the approximant, one obtains a global approximant with a Levin-like transform. It may so happen that the approximant globally represents the function for more than one solution set. On the other hand, one can have a solution set with which the approximant does not globally represent the function.

Alternatively, as the constant term b_0 in the asymptotic expansion-57 is absent, one can start with the series

$$b_1 y + b_2 y^2 + \cdots + b'_{k-n+1} y^{k-n+1} + \cdots + b'_{k+1} y^{k+1},$$

where the b's are the coefficients of the asymptotic series and the b''s are still to be determined. One can construct an approximant with the above series and the orders of the polynomials in the numerator and denominator are equal. However, the constant term in the numerator will be absent. We now replace y by $1/z$ in this approximant, expand it about $z = 0$ and equate the coefficients of this with those of the usual expansion of the function. This gives a set of nonlinear equations in b''s . Substituting the values of b''s in the approximant one obtains a global approximant for the function.

The construction of global approximants with Levin-like transforms is not as straightforward as in the case of Padé approximants. With Levin-like transforms there may not be a single successful method, and one has to tailor the global approximant to the properties of the available expansions. That this should be possible in most cases is illustrated in [34]

Global Approximant for the Integral $\mathbf{I\,(m) = \int_0^\infty e^{-x^2-m^4x^4} dx}$

Consider the integral $I\,(m) = \int_0^\infty e^{-x^2-m^4x^4} dx$ which one encounters in a mechanical model for quantum field theory [33]. Expanding $e^{-m^4x^4}$ and integrating term by term one gets

$$s = 1 - \frac{3}{4}m^4 + \frac{105}{32}m^8 - \frac{3465}{128}m^{12} + \cdots$$

where $I\,(m) = \dfrac{\sqrt{\pi}}{2}s$. The above series is a Stieltjes series and is formally divergent with zero radius of convergence. The asymptotic expansion for the integral can be obtained by expanding e^{-x^2} and integrating term by term. The asymptotic series for $\dfrac{2}{\sqrt{\pi}} I\,(m)$ is given by

$$s_1 = 1.022766y - 0.345684y^3 + 0.255691y^5 - 0.259265y^7 + 0.319614y^9 - \cdots$$

where $y = 1/m$. To obtain a global approximant with the τ-transform, we start with the series

$$1.02276567y + a_1 y^3 + a_2 y^5 + a_3 y^6 + a_4 y^7$$

and construct a τ-approximant of order 4 and adjust the constants so the series expansion of the approximant agrees with s. With $\beta = 20$ this gives $a_1 = -1.611880$, $a_2 = 2.810072$, $a_3 = -1.871834$ and $a_4 = 0.917793$. The value of β is adjusted so that better agreement is obtained over the entire range. The global τ_4-approximant is given by

$$g_{\tau_4} = \frac{\sqrt{\pi}}{2}\left(\frac{1 + 2.729969m^3 + 2.871267m^4 + 1.497256m^5}{1 + 2.729969m^3 + 2.669202m^4 + 2.807355m^5 + 1.463929m^6}\right).$$

This approximant reproduces the integral over the entire range. $\bullet\triangleleft$

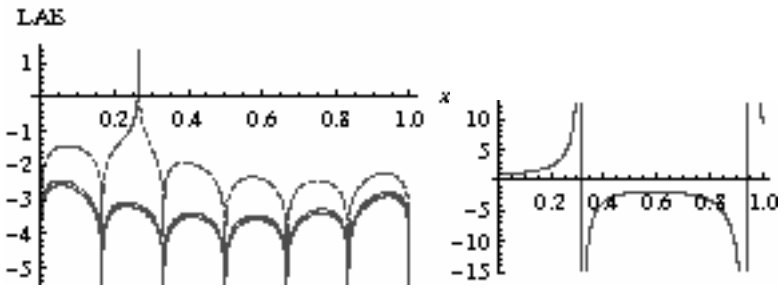


Figure 5: Figure on the left shows the logarithm (to the base 10) of the absolute error (LAE) for different interpolants for $e^x \cos(5x)$. Solid line - τi_4; dotted line - ui_4 and the dashed line - $r22$. Figure on the right shows the plots of $e^x \sec(5x)$ and the reciprocal of τi_6.

4 Applications to Numerical Analysis

4.1 Interpolation using Levin and Weniger transforms

In numerical computation one often has to approximate functions. The need arises when a function is known in the form of a table of values and one needs some closed form of representation so that required manipulations like differentiation and integration can be performed. Another reason for this approximation could be that the function may be defined implicitly and an analytical expression is too complicated to evaluate. The most commonly used interpolation methods are the polynomial interpolations of Newton and Lagrange or interpolation by continued fraction can be found in [37].

For interpolation with the Levin-Weniger transforms, one faces a set of nonlinear equations for the coefficients a_j's and poses a formidable problem. The problem was solved by the method of successive expansion and multi-point Levin-Weniger approximants can be obtained [36].

As an example, we consider the function $e^x \sec(5x)$, which is the reciprocal of the function $e^{-x} \cos(5x)$ and has two poles between $(0, 1)$. The interpolation formula for $e^{-x} \cos(5x)$ using the u and τ-transforms of order 6 are given by

$$ui_6 = \frac{1 + 0.2826x - 10.5612x^2 - 14.2329x^3 + 48.1575x^4 - 24.1517x^5}{1 + 1.4461x + 0.6895x^2 + 1.8020x^3 - 0.2907x^4 + 0.08981x^5 + 0.0006320x^6}$$

$$\tau i_6 = \frac{1 + 0.1027x - 10.8847x^2 - 9.1138x^3 + 39.7509x^4 - 20.3830x^5}{1 + 1.2220x + 0.7312x^2 + 1.5271x^3 - 0.2241x^4 + 0.02596x^5 + 0.007901x^6}.$$

Table 6: Determination of the unstable fixed point of the functional iteration given by equation-66 using the u_2-transform (with $\omega_n = \Delta S_n$).

		$\mu = 1$	$\mu = 2$	$\mu = 3$	$\mu = 4$	$\mu = 5$
Seed	$x_1^{(\mu)}$	5.0	$0.519\cdots$	$0.423\cdots$	$0.42924\cdots$	$0.4293823\cdots$
	$x_2^{(\mu)}$	$9.4\cdots$	$0.582\cdots$	$0.419\cdots$	$0.42915\cdots$	$0.42938234\cdots$
	$x_3^{(\mu)}$	$18.4\cdots$	$0.694\cdots$	$0.412\cdots$	$0.42901\cdots$	$0.42938228\cdots$
	$x_4^{(\mu)}$	$36.3\cdots$	$0.889\cdots$	$0.402\cdots$	$0.42877\cdots$	$0.42938217\cdots$
Limit		$0.519\cdots$	$0.423\cdots$	$0.4292\cdots$	$0.4293823\cdots$	$0.42938244899455\cdots$

The rational interpolant with the same number of inputs is

$$r33 = \frac{1 - 7.8775x + 18.8132x^2 - 12.2693x^3}{1 - 5.7881x + 9.7591x^2 - 8.1674x^3}.$$

Reciproals of these interpolants give the interpolant for $e^x \sec(5x)$. Figure- 5 shows the plots of the logarithm (to the base 10) of the absolute error for these interpolants as well as the function. It may be mentioned that the rational interpolant $r33$ gives a pole at about $x = 0.25$. A plot of the reciprocal of τi_6 and $e^x \sec(5x)$ is also shown in the figure- 5.

One great disadvantage of the rational interpolants is that they give, in some cases, spurious poles even if the function itself has no pole. For example, the rational interpolants. R_{11}, R_{33} and R_{55} for the function $e^{-x}\cos 5x$ predict poles at 0.284305, 0.264782 and 0.977217 respectively in the range (0,1). As the Padé-type rational interpolants is unique for a given number of interpolating points, it is not possible to remove the poles without changing the interpolating points. For interpolants with Levin-like transforms, the situation is favourable as one has the free parameter β to remove the poles.

4.2 Finding Roots Using Divergent Iteration

As we have found that we can find the sum of a divergent series using the convergent accelerating transforms, we can find the root of an equation even when the functional iteration diverges by using these transforms [38]

Consider the functional iteration

$$x_{n+1} = \frac{1}{4}\ln\left(\cosh^2(2x_n)\,\cosh(4x_n)\right) \tag{66}$$

The two stable fixed points of this functional iteration are 0 and ∞, there being an unstable one at $0.42938244899456\ldots$. . A trial value less than this moves towards zero through successive iterations, while a value greater than this moves towards infinity. However, let us start with an arbitrary initial value of $x_1^{(1)} = 5$. Then the numbers of the sequence $\{x_n^{(1)}\}$ generated by the iteration scheme are shown in table-6. The limit at the bottom of each column is the value obtained by the application of u_2-transform (with $\omega_n = \Delta S_n$)on the four

values in that column. We use this limit as the initial value for the next stage of iteration. As can be seen from the table , the repetition of this procedure very quickly leads to the desired fixed point starting from a wide range of initial values. In the present case five successive applications of the procedure enables one to determine the unstable fixed point to the limit of available precision (to 14 digits in the present case). The number of successive applications of the procedure needed to obtain the limit depends, to some extent, on the initial choice of the seed.

4.3 Numerical Integration and Convergence Accelerating Transforms

The Riemann sum (mid-point rule) for an integral is defined as

$$\int_a^b f(x)\,dx \approx R_n = h\sum_{r=0}^{n-1} f\left(a+(2r+1)\,\frac{h}{2}\right) \tag{67}$$

where $h = \dfrac{(b-a)}{n}$. One can, however, define the sequence in a number of other ways. For example, instead of the midpoint rule one can use the simple Riemann sum. If the convergence is too slow, one can apply the iteration of the the transforms to obatin an accurate result.

Evaluating Highly Oscillating Integrals

Consider another integral

$$I = \int_{-\infty}^{\infty} \sin\left(x^2+x\right)dx = 0.904276756189027. \tag{68}$$

We divide the integral into two parts as follows:

$$I = I' + I'' = \int_{-\infty}^{0} \sin\left(x^2+x\right)dx + \int_{0}^{\infty} \sin\left(x^2+x\right)dx. \tag{69}$$

The zeros of the integrand are given by the roots of the equating $x^2+x-n\pi=0$ and are as follows:

Roots	for $x \leq 0$	Roots	for $x \geq 0$
n	x	n	x
0	0	0	0
1	-1.0	1	1.34162772
2	-2.34162772	2	2.05600965
3	-3.05600965	3	2.61043051
4	-3.61043051	4	3.07999590
5	-4.07999590	5	3.49471953
6	-4.49471953	6	3.87030387
7	-4.87030387	7	4.21605222
8	-5.21605222	8	4.53812874
9	-5.53812874	9	4.84081772
10	-5.84081772	10	5.12724858

We can now integrate between successive zeros and as the integrand is oscillating these alternate in sign. The values of the integral between successive zeros for $x \leq 0$ are

-0.16547919	0.79441336	-0.45220196	0.35222622	-0.29861682
0.26386470	-0.23898612	0.22004145	-0.20499203	0.19266241

and those for $x \geq 0$ are

0.79441336	-0.45220196	0.35222622	-0.29861682	0.26386470
-0.23898612	0.22004145	-0.20499203	0.19266241	-0.18232071

The partial sums of these forms sequences and results of applying the $\tau-$transform (with $\beta = 0$) of different orders on the sequences are as follows:

tr. ord.	2	3	4	5	6	7
$x \leq 0$	0.189	0.329	0.3622	0.3681	0.36917	0.369359
$x \geq 0$	0.534	0.535	0.5349	0.5349	0.53487	0.534878
Total	0.723	0.864	0.8971	0.9030	0.90404	0.904237

Using twenty partial sums one can evaluate the integral accurate up to twelve significant digits. •◁

4.4 Definite integrals involving parameters

Consider the example

$$g(a) = \int_0^a \tan x dx \tag{70}$$

where a has a value close to $\frac{\pi}{2}$. It is difficult to evaluate this integral by any standard quadrature when a is close to $\frac{\pi}{2}$, as the integrand increases rapidly near $\frac{\pi}{2}$ and goes to infinity at $\frac{\pi}{2}$. Though the integrand is continuous over

the range for any value of a ($a < \frac{\pi}{2}$), the singularity at $\frac{\pi}{2}$ results in a very slow convergence. In fact, the evaluation of $\tan x$ close to the singularity will involve a significant round-off error and a slight error in calculating the abscissas will cause a significant error in the function values. It is well known that an approximant, built from a series expansion of the function, reproduces the function better near the point about which the expansion is made. As the integrand has very large value near $\frac{\pi}{2}$, the integral will be better evaluated if we approximate the integrand by a series or an approximant which reproduces it better near $\frac{\pi}{2}$. We, thus, make a Laurent expansion of $\tan x$ and is given by

$$\tan x = \frac{1}{\left(\frac{\pi}{2}-x\right)} - \frac{\left(\frac{\pi}{2}-x\right)}{3} - \frac{\left(\frac{\pi}{2}-x\right)^3}{45} - \frac{2\left(\frac{\pi}{2}-x\right)^5}{945} - \frac{\left(\frac{\pi}{2}-x\right)^7}{4725} - \frac{2\left(\frac{\pi}{2}-x\right)^9}{93555} - \ldots \tag{71}$$

Integrating equation-71 term by term we get

$$\int \tan x dx = -\ln\left(\frac{\pi}{2}-x\right) + \frac{\left(\frac{\pi}{2}-x\right)^2}{6} + \frac{\left(\frac{\pi}{2}-x\right)^4}{180} + \frac{\left(\frac{\pi}{2}-x\right)^6}{2835} + \ldots$$

Putting the limits we have

$$\begin{aligned} g(a) &= \int_0^a \tan x dx \approx \ln\left(\frac{\pi}{(\pi-2a)}\right) + \frac{1}{6}\left(\left(\frac{\pi}{2}-a\right)^2 - \left(\frac{\pi}{2}\right)^2\right) \\ &+ \frac{1}{180}\left(\left(\frac{\pi}{2}-a\right)^4 - \left(\frac{\pi}{2}\right)^4\right) \\ &+ \frac{1}{2835}\left(\left(\frac{\pi}{2}-a\right)^6 - \left(\frac{\pi}{2}\right)^6\right) + \ldots \end{aligned} \tag{72}$$

This series is highly convergent for values of a near $\frac{\pi}{2}$ and a few terms of the series is good enough to reproduce the integral up to a few decimal places. If we leave aside the first term and form an approximant of order 2 with the τ-transform ($\beta = 0$) and then put the limits, we obtain the following expression for the integral

$$\begin{aligned} \int_0^a \tan x \, dx &= \ln\left(\frac{\pi}{(\pi-2a)}\right) + \frac{1890(\frac{\pi}{2}-a)^2 - 97(\frac{\pi}{2}-a)^4}{4\left(2835 - 240(\frac{\pi}{2}-a)^2 + 2(\frac{\pi}{2}-a)^4\right)} \\ &\quad - \frac{1890(\frac{\pi}{2})^2 - 97(\frac{\pi}{2})^4}{4\left(2835 - 240(\frac{\pi}{2})^2 + 2(\frac{\pi}{2})^4\right)} \\ &= \ln\left(\frac{\pi}{(\pi-2a)}\right) - 0.4515349995 \\ &\quad + \frac{1890(\frac{\pi}{2}-a)^2 - 97(\frac{\pi}{2}-a)^4}{4\left(2835 - 240(\frac{\pi}{2}-a)^2 + 2(\frac{\pi}{2}-a)^4\right)} \end{aligned} \tag{73}$$

Table 7: Values of the integral $\int_0^a \tan x dx$ obtained from equation-72 and those obtained by the τ_2-approximant given by equation-73 .

a	exact value	eqn. 72	eqn. 73
0.5	0.130584	0.121969	0.130567
0.7	0.268086	0.258066	0.268106
0.9	0.475424	0.464717	0.475489
1.1	0.790548	0.779533	0.790604
1.3	1.318640	1.307544	1.318693
1.5	2.648784	2.637678	2.648832
1.57	7.135501	7.124395	7.135549

It is seen from table-7 that the expression given by 73, which uses only three terms of the direct series excepting the first term, is a much fairly good representation of the integral.. One advantage of the approaches discussed here is that one obtains an expression for the integral in a closed form in terms of the parameter a and this may greatly simplify the manipulation with the parameter.

Approximate closed form for Bose-Einstein and Fermi-Dirac integrals using Levin-like transforms has been developed by Bhagat *et, al* [39] . These are utilized to obtain closed form expressions for generalized Bose-Einstein and Fermi-Dirac integrals. With these expressions it is possible to obtain values for the integrals to an accuracy of 5 to 8 significant digits with low order transforms, the added advantage being that these results are amenable to analytic manipulations.

4.5 Summing a Fourier Series

One needs a large number of terms to evaluate a periodic function by directly summing the Fourier series corresponding to the function. We have already mentioned that the nonlinear sequence transforms can find the limit of a sequence of complex numbers. This is well illustrated by summing a Fourier series by a nonlinear sequence transform.

Let us consider a periodic function

$$\begin{aligned} f(x) &= x, \qquad 0 < x < 1 \\ &= (x-2) \quad 1 < x < 2. \end{aligned} \tag{74}$$

The Fourier series expansion of the function is given by

$$f(x) = \frac{2}{\pi} \sum_{n=1}^{\infty} (-)^{n+1} \frac{\sin(n\pi x)}{n} \tag{75}$$

We note that

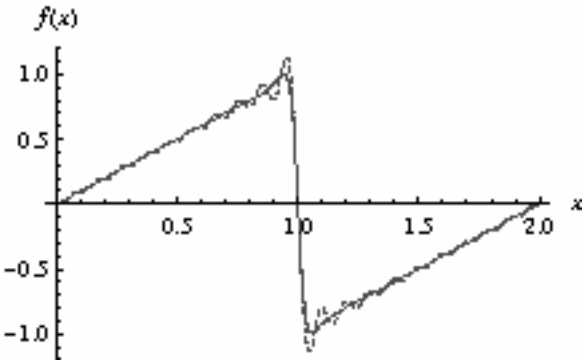


Figure 6: τ_3-approximant along with the direct sum of 20 terms of the series given by equation- 75 for the function given by equation -74.

$$\begin{aligned} f(x) &= \mathrm{Im}\left[\frac{2}{\pi}\sum_{n=1}^{\infty}(-)^{n+1}\,\frac{e^{in\pi x}}{n}\right] \\ &= \mathrm{Im}\left[\frac{2}{\pi}\sum_{n=1}^{\infty}(-)^{n+1}\,\frac{y^n}{n}\right] = \mathrm{Im}\left[\frac{2}{\pi}S\right] \end{aligned} \tag{76}$$

where $y = e^{i\pi x}$ and $S = \sum_{n=1}^{\infty}(-)^{n+1}\,\dfrac{y^n}{n}$.

This is because $\sin\theta$ is the imaginary part of $e^{i\theta}$. The infinite series S can be summed by some suitable transform and this gives a representation of S as a rational function in term of y. The imaginary part of this multiplied by $\frac{2}{\pi}$ gives a representation of $f(x)$. The τ-transform of order 3 (with $\beta = 0$), which needs only four terms of the series, gives

$$f(x) \approx \tau_3 = \left(\frac{2}{\pi}\right)\frac{2760\sin(\pi x) + 1554\sin(2\pi x) + \frac{520}{3}\sin(3\pi x)}{4841 + 6300\cos(\pi x) + 1548\cos(2\pi x) + 80\cos(3\pi x)} \tag{77}$$

It may be remarked that the sum given by equation-75 is the imaginary part of the series for S. Now $S = \ln(1+y) = \ln(1+\cos\pi x + i\sin\pi x)$. Extracting the imaginary part of this and multiplying by $\frac{2}{\pi}$, one gets

$$f(x) = \frac{2}{\pi}\tan^{-1}\frac{\sin\pi x}{1+\cos\pi x} = \frac{2}{\pi}\tan^{-1}\tan\frac{\pi x}{2}.$$

Figure-6 shows the function and τ_3 approximant along with the direct sum of 20 terms of the series given by equation-75.

It is seen from the figure that τ_3 with only 4 terms reproduces the function remarkably well over the entire range. To have an idea of the accuracy with which the function is reproduced, we present in table-8 the values of the function

Table 8: Values of the function given by equation-74 using τ_3 and τ_4 along with the absolute relative error.

x	τ_3	absolute rel. error	τ_4	absolute rel. error
0.1	0.100004402	4.4×10^{-4}	0.10000172	1.7×10^{-5}
0.2	0.20003128	1.6×10^{-4}	0.19999928	3.6×10^{-6}
0.3	0.29995055	1.6×10^{-4}	0.29999722	9.3×10^{-6}
0.4	0.39989435	2.6×10^{-4}	0.40000404	$\times10^{-5}$
0.5	0.50006776	1.4×10^{-4}	0.50000538	1.0×10^{-5}
0.6	0.60045653	7.6×10^{-4}	0.59996774	5.4×10^{-5}
0.7	0.69964224	5.1×10^{-4}	0.70005904	8.5×10^{-5}
0.8	0.79604379	4.9×10^{-3}	0.80010749	1.3×10^{-4}
0.9	0.92790777	3.1×10^{-2}	0.89776638	$\times10^{-3}$
0.95	0.98626653	3.8×10^{-2}	0.99041719	4.3×10^{-2}
1.0	0		0	

obtained by the τ_3 and τ_4 approximants for some specific values of x along with the absolute relative error. It can be seen from the table as well as from figure-6 that the function is very well reproduced except at points very close to the point of discontinuity. At the points of discontinuity, all the transforms give the mean value zero at that point. To achieve higher accuracy one can use transforms of higher order. $\bullet\triangleleft$

4.6 Solution of Differential Equations

Numerical solution of differential equations is a vast field. Many problems in engineering and science can be formulated in terms of differential equations. A differential equation involving the relation between a function and one or more of its derivatives can be formally written as

$$y^{(n)} = f\left(x,\, y\left(x\right),\, y'\left(x\right) \cdots y^{(n-1)}\left(x\right)\right) \tag{78}$$

where $y^{(n)}\left(x\right)$ is the n-th derivative of $y\left(x\right)$. As the order of the highest derivative involved in the above equation is n, the above equation is a differential equation of order n. Differential equations are classified as linear or nonlinear. If the function f in equation-78 involves y and its higher derivatives linearly, then the equation is said to be a linear one. Though it is easier to handle the linear equations analytically, from a view point of solving them numerically both the linear and nonlinear equations can be treated on the same footing.

The general solution of equation-78 will, in general, contain n arbitrary constants and consequently there exists an n-parameter family of solutions. If the values of $y\left(x\right), y'\left(x\right) \cdots y^{(n-1)}\left(x\right)$ are prescribed at $x = x_0$, we have an initial value problem. If, on the other hand, conditions are specified at more than one points it is known as a boundary value problem. The boundary conditions of an equation may be linear or nonlinear For example, the equation

$y''(x)+y=1$ with the boundary conditions $y'(0)=y(0)^2$ and $y\left(\frac{3\pi}{2}\right)=0$ is an example of a linear equation with nonlinear boundary conditions and has two solutions $y(x)=1+\sin x$ and $y(x)=1+\sin x-2\cos x$ and we shall discuss this subsequently.

There exists a large number of methods for numerically solving differential equations. Any method of solving a first order equation is equally applicable to a higher order equation. This is because of the fact that an equation of order n can be rewritten as a system of n first order equations.

Thus, without any loss of generality, we shall mostly confine our discussion on first order equations of the form

$$y'(x)=f(x,\,y)\,,\qquad y(x_0)=y_0 \tag{79}$$

where the function f may be linear or nonlinear, but it is assumed that f is sufficiently differentiable with respect to both x and y.

The Taylor series method consists of approximating the solution by a truncated Taylor series in the neighborhood of some initial point x_0, where the initial value is known. Successive differentiation of the given differential equation is used to generate the necessary derivatives. A new Taylor series can then be constructed about $x_1=x_0+h$. This process generates the solution along the path $(x_0,\,x_1,\,x_2\cdots)$. If $y(x)$ be the exact solution of the equation-79, then to find the value of $y(x)$ at a point near x_i, a Taylor series expansion of $y(x)$ about x_i can be written as

$$\begin{aligned} y(x) &= y(x_i)+(x-x_i)\,y'(x_i)+\frac{(x-x_i)^2}{2!}y''(x_i)+\cdots \\ &\quad ++\frac{(x-x_i)^n}{n!}y^{(n)}(x_i)+\cdots \end{aligned} \tag{80}$$

where y' and y'' etc. are the total derivatives of y evaluated at x_i. Remembering that $y(x)$ is not known explicitly but $y'(x)=f(x,y)$ is known and keeping in mind that f is sufficiently differentiable one can express the total derivatives of y in terms of the partial derivatives of f, *i.e.,*

$$\begin{aligned} y' &= f \\ y'' &= f'=f_x+f_y y'=f_x+f_y f \\ y''' &= f''=f_{xx}+2f_{xy}f+f_{yy}f^2+f_x f_y+f_y^2 f \end{aligned}$$

and so on, where f_x, f_y, f_{xy} etc. are the partial derivatives of f. If $y(x)$ is known at $x=x_0$ and if we assume that the truncated series is a good approximation for a step length h, where $h=x-x_0$, then we can evaluate $y(x_0+h)$ from the equation

$$y(x_0+h)=y(x_0)+hT_k(x_0,\,y_0) \tag{81}$$

where

$$T_k(x_0,\,y_0)=f(x_0,\,y_0)+\frac{h}{2!}f'(x_0,\,y_0)+\cdots+\frac{h^{(k-1)}}{k!}f^{(k-1)}(x_0,\,y_0) \tag{82}$$

Table 9: Expressions obtained by using different transforms.

transform used	expressions
$[1/1]$	$y_{n+1} = y_n + h\dfrac{2f_n}{2 - h\dfrac{f'_n}{f_n}}$
u_2	$y_{n+1} = y_n + h\dfrac{(2f_n - hf'_n)}{(2 - 2h\dfrac{f'_n}{f_n} + h^2\dfrac{f'_n}{y_n})}$
τ_2	$y_{n+1} = y_n + h\dfrac{(6f_n - hf'_n)}{(6 - 4h\dfrac{f'_n}{f_n} + h^2\dfrac{f'_n}{y_n})}$

We can now proceed for the next step. Continuing in this manner we obtain a set of discrete values of $y_n = y(x_0 + nh)$ which are approximation for the true solution at the points $x_n = x_0 + nh$. Formally we can write

$$y(x_{n+1}) = y(x_n) + hT_k(x_n,\, y_n) \tag{83}$$

As we already know that the sum of an infinite series, of which only a few terms are known, can be best approximated by using the nonlinear sequence transforms. If we calculate only one derivative of $f(x, y)$, then three terms of the series are known and we can employ the different nonlinear transforms on these three terms to obtain formulas for the numerical solution of a first order differential equation using Levin-Weniger transforms [90] of order 2 or $[1/1]$ Padé approximant. These are shown in table- 9. As u_2 and y_2 transforms are equivalent and so are τ_2 and t_2 transforms, we show the formulas obtained with u_2 and τ_2 transforms. If the two derivative of $f(x, y)$ can be calculated then transforms of a higher order can used to obtain the solution and these as well are shown in table- 9.

Consider the differential equation $y' = 1 + y^2$ with the initial condition $y(0) = 1$, for which the exact solution is $y(x) = \tan\left(x + \frac{\pi}{4}\right)$. Any standard linear method will not be able to find the solution of the equation for $x \geq \pi/4$. Figure-7 shows the the numerical solution along with the exact result.

Let us consider the differential equation

$$y' = \lambda_1 y + e^{\lambda_2 x}$$

. This equation has the general solution

$$y(x) = \frac{e^{\lambda_2 x}}{\lambda_2 - \lambda_1} + \epsilon e^{\lambda_1 x},$$

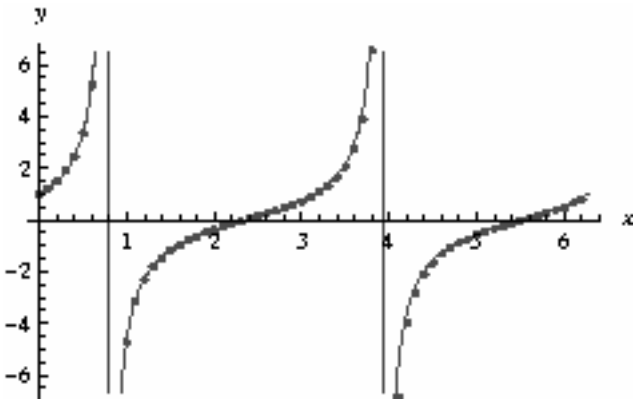


Figure 7: Solution of $y' = 1 + y^2$ using τ_2-approximant.

where ϵ is a constant. If we now use the boundary condition $y(0) = 1/(\lambda_2 - \lambda_1)$, one obtains $\epsilon = 0$. However, if in any numerical method of solution there is even a small error in implementing this boundary condition, the term $\epsilon e^{\lambda_1 x}$ will ultimately dominate. This ill-conditioning generates a solution completely different from the one sought. We demonstrate this with the choice $\lambda_1 = 9$ and $\lambda_2 = -1$. More specifically, we consider the differential equation

$$y' = 9y + e^{-x}, \quad y(0) = -\frac{1}{10}$$

the general solution for which is given by $y(x) = -\frac{e^{-x}}{10}$. Using Runge-Kutta method of order 4 and with different step size, it is found that the method becomes unstable after a certain value x depending on the step size. A decrease in the step size shifts the instability to a larger value of x. A similar feature is present in the solution with formulas using the nonlinear transforms, the only difference being that the instability is shifted to a larger value of x on increasing the order of the transform. Figure- 8 shows $y(x)$ obtained by τ_8 approximant along with exact result. The figure also shows the solution obtained by Runge-Kutta method of order 4 with step size 0.01 and 0.001 .

One natural question that arises is that, if one takes the pain the calculating a few derivatives, is not it possible to form an approximant of higher order which approximates the true solution upto a reasonable value of x ? To check this we calculate nine terms of the Taylor series and form the $\tau-$approximant of order 8 (with $\beta = 0$) which is given by

$$\tau_8 = \frac{-1}{10}\left(\frac{1 - \frac{7x}{15} + \frac{x^2}{10} - \frac{x^3}{78} + \frac{x^4}{936} - \frac{x^5}{17160} + \frac{x^6}{514800} - \frac{x^7}{32432400}}{1 + \frac{8x}{15} + \frac{2x^2}{15} + \frac{4x^3}{195} + \frac{x^4}{468} + \frac{x^5}{6435} + \frac{x^6}{128700} + \frac{x^7}{4054050} + \frac{x^8}{259459200}}\right)$$

Boundary value problem

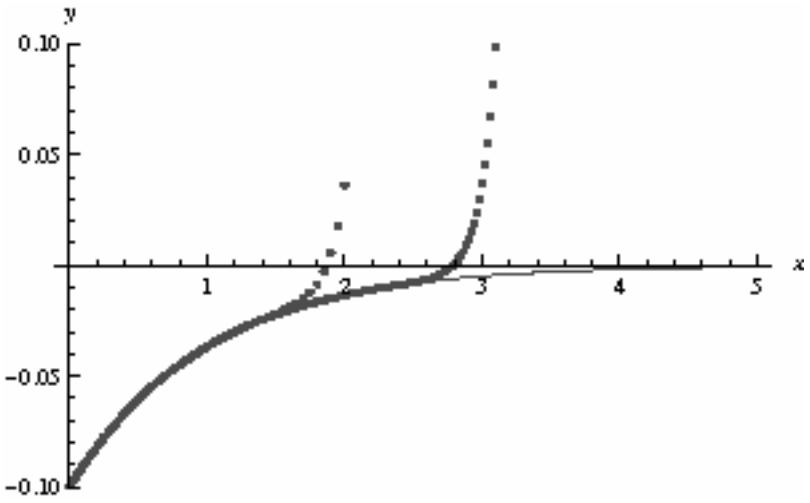


Figure 8: Solution of the differential equation $y' = 9y + e^{-x}$ by Runge-Kutta method of order 4 with step sizes 0.01 and 0.001. The solid line represents the solution obtained with τ_8.

Let us now consider the boundary value problem

$$y'' + k^2 y = 1; \quad y(0) = 0, \qquad y(1) = 0$$

The exact solution for the problem is given by

$$y(x) = \frac{1}{k^2} + \frac{(\cos k - 1)\sin(kx)}{k^2 \sin k} - \frac{\cos(kx)}{k^2}$$

If we take $k = 3.141$ and $k = 3.142$, the solutions are entirely different as these values lie on opposite sides of π as may be seen from the figure-9 . It is for this reason that any error incurred at some intermediate point may lead to a completely wrong solution and this is true for any numerical prescription. Let us demonstrate how, by using the convergence accelerating transforms, we obtain a solution with much ease.

As in the "shooting" process, we start with the initial value problem

$$y'' + k^2 y = 1; \quad y(0) = 0, \qquad y'(0) = \alpha$$

and obtain the series

$$\begin{aligned} y(x) &= \alpha x + \frac{x^2}{2} - \frac{\alpha k^2 x^3}{6} - \frac{k^2 x^4}{24} + \frac{\alpha k^4 x^5}{120} + \frac{k^4 x^6}{720} - \frac{\alpha k^6 x^7}{5040} - \frac{k^6 x^8}{40320} + \\ &\quad + \frac{\alpha k^8 x^9}{362880} + \frac{k^8 x^{10}}{3628800} - -\frac{\alpha k^{10} x^{11}}{39916800} - \frac{k^{10} x^{12}}{479001600} + \cdots \end{aligned}$$

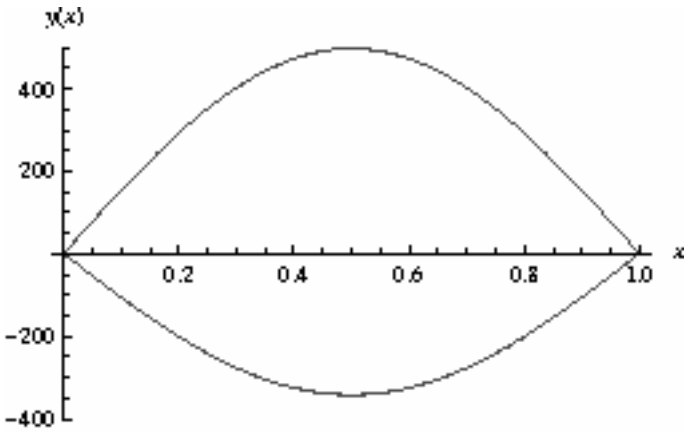
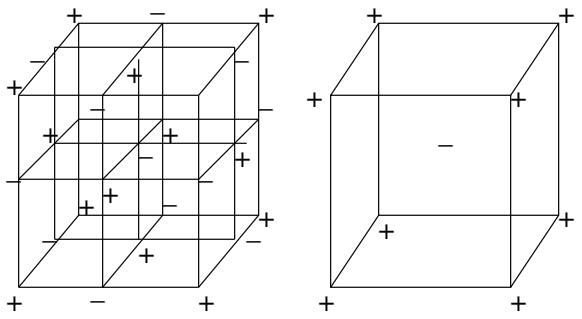


Figure 9: Solution of the differential equation $y'' + k^2 y = 1$with the boundary conditions $y(0) = 0$ and $y(1) = 0$ using the τ_5 transform (dashed curve) along with the exact solution {solid line). The lower curve corresponds to $k = 3.141$ and the upper one corresponds to $k = 3.142$.

Here also the successive pairs of terms of the series alternate in sign. As in the previous example, we consider the sum of approximants obtained separately for series constructed out of the even and odd numbered terms as representation of the solution and the one obtained with τ-transform of order 5 is given by

$$\tau_5 = \frac{\dfrac{x^2}{2} - \dfrac{37k^2x^4}{1188} + \dfrac{269k^4x^6}{427680} - \dfrac{139k^6x^8}{31434480} + \dfrac{19k^8x^{10}}{2155507200}}{1 + \dfrac{25k^2x^2}{1188} + \dfrac{5k^4x^4}{21384} + \dfrac{5k^6x^6}{2794176} + \dfrac{k^8x^8}{100590336} + \dfrac{k^{10}x^{10}}{30177100800}} + \frac{\alpha x - \dfrac{14\alpha k^2x^3}{99} + \dfrac{29\alpha k^4x^5}{6480} - \dfrac{449\alpha k^6x^7}{10478160} + \dfrac{(17\alpha k^8x^9}{167650560}}{1 + \dfrac{5k^2x^2}{198} + \dfrac{5k^4x^4}{14256} + \dfrac{5k^6x^6}{1397088} + \dfrac{k^8x^8}{33530112} + \dfrac{k^{10}x^{10}}{5029516800}}$$

If we now assign to k any one of the two values mentioned and force the approximant to be zero at $x = 1$, the approximant gives a linear equation for α and consequently can be easily solved. With the τ_5-approximant, the values of α, corresponding to $k = 3.141$ and 3.142 are respectively given by -1075.5245 and 1560.2348. Figure 9 shows the plots of the τ_5-approximant with $k = 3.141$ and 3.142 along with the exact solution. If one has to solve the equation by the shooting method for values of k close to π, one will face instability, as the value of the initial slope changes drastically as one crosses π. The values of α for $k = 3.1415$ and 3.1416, as obtained from the τ_5-approximant, are respectively -6918.03 and 79834.30, the exact values of the initial slopes being -6871.17 and 86657.1. Thus the same τ_5-approximant will fairly represent the solutions of the



(a) NaCl (b) CsCl

Figure 10: First Evjen cell for NaCl and CsCl lattices.

equation with these values of k as well. A better representation can obtained with a higher order approximant.

At this point one may ask - how to know to the order of the transform? This can be judged by comparing two approximants of successive orders. If they agree within a reasonable accuracy, then either of them can be considered as a reasonable approximant. For example, τ_5-approximant with $k = 3.141$ and $x = 0.5$ gives the value -342.3133 and the τ_6-approximant gives -341.9548. For $k = 3.142$ the corresponding values are 496.6751 and 497.4347. With τ_5-approximant the error over the entire range is about 0.15 percent. $\bullet\triangleleft$

5 Applications to Physical Problems

5.1 Evaluation of Lattice Sums

The problem of evaluating lattice sums is frequently encountered in condensed matter physics. The problem of determining the electrostatic potential within a lattice of point charges is made particularly difficult due to the fact that these sums are slowly and conditionally convergent. A number of methods have been proposed for evaluating them. The classical methods for the evaluation of Madelung sums are those of Evjen [40] and Ewald [41] and these are reviewed in the review article by Tosi [42].m. There exist a number of modifications and refinements of the Evjen and Ewald procedure and these are extensively discussed in the review article by Glasser and Zucker [44]. However, none of

these methods has really made the evaluation of lattice sums as simple as might be expected. This is because of the fact that most of these methods, except perhaps the Evjen method, express the lattice sums in terms of tabulated functions. In the study of stability of a particular lattice, one needs to know the value of lattice sums for competing structures, for which the sums may be very nearly equal and the difference between the sums may be of the same order as the error arising from rounding-off numbers or truncating sums; thus the need arises for an accurate evaluation of lattice sums.

A direct method of evaluating the lattice sums was proposed by Bhowmick, Roy and Bhattacharya [43]. The method consists in accelerating the contribution of different neighbours to the lattice sum in some sequential order, such that the limit of the virtually infinite sequence is the desired lattice sum and apply the convergence accelerating transforms on this sequence. This method permits the evaluation of lattice sums with a high degree of precision as will be illustrated below.

5.1.1 Madelung sums for NaCl and CsCl lattices

We define the Madelung constant as

$$\alpha = \sum{}' \frac{(-1)^m}{\sqrt{m_1^2 + m_2^2 + m_3^2}} \tag{84}$$

where $m = m_1 + m_2 + m_3$.

For NaCl lattice (m_1, m_2, m_3) run over all integer values and for CsCl lattice (m_1, m_2, m_3) are either all odd or all even. The prime over the summation implies that the term for which $m_1 = m_2 = m_3 = 0$ is excluded from the sum. One can build the sequence for the lattice sum in a variety of ways. For example, we can sum over expanding cubes to build the sequence. Alternatively, we can build the sequence by summing over expanding cubes which are electrically neutral and this is basically the Evjen sequence.

It may be remarked that a very rapidly convergent series for the Madelung sum of NaCl lattice was discovered by Benson *et. al.* [45] using a physical argument and was proven analytically by Mackenzie [46] and is given by

$$\alpha = -12\pi \sum_{m,n=1(\text{odd})}^{\infty} \operatorname{sech}^2\left(\frac{\pi}{2}\left(m^2 + n^2\right)\right). \tag{85}$$

The above sum is highly convergent. For example, only the first term of the series gives $\alpha = -1.73267$. Considering terms up to $m = 5$ and $n = 5$, it gives $\alpha = -1.74756451$, which is correct up to eight significant digits. A similar type of expression for CsCl structure was given by Benson *et. al.* [47]. Extension to all rhombohedral lattices was made by Mackenzie [48]. Though the Madelung sum for NaCl and CsCl lattices can be expressed as very rapidly convergent series, this is not true for all slowly convergent lattice sums. However, one can find the lattice sums, irrespective of whether it can be expressed as rapidly convergent

Table 10: Iteration of u_2-transform (with $\omega_n = \Delta S_n$) for α(NaCl) using expanding cubes without sharing of charges.

n	S_n	$u_2^{n,1}$	$u_2^{n,2}$	$u_2^{n,3}$	$u_2^{n,4}$
1	2.13352 07792 784	1.749..	1.74756..	1.74756 4584..	1.74756 45946
2	1.51664 63362 669	1.7469..	1.74756 3..	1.74756 4592..	
3	1.91250 39789 592	1.7478..	1.74756 48..	1.74756 45947..	
4	1.61926 96788 704	1.7474..	1.74756 44..	1.74756 45945..	
5	1.85253 54904 123	1.7476..	1.74756 46..		
6	1.65874 22894 727	1.74752..	1.74756 57..		
7	1.82454 42337 282	1.74758..	1.74756 60..		
8	1.67964 12454 745	1.75754..			
9	1.80833 81857 782	1.74757..			
10	1.69257 89282 595	1.74755..			
11	1.79776 89192 232				
12	1.70137 66038 269				
13	1.79033 12603 333				

Table 11: Iteration of u_2-transform (with $\omega_n = \Delta S_n$) for α(CsCl) using expanding cubes without sharing of charges.

n	S_n	$u_2^{n,1}$	$u_2^{n,2}$	$u_2^{n,3}$	$u_2^{n,4}$
1	4.61880 21535 17	0.95..	1.0178..	1.01765..	1.01768 076
2	-4.93323 96103 61	1.05..	1.0177..	1.01768 13..	
3	9.34861 09902 38	0.99..	1.01765..	1.01768 077..	
4	-9.69295 25236 67	1.03..	1.01769..	1.01768 076..	
5	14.10826 26595 37	1.00..	1.01767..		
6	-14.45291 64752 90	1.02..	1.01768 4..		
7	18.86832 22709 63	1.01..			
8	-19.21301 88720 43	1.012..			
9	23.62844 57854 21	1.0216..			
10	-23.97315 38210 79				
11	28.38858 73683 74				
12	-28.73329 94699 64				
13	33.14873 56230 11				

series or not, using the convergent accelerating transforms and in the following section we demonstrate this considering the NaCl and CsCl lattices as prototype examples for which the sums are known accurately.

Table-10 shows that the Madelung sum for NaCl lattice, where the sequence is built by summing over expanding cubes without sharing of charge and converge too slowly. It is evident from the table that the Madelung sum can be reproduced to fourth decimal places by using only seven partial sums. Though it is not shown in the table, it may be mentioned here that sixteen partial sums give, with an available precision of 15 digits, the value -1.7475645646332 for the Madelung sum, which we believe is correct upto 14 significant digits.

It is interesting to observe that the sequence obtained by using cubic blocks without sharing of charges in the case of CsCl is formally divergent as is evident from table- 11. The value obtained by the sequence to sequence transforms is exactly the value obtained by using analytic continuation in a complex plane. It is seen from table-11 that the successive iterates of this formally divergent series approaches the Ewald sum for CsCl. The number of terms of the sequence that is needed to obtain the value of the limit correct to 14 significant places is 22, and the value obtained is 1.01768 07547 263.

5.2 Non-linear Simple Pendulum

The differential equation of a free undamped simple pendulum is given by

$$\frac{d^2\theta}{dt^2} + \frac{g}{l}\sin\theta = 0 \tag{86}$$

where θ is the angular displacement from the equilibrium position, l is the length of the pendulum and g is the acceleration due to gravity. The equation is nonlinear due to presence of the term $\sin\theta$.

The common approach is to linearise the equation by replacing $\sin\theta$ by θ. For the nonlinear equation, one can obtain an expression for the time period of the pendulum in terms of elliptic functions and the problem is shifted to that of evaluating the function which is expressed in terms of a definite integral. There are other approaches approximating nonlinear systems. The most common and widely used method for tackling nonlinear systems is the perturbation method [49] and different authors [50-57] have used this method and other simple pedagogic approach to the nonlinear simple pendulum. Another approach for obtaining analytical approximation to periodic solution of the differential equation is the harmonic balance method [58-59]. Recently Belendez et. al [60] has used this technique to obtain analytic approximate expressions for the period of the pendulum for large amplitude. We shall see presently that one can obtain analytic expressions for the period of the nonlinear pendulum which are very accurate and is better than those obtained by other methods .

If the pendulum is displaced through an angle θ_0 and then released, the initial conditions are given by $\theta(0) = \theta_0$ and $\left(\frac{d\theta}{dt}\right)_{t=0} = 0$ and θ_0 is the amplitude of oscillation. If one linearise the equation by replacing $\sin\theta$ by θ, it can be easily solve and the solution is $\theta = \theta_0\cos\omega t$ where $\omega = \sqrt{\frac{g}{l}}$ and the time period is

given by $T_0 = 2\pi\sqrt{\frac{l}{g}}$. To obtain the time period of the nonlinear pendulum, we multiply equation-86 by $\frac{d\theta}{dt}$ and integrate with respect to t to get

$$\left(\frac{d\theta}{dt}\right)^2 - \frac{2g}{l}\left(\cos\theta - \cos\theta_0\right) = 0 \tag{87}$$

where we have used the boundary condition $\theta = \theta_0$ at $t = 0$. Integrating once more from $\theta = 0$ to θ_0 yields

$$\sqrt{\frac{2g}{l}}\,\tau = \int_0^{\theta_0} \frac{d\theta}{\sqrt{(\cos\theta - \cos\theta_0)}} = \int_0^{\theta_0} \frac{d\theta}{\sqrt{2}\sqrt{\sin^2\frac{\theta_0}{2} - \sin^2\frac{\theta}{2}}} \tag{88}$$

This is $\frac{1}{4}$ of a cycle and therefore τ is $\frac{1}{4}$ of the time period. Trying the half-angle substitution $\sin\frac{\theta}{2} = \sin\frac{\theta_0}{2}\sin\phi$, we get

$$T = 4\sqrt{\frac{l}{g}}\int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - \sin^2\frac{\theta_0}{2}\sin^2\phi}} = 4\sqrt{\frac{l}{g}}\,K\left(m\right). \tag{89}$$

$K\left(m\right)$ is the elliptic integral of the first kind and is defined as follows

$$K\left(m\right) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - m\sin^2\phi}} \tag{90}$$

where $m = \sin^2\frac{\theta_0}{2}$. For $m = 1$, the integrand goes to infinity at the upper limit. To obtain the behavior of the integral near $m = 1$, we change the variable θ to $\frac{\pi}{2} - \theta$ and write

$$K\left(m\right) = \int_0^{\theta_0} \frac{d\theta}{\sqrt{1 - m\cos^2\theta}} + \int_{\theta_0}^{\pi/2} \frac{d\theta}{\sqrt{1 - m\cos^2\theta}} \approx \int_0^{\theta_0} \frac{d\theta}{\sqrt{(1-m) + m\theta^2}} + \int_{\theta_0}^{\pi/2} \frac{d\theta}{\sin\theta}$$

where θ_0 is so chosen that θ_0^2 is very large compared to $(1 - m)$ but very small compared to 1 and obtain

$$K\left(m\right) = \ln\frac{\theta_0 + \sqrt{(1-m) + \theta_0^2}}{\sqrt{(1-m)}} - \ln\tan\frac{\theta_0}{2} \approx \ln\frac{2\theta_0}{\sqrt{(1-m)}} - \ln\frac{\theta_0}{2}$$

$$= \ln\frac{4}{\sqrt{1-m}} = \frac{1}{2}\ln\frac{16}{(1-m)}$$

We now subtract the series for $\frac{1}{2}\ln\frac{16}{(1-m)}$ from the series for $K\left(m\right)$ and considering only three terms of the series construct τ_2 approximant and add $\frac{1}{2}\ln\frac{16}{(1-m)}$ to obtain a global approximation for $K\left(m\right)$ [34].

$$g\tau_2 = \frac{\pi}{2}\left(\frac{0.117458 - 0.110792m}{1 - 0.361684m - 0.0525862m^2}\right) + \frac{1}{2}\ln\left(\frac{16}{1-m}\right). \tag{91}$$

Table 12: $\frac{T}{T_0}$at different amplitude of oscillation.

θ	$g\tau_2$	exact	θ	$g\tau_2$	exact
10^o	1.0019076	1.0019072	30^o	1.0174087	1.0174088
50^o	1.049773	1.049784	70^o	1.102086	1.102145
90^o	1.18018	1.18034	110^o	1.29519	1.29534
130^o	1.4705	1.4698	150^o	1.7659	1.7622
170^o	2.4487	2.4394	172^o	2.5900	2.5801
174^o	2.772	2.762	176^o	3.030	3.019
178^o	3.471	3.460	179^o	3.912	3.901

Table-12 shows the values of $\frac{T}{T_0}$ for various amplitudes obtained by using the approximant given by equation-91 along with the exact value. It is seen that the simple expression represents $\frac{T}{T_0}$ over the entire range with fair accuracy.

5.3 Excluded Volume Problem in Polymer

Macro-molecules are molecules with very high molecular weights and include cellulose, proteins, starch and many other molecules that are polymerized from monomers. Their wide variety of sizes and shapes make them suitable for the basic ingredients in living as well as inanimate objects. When a chain polymer is made to float in a supporting medium, its shape depends on the molecular weight, its repeating units, the temperature and the solvent. Such an object has overall geometrical properties, such as a characteristic radius, which are directly associated with the directly measurable physical properties of the macro-molecules in the dilute solution. For instance, the small angle scattering of light or x-rays gives direct information about the radius of gyration of the scattering molecules. It is well known that the presence of polymeric molecules in small concentration has a dramatic effect on the viscosity of the solvent and this can be explained with the simple assumption that each macro-molecular globule behaves as a *non-draining* sphere, within which the solvent molecules are entrained. It has been experimentally confirmed that the apparent radius of this sphere, for a given solute and solvent, is a standard multiple of the radius of gyration found in light scattering on the same solution. All these point to the fact that a study of the theory of the geometrical properties of a random coil is of immediate physical interest.

A physical quantity relevant for such a study is the mean-square distance between the ends of the long polymer chain. If $\vec{l_i}$ is the vector representing the i-th segment of the chain then

$$\langle R^2 \rangle = \langle \left(\sum_i \vec{l_i} \right)^2 \rangle = \langle \left(\sum_i l_i^2 \right) \rangle + \langle \sum_{i \neq j} \vec{l_i}.\vec{l_j} \rangle$$

where the average $\langle\ \rangle$ is taken over the ensemble of the allowed chains.

For a freely rotating chain there is no correlation between the orientations and one has $\langle \vec{l_i}.\vec{l_j} \rangle = 0$ and consequently

$$\langle R^2 \rangle_0 = Nl^2 \tag{92}$$

where l^2 is the average squared bond length and N is the number of segments in the molecule.

Another quantity relevant to the characterization of a configuration is the radius of gyration S. It is defined as the root mean square distance of the segments or groups from their common center of gravity. If s_i be the distance of the i-th atom from the center of gravity of the chain in a specified configuration, then

$$\langle S^2 \rangle_0 = \frac{1}{N} \sum_i s_i^2. \tag{93}$$

It is easy to prove that for large values of N the radius of gyration of a chain (assigning equal mass to each segments) is related to the end-to-end distance as follows:

$$\langle S^2 \rangle_0 = \frac{1}{6} \langle R^2 \rangle_0 \tag{94}$$

Optical and viscosity experiments confirm quite satisfactorily that the apparent radius of a macro-molecular globule is proportional to the square root of the number of segments in the chain. This proportionality remains valid even if one calculate $\langle R^2 \rangle_0$ or $\langle S^2 \rangle_0$ for more complicated molecular chain models only with a different proportionality constant.

To evaluate $\langle R^2 \rangle_0$ for more complicated molecular chain models it is convenient to introduce a transformation tensor $\mathbf{T_i}$ such that $\mathbf{T_i} \vec{l_i} = \vec{l}_{i+1}$. In other words, $\mathbf{T_i}$ rotates the i-th segmental vector $\vec{l_i}$ into the direction of its successor. In can be shown that for a free rotation model with a fixed bond angle θ

$$\langle R^2 \rangle = \frac{1 + \langle \cos\theta \rangle}{1 - \langle \cos\theta \rangle} Nl^2 \tag{95}$$

where $\langle \mathbf{T} \rangle = \langle \cos\theta \rangle$.

The configuration of a chain molecule has a close analogy with the random flight or walk, consisting steps of fixed length. However, they differ in a most important respect; whereas a random flight may cross its own path, a chain molecule is obviously forbidden from doing so. Out of the total number of random walk configurations only a fraction will be altogether free of self-intersection and consequently acceptable configuration for a real chain molecule. As a consequence of retention of only the non-intersecting configuration to the exclusion of all others, the average spatial configuration of the real molecule is perturbed relative to its random flight analog and the average dimension of the chain (i.e., $\langle R^2 \rangle_0$ and $\langle S^2 \rangle_0$ are increased.

The problem of spatial configuration of a macro molecule separates into two fairly distinct parts. One of them deals with the bond structure and local interactions between atoms or groups which are near neighbors in sequence along

the chain and is referred to as the short range interaction. The mean square end-to-end distance of a polymer chain with short range interference may be expressed in the form

$$\langle R^2 \rangle = \langle R^2 \rangle_0 \ \sigma_R^2 \tag{96}$$

where $\langle R^2 \rangle$ is the mean square end-to-end distance of the freely rotating state and σ_R, is referred to as the conformation factor, represents the effect of steric hindrances to internal rotations, a special case of which is given by equation-95. This conformation factor depends generally on the temperature and sometimes on the solvent, while $\langle R^2 \rangle_0$ is a geometrical quantity independent of thermodynamic variables. For high molecular weight polymers of ordinary interest $\langle R^2 \rangle_0$ is proportional to N, but σ_R is independent of N and therefore the Markoff nature of the chain is still preserved. It may be mentioned here that one can define a similar quantity σ_S related to the radius of gyration $\langle S^2 \rangle$ and have properties very similar to σ_R.

The excluded volume effect, on the other hand, represents the effect of interaction between the segments which are far apart along the chain and is often called the "long range interaction" in contrast to the "short range interaction" due to steric hindrance. In real polymers, the nature of the long range interaction may also involve other specific interaction mediated by solvent molecules. Starting with the work of Flory [61, 62] a large number of methods [63-67] exist in the literature to account for the excluded volume effect. Once the long range interaction is introduced, the exact calculations becomes impossible and a great deal of effort has been expended on working out the valid approximations. When the long range effect is taken into account $\langle R^2 \rangle$ is no longer proportional to N but to a higher power of N, i.e.,

$$\langle R^2 \rangle \propto N^{2\nu}, \quad \nu < 1. \tag{97}$$

The exponent ν is about $3/5$, so that the excluded volume effect is important in long chains.

In the model used by Flory, the polymer molecule is regarded as a continuous cloud of segments distributed about the molecular center of the mass. For this model, the expansion factors σ_R and σ_S cannot be distinguished from each other and we represent them by the common symbol σ.

Using thermodynamic argument [61] it can be proved

$$\sigma^5 - \sigma^3 = CN^{1/2} \tag{98}$$

and represents the relationship between the length N of a polymer chain and its expansion factor σ under the influence of the mutual exclusion of its segments and its referred to as the Flory's formula. Stockmayer [68] recommended an adjustment of the constant on the right hand side of equation-98 so that it correctly reproduces the first order perturbation term given by equation-103 and this gives

$$\sigma_R^5 - \sigma_R^3 = \frac{4}{3} z \tag{99}$$

and a similar expression for σ_s. In the above, the excluded volume parameter z is given by

$$z = \left(\frac{3}{2\pi}\right)^{3/2} \left(\frac{\beta N^{1/2}}{l^3}\right) \tag{100}$$

where β is called the binary cluster integral for a pair of segments and represents the effective volume excluded to one segment by the presence of another. Equation-99 is referred to as the modified Flory's equation.

A number of formulas similar to the Flory's equation have been suggested by various authors and a summary of these can be found in the book by Yamakawa [69]. Of the various formulas which expresses σ_R in closed form, those predicted by Buecher [71] and by Yamakawa and Tanaka [72] gives values of σ_R which are close to those predicted by perturbation theory and these are respectively given by

$$\sigma_R^4 - \sigma_R^2 = \frac{48}{69} z \left(1 + \frac{2}{3\sigma_R^2} + \frac{1}{4\sigma_R^4}\right) \tag{101}$$

$$\sigma_R^2 = 0.572 + 0.428\,(1 + 6.23z)^{1/2} \tag{102}$$

Of the various methods which consider the excluded volume effect, the perturbation calculation deserves attention because it represents the exact and standard theory of the excluded volume effect. The perturbation approach to the problem was initiated by Teramota [74] and a brief summary of the work being given in the article by Flory [73] and in the book by Yamakawa [69]. It has subsequently been pursued by many workers [70-71]. The perturbation series for the expansion factor is formally given in the form of an infinite series and is given by

$$\sigma_R^2 = 1 + a_1 z + a_2 z^2 + a_3 z^3 + \cdots \tag{103}$$

The calculation of the coefficients, though straightforward, is quite tedious. Some of the coefficients as calculated by Muthukumar and Nickel [75] are as follows:

$$a_1 = 4/3, \quad a_2 = -2.075385396, \quad a_3 = 6.296879676$$
$$a_4 = -25.05725072, \quad a_5 = 116.134785, \quad a_6 = -594.71663$$

It is seen that the coefficients increase explosively and the increase is roughly like n^n. It may be mentioned that the above power series has zero radius of converge.

As we know that the Padé approximants can find the *sum* of a divergent series, we can form different Padé approximants with the available terms of the series given by equation-103 and these are shown in table-13. The plots for these approximants are shown in figure- 11. It is seen that [2/2] and [2/3] approximants give bounds to the *sum* and so also [2/3] and [3/3] but none of these approximants can be considered as a representation of the function.

Table 13: Some approximants for the series given by equation-103. For τ approximants we have used $\beta = 0$.

Transform used	Approximant
[2/2]	$\frac{1 + 6.308z + 7.579z^2}{1 + 4.975z + 3.021z^2}$
[2/3]	$\frac{1. + 7.614z + 12.390z^2}{1 + 6.280z + 6.092z^2 - 1.385z^3}$
[3/3]	$\frac{1. + 10.159z + 28.444z^2 + 19.288z^3}{1 + 8.825z + 18.753z^2 + 6.304z^3}$
τ_4	$\frac{1. + 10.43z + 30.75z^2 + 23.61z^3}{1. + 9.096z + 20.697z^2 + 8.59 * z^3 - 0.7159z^4}$
τ_5	$\frac{1. + 14.21z + 66.32z^2 + 114.50z^3 + 55.79z^4}{1. + 12.87z + 51.23z^2 + 66.62z^3 + 17.28z^4 - 0.9217z^5}$
τ_6	$\frac{1. + 18.093z + 117.365z^2 + 329.935z^3 + 379.626z^4 + 127.667z^5}{1. + 16.759z + 97.095z^2 + 228.961z^3 + 195.38z^4 + 34.76z^5 - 1.2873z^6}$

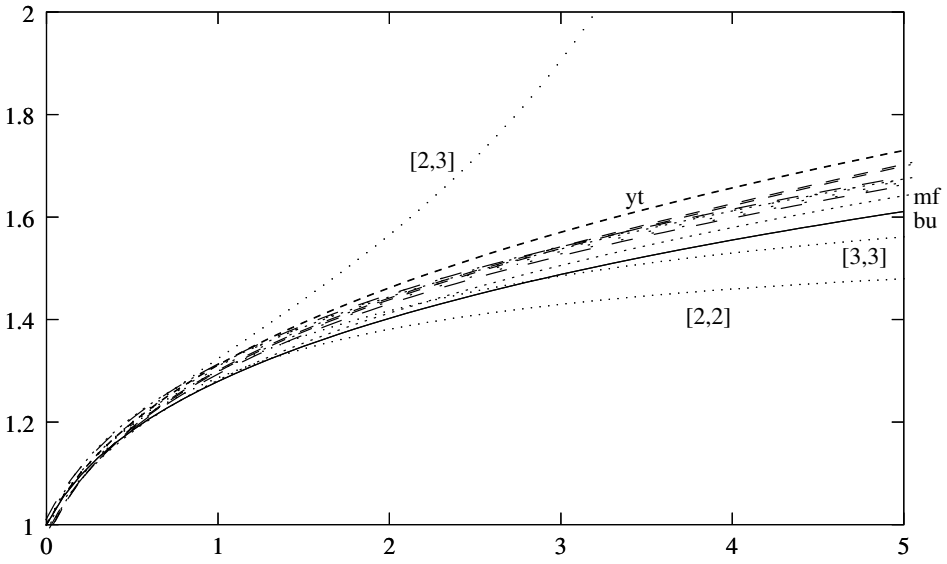


Figure 11: Conformation factor using different approximants and phenomenological models. yt - Yamakawa and Tanaka [72]; bu - Buecher [71]; mf - modified Flory (equation 99). The different τ-approximants by shown by the dashed lines.

However, the τ_5 and τ_6 approximants, which use the same number of terms as the [2/3] and [3/3] Padé approximants, are almost coincident over a wide range of z and the values predicted by these approximants lie with those predicted by equations- 99, 101 and 102. A similar result is obtained using the u-transform as well [76]. Thus by using the Levin-like transforms it is possible to obtain a good representation for the conformation factor over a wide range even with a small number of terms of the perturbation series.

5.4 Quantum Harmonic Oscillator

We shall now consider a somewhat less trivial problem of finding the energy eigenvalues of harmonic oscillator. Though the problem is exactly solvable, we shall demonstrate that by making use of the Levin-like transforms we can find the energy eigenvalues much easily. The Schrödinger equation for the harmonic oscillator is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}kx^2\psi = E\,\psi \tag{104}$$

and the eigenvalues are $E=\left(n+\frac{1}{2}\right)\hbar\omega$ where $\omega=\sqrt{k/m}$ [77]. Introducing the variables $\xi=\sqrt{\frac{m\omega}{\hbar}}\,x$ and $\epsilon=\frac{2E}{\hbar\omega}$, the equation-104 reduces to

$$\frac{d^2\psi}{d\xi^2}=\left(\xi^2-\epsilon\right)\psi, \tag{105}$$

and the eigenvalues for this equation are given by $\epsilon=(2n+1)$. The boundary conditions for the problem are $\psi=0$ for $\xi\to\pm\infty$. In making a series solution about $\xi=0$ we set $\psi'(0)=0$ and $\psi(0)=1$ for the solution with even parity. For the odd solution we set $\psi(0)=0$ and $\psi'(0)=1$. First few terms of these series are given by

$$\begin{aligned} s_{ev} &= 1-\frac{\epsilon\xi^2}{2}+\frac{\left(2+\epsilon^2\right)\xi^4}{24}+\frac{\left(-14\epsilon-\epsilon^3\right)\xi^6}{720}+ \\ &\quad \frac{\left(60+44\epsilon^2+\epsilon^4\right)\xi^8}{40320}-\frac{\left(-844\epsilon-100\epsilon^3-\epsilon^5\right)\xi^{10}}{3628800} \\ &\quad +\frac{\left(5400+4804\epsilon^2+190\epsilon^4+\epsilon^6\right)\xi^{12}}{479001600}+\cdots \end{aligned} \tag{106}$$

$$\begin{aligned} s_{odd} &= x-\frac{\epsilon x^3}{6}+\frac{\left(6+\epsilon^2\right)\xi^5}{120}+\frac{\left(-26e-\epsilon^3\right)\xi^7}{5040}+ \\ &\quad \frac{\left(252+68\epsilon^2+\epsilon^4\right)\xi^9}{362880}-\frac{\left(-2124\epsilon-140\epsilon^3-\epsilon^5\right)\xi^{11}}{39916800} \\ &\quad +\frac{\left(27720+9604\epsilon^2+250\epsilon^4+\epsilon^6\right)\xi^{13}}{6227020800}+\cdots \end{aligned} \tag{107}$$

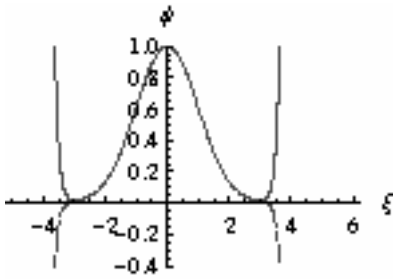


Figure 12: Plot of truncated series for s_{ev} with $\epsilon = 1$; solid curve - 15 terms of the series, dotted curve - 16 terms of the series.

Table 14: First few eigenvalues (ϵ) of different parity for the harmonic oscillator obtained by equating to zero the u-approximants ($\beta = 0$) of different orders on the series given by equations 106 and 107 evaluated at at $\xi = 10^6$.

order of transform	ϵ even parity	ϵ odd parity
2	1	3
4	1, 5.1047, 11.2062	3, 7.0227, 11.89
6	1, 5.0007, 9.0501,	3, 7.00002, 10.97
	13.65, 23.18	14.48, 22.89
8	1, 5.000002, 9.00009	3, 7, 11.0001, 15.0359
	12.9830, 16.78, 22.23	18.00006, 21.62, 38.0071
10	1, 5, 9, 12.99995	3, 7, 11, 14.9997, 19.0606
	17.0022, 20.52, 23.47, 32.30	31.38, 57.45

The boundary condition that $\psi = 0$ for $\xi \to \pm\infty$ cannot be satisfied by any polynomial function. If one truncates the series s_{ev} and plots it for $\epsilon = 1$ (or any other eigenvalue with even parity), the curves with odd and even number of terms will blow in opposite directions as shown in figure-12 and similar behaviour will be observed for s_{odd} as well. The u_2-approximant (with $\beta = 0$) built with the even and odd series are respectively give by the following expressions:

$$u_{2ev} = \frac{1 + \dfrac{\xi^2}{3\epsilon} - \dfrac{\epsilon\xi^2}{3}}{1 + \dfrac{\xi^2}{3\epsilon} + \dfrac{\epsilon\xi^2}{6} + \dfrac{\xi^4}{12} + \dfrac{\epsilon^2\xi^4}{24}} \tag{108}$$

$$u_{2odd} = x\frac{1 + \dfrac{3\xi^2}{5\epsilon} - \dfrac{\epsilon\xi^2}{15}}{1 + \dfrac{3\xi^2}{5\epsilon} + \dfrac{\epsilon\xi^2}{10} + \dfrac{\xi^4}{20} + \dfrac{\epsilon^2\xi^4}{120}} \tag{109}$$

If we now demand that u_{2ev} vanishes at a large distance, say $\xi = 10^6$, then we obtain an equation for ϵ , and solving for ϵ, we obtain the ground state

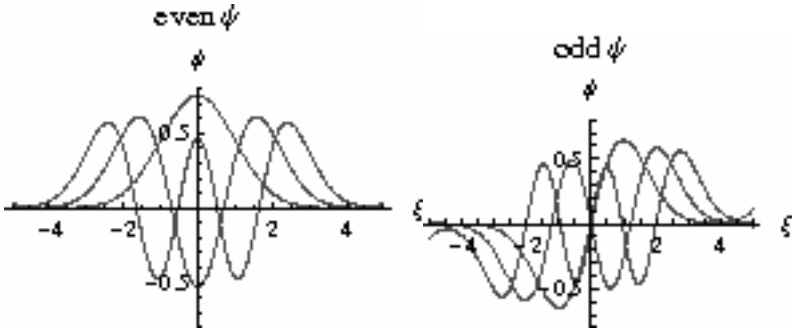


Figure 13: First few normalized eigenfunctions obtained with $u_{10}(\beta = 0)$ along with the exact eigenfunctions.

eigenvalue. Table-14 shows the eigenvalues obtained with transforms of different orders. The solution will contain, apart from the approximate eigenvalues, some complex and negative values as well and we ignore those. As can be seen from the table that, as the order of the transform is increased, one gets larger number of eigenvalues, and the lower eigenvalues becomes more and more accurate. If some eigenvalue is accurate up to eight decimal places, it is shown as an exact eigenvalue in the table. One may now ask, what about the eigenfunctions? For approximant of any order, the eigenfunction (un-normalized) is obatined by substituting the corresponding eigenvalues in the approximant. It is seen from the table that u_{10} correctly reproduces the first three eigenvalues at least. The first three eigenfunctions (both odd and even parity), properly normalized, along with the exact wave functions are shown in figure-13.

The eigenfunctions corresponding to ground state and the first excited state, as given by the u_2- transform, is obtained by substituting 1 and 3 for ϵ in the expressions for u_{2ev} and u_{2odd} in equations- 108 and 109 respectively and are given by

$$\psi_0 \approx \frac{1}{1 + \frac{\xi^2}{2} + \frac{\xi^4}{8}} \tag{110}$$

$$\psi_1 \approx \xi \frac{1}{1 + \frac{\xi^2}{2} + \frac{\xi^4}{8}} \tag{111}$$

These eigenfunctions are distinctly different from the actual eigenfunctions. However, a plot of these functions (properly normalised) shows that these fairly represents the actual eigenfunctions as can be seen from figure-14.

It is well known that, for a harmonic oscillator, the operator $(\xi - D)$ operating on the eigenfunction ψ for any state gives the next excited state. Thus, if we operate $(\xi - D)$ on ψ_0, we must get the eigenfunction of the first excited state.

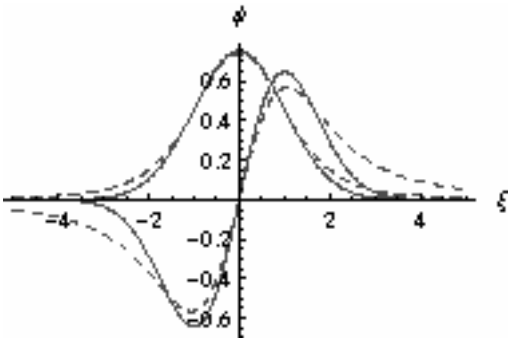


Figure 14: The ground state and the first excited states wave functions (normalised) obtained by the u_2-transform (equations-110 and 111) by shown by the dotted line and the exact wave functions by the solid lines.

If we designate it by $\psi_0^{(1)}$ we get

$$\psi_0^{(1)} = x\,\frac{8\left(16+8\xi^2+\xi^4\right)}{\left(8+4\xi^2+\xi^4\right)^2}. \tag{112}$$

It may noted that ψ_1 and $\psi_0^{(1)}$ looks distinctly different although both of them represents the first excited state and when properly normalised these two qualitatively describes the first excited states. One may ask at this point - can we find the eigenvalue for the first excited state from a knowledge of this eigenfunction? Yes, we can and let us see how. It is evident from equation-105 that $(-D^2+\xi^2)\psi/\psi$ should give the eigenvalue for the corresponding state for any value of ξ. If we remember that we made the series expansion about $\xi = 0$ and as such the approximants will better represent the function near the origin. Thus if one evaluates $(-D^2+\xi^2)\psi_0^{(1)}/\psi_0^{(1)}$ for some small value of ξ one must get eigenvalue for the first excited state. With $\xi = 10^{-6}$ one gets eigenvalue for the first excited state correct to 12 significant digits. One can go on operating $(\xi - D)$ to get subsequent states. For example, operating $(\xi - D)$ on $\psi_0^{(1)}$ one should get the eigenfunction for the second excited state and is given by

$$\psi_0^{(2)} = \frac{8\left(-128+128\xi^2+232\xi^4+92\xi^6+15\xi^8+\xi^{10}\right)}{\left(8+4\xi^2+\xi^4\right)^3} \tag{113}$$

and $\left(-D^2+\xi^2\right)\psi_0^{(2)}/\psi_0^{(2)}$evaluated at $\xi = 10^{-6}$ gives the second excited state correct to 11 significant digits. As one goes on repeating the procedure, the eigenfunctions become less and less accurate and consequently the accuracy of the eigenvalues obtained in this way decreases. This is not unexpected as one starts with an approximate eigenfunction and not the exact eigenfunction. The ground state eigenfunction given by equation-110 and the first three excited states $\psi_0^{(1)}$, $\psi_0^{(2)}$ and $\psi_0^{(3)}$ (properly normalised) fairly represent the states. It

Table 15: Perturbation series coefficients $b_n^{(2)}$ for the quartic anharmonic oscillator. Numbers in the parentheses correspond to the powers of 10 for the coefficients.

n	$b_n^{(2)}$	n	$b_n^{(2)}$
1	0.75 (00)	2	-1.3125 (00)
3	5.203125 (00)	4	-3.01611328125 (01)
5	2.23811279296875 (02)	6	-1.999462921142578 (03)
7	2.077708948516846 (04)	8	-2.456891772873402 (05)
9	3.256021887746751 (06)	10	-4.781043106012490 (07)

may be remarked that if one repeats the procedure starting with ψ_1 one gets similar results. For example, operating $(\xi - D)$ repeatedly on ψ_1 one should get the eigenfunctions for the second and higher excited states and the eigenfunctions for the second and third excited states obtained in this way are given by

$$\begin{aligned}
\psi_1^{(1)} &= \frac{8\left(-8+12\xi^2+7\xi^4+\xi^6\right)}{\left(8+4\xi^2+\xi^4\right)^2} \\
\psi_1^{(2)} &= \xi\,\frac{8\left(-384-128\xi^2+120\xi^4+68\xi^6+13\xi^8+\xi^{10}\right)}{\left(8+4\xi^2+\xi^4\right)^3}
\end{aligned}$$

and the eigenvalues corresponding to these states obtained by the method prescribed above are correct to 15 and 12 significant digits respectively. Thus, starting with only three terms of the direct series, one can obtain correct values for a number of states.

5.5 Quantum Anharmonic Oscillators

Anharmonic oscillators serve as simple model systems in many branches of physics and are also of particular interest as model systems in quantum field theory.. An overview of the work on anharmonic oscillators before 1980 can be found in the article by Killingbeck [78] and a number of subsequent references can be found in [79, 80, 81, 82-85]. Though seemingly simple, it is not an easy problem to find the energy spectrum and eigenfunctions of the anharmonic oscillators. One of the standard ways of solving the problem is to invoke perturbation theory. We briefly discuss this in the floowing section.

The anharmonic oscillators are defined by the Hamiltonian

$$H^{(m)}(\gamma) = H_0 + \gamma x^{2m}, \tag{114}$$

where

$$H_0 = p^2 + x^2 \tag{115}$$

The cases $m = 2, 3, 4$ correspond respectively to the quartic, sextic and octic oscillators respectively. The Rayleigh-Schrödinger perturbation theory for the ground state energies of the Hamiltonian is given by

$$E^{(m)}(\gamma) = \sum_{n=0}^{\infty} b_n^{(m)} \gamma^n, \tag{116}$$

with $b_0^{(m)} = 1$ for all m. A few coefficients $b_n^{(2)}$for the oscillators are shown in tables-15 and similar coefficients for $b_n^{(3)}$ and $b_n^{(4)}$are also available. The coefficients $b_n^{(m)}$ can be computed with the help of difference equation and is described in the article by Weniger *et. al* [79]. The coefficients $b_n^{(m)}$ tend to infinite for all m as $n \to \infty$. This divergence was confirmed numerically by Bender and Wu [86-88]. and $E^{(2)}(\gamma)$ diverges quite strongly for every $\gamma \neq 0$. Presently, we shall consider only the quartic oscillator as the conclusions for other oscillators are very similar though somewhat difficult.

Ever since the seminal work of Bender and Wu, Rayleigh-Schrödinger perturbation expansion of the an-harmonic oscillators have been textbooks examples of strongly divergent perturbation series. A large number of works on the summation of these perturbation series with the help of Padé approximants exist in the literature. It can be proved that the perturbation series for the quartic an-harmonic oscillators are Padé summable.

We now show that the divergent perturbation series for the quartic oscillator can be *summed* much more effectively by Levin-Weniger transforms. We note that, apart from the first term, the perturbation series is an alternating one. Thus, we leave aside the first term and form an approximant with the rest of the series. Using the perturbation series for $E^{(2)}(\gamma)$ given by equation-116 the τ_6-approximant (with $\beta = 0$) is given by

$$\tau_6 = 1+$$

$$\frac{0.75\gamma + 24.1935\gamma^2 + 245.396\gamma^3 + 900.827\gamma^4 + 1024.21\gamma^5 + 198.404\gamma^6}{1 + 34.008\gamma + 379.772\gamma^2 + 1669.99\gamma^3 + 2722.63\gamma^4 + 1233.52\gamma^5 + 59.9627\gamma^6}. \tag{117}$$

Figure-15 shows the plots of τ_4, τ_6 and τ_8 along with the exact eigenvalues. The figure also shows the plots of [3/4] and [4/4] Padé approximants. It is evident that the τ-transform can *sum* the series much more effectively.

However, the eigenvalues can be determined much more efficiently by using the re-normalized perturbation series. For large values of the coupling parameter it is better to use the strong coupling expansion. Using Symanzik scaling it can be shown that $E^{(m)}(\gamma)$ possesses also a strong coupling expansion which is convergent:

$$E^{(m)}(\gamma) = \gamma^{\frac{1}{m+1}} \sum_{n=0}^{\infty} K_n^{(m)} \gamma^{\frac{-2n}{m+1}} \tag{118}$$

where $K_n^{(m)}$ are the coefficients of the strong coupling expansion. As equation-117 is a power series in γ and the above strong coupling expansion is a power

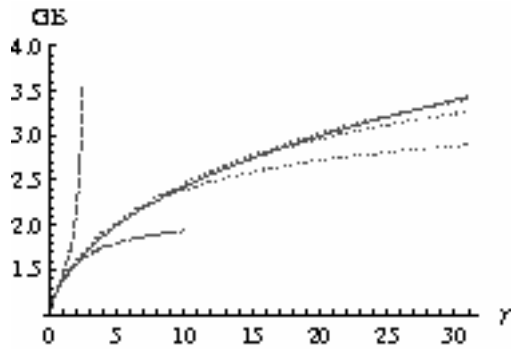


Figure 15: Ground state energy (GE) of the quartic an-harmonic oscillator *vs* γ. Solid line -exact; dotted curves - τ-transforms of orders 4, 6 and 8 ($\beta = 0$); dashed curves - [3/4] and [4/4] Padé approximants.

in $\gamma^{-\frac{2}{m+1}}$ and these two expansions have incompatible variables and cannot be used for constructing two-point approximant which will be valid over the entire range.

It is obvious that the energy eigenvalues of the an-harmonic oscillators can be efficiently computed if the asymptotic behavior can somehow be incorporated into the perturbation scheme. This is accomplished with the help of the re-normalization scheme of Vinette and Cizek [91]. The re-normalized Hamiltonian can be written

$$\begin{aligned} H^{(m)}(\kappa) &= (1-\kappa)^{-1/2}\left[p^2 + x^2 + \frac{\kappa}{B_m}\left(x^{(2m)} - B_m x^2\right)\right] \\ &= (1-\kappa)^{-1/2} H_R^m(\kappa) \end{aligned} \tag{119}$$

where $B_m = \frac{m(m-1)!!}{2^{m-1}}$ and the re-normalized coupling constant k is related to γ through the equation $\gamma = \frac{1}{B_m}\frac{\kappa}{(1-\kappa)^{\frac{(m+1)}{2}}}$. The energy can be written as

$$E_R^m(\kappa) = \sum_{n=0}^{\infty} c_n^{(m)} \kappa^n \tag{120}$$

.The energy $E_R^{(m)}(\kappa)$ of the re-normalized Hamiltonian $H_R^{(m)}(\kappa)$ possesses an additional perturbation series in powers of $(1-\kappa)$ and can be written as

$$E_R^{(m)}(\kappa) = \sum_{0}^{\infty} (1-\kappa)^n \ \Gamma_n^{(m)} \tag{121}$$

where $\Gamma_n^{(m)}$ is related to $c_n^{(m)}$ through the equation

$$\Gamma_n^{(m)} = \frac{(-1)^n}{n!} \sum_{\nu=0}^{\infty} (\nu+1)_n c_{n+\nu}^{(m)} \tag{122}$$

Table 16: Two-point τ-approximants for $E_R^{(m)}(\kappa)$ for an-harmonic oscillators. m=2, 3 and 4 correspond respectively to the quartic, sextic and octic anharmonic oscillators.

m	Two-point approximants
2	$\tau_2 = \dfrac{1 + 0.098951398448695\kappa - 0.111867731520187\kappa^2}{1 + 0.348951398448695\kappa - 0.006371342766916\kappa^2}$ $\tau_3 = \dfrac{1 + 1.837798720289505\kappa - 0.365284914180951\kappa^2 - 0.073030161413163\kappa^3}{1 + 2.087798720289505\kappa - 0.177498099224758\kappa^2 - 0.001643500918748\kappa^3}$
3	$\tau_2 = \dfrac{1 + 0.233708765896205\kappa - 0.269105045615645\kappa^2}{1 + 0.567042099229538\kappa - 0.023897896753149\kappa^2}$ $\tau_3 = \dfrac{1 + 5.444109045278168\kappa - 1.494165870971539\kappa^2 - 0.396769776998241\kappa^3}{1 + 5.7774423786115\kappa + 0.522388995973074\kappa^2 - 0.015800654816468\kappa^3}$
4	$\tau_2 = \dfrac{1 + 0.181221984340383\kappa - 0.336533753511279\kappa^2}{1 + 0.556221984340383\kappa - 0.0346131480068169\kappa^2}$

Because of the presence of the Pochhammer symbol $(\nu + 1)_n$ and the fact that $c_{n+\nu}^{(m)}$ grows rapidly with increasing index, the above infinite series grows much more rapidly. However the Levin-like transforms can be used to obtain $\Gamma_n^{(m)}$.

Since there exist two expansions of $E_R^{(m)}(\kappa)$ in terms of κ and $(1-\kappa)$, as given above, they can be used to construct two-point Padé or Levin-like transforms. We give the two-point τ_2 and τ_3 approximants in table-16 for $m = 2$, 3 and τ_2 approximant for $m = 4$ as the coefficients of the expansion of $E_R^{(4)}$ about $\kappa = 1$ (i.e., $\Gamma_n^{(4)}$) for the octic oscillator are not known with sufficient accuracy,.

Ground state energy eigenvalues of the quartic oscillator for some specific values of γ, along with the exact values are given in table-17 . It is seen from the table that, for a given input, the two-point τ-approximants [92] reproduce better the energy eigenvalues than the two-point Padé approximants. The simple expression using the τ_2-transform reproduces the energy eigenvalues of the quartic oscillator over the entire range of the coupling parameter shown. The number of significant digits obtained with the two-point τ-approximant for γ= 0.2 and 2000 are respectively 5 and 9. The agreement is better for higher values of the coupling parameter. Table-18 gives the values of the error for quartic, sextic and octic oscillators with two-point Padé and τ approximants. In all cases it is found that the τ approximants reproduce the energy eigenvalues better than Padé approximants.

It is evident from the above discussion that it is really difficult to calculate even the ground state energy of the an-harmonic oscillators, not to speak of the

Table 17: Calculated values of the ground state energy eigenvalues of the quartic oscillator using two-point approximants. In each case two coefficients are used from the expansion about $\kappa = 1$ and the other coefficients are determined from the expansion about $\kappa = 0$ (excluding the $c_0 = 1$ term). The last column gives the exact energy eigenvalues.

γ	Approximants used				Exact
	τ_2	[1/1]	τ_3	[1/2]	
0.2	1.11838	1.11818	1.1183026	1.1182811	1.118292654
1.0	1.39244	1.39194	1.3923695	1.3923346	1.392351642
4.0	1.90317	1.90264	1.9031467	1.9031283	1.903136945
100.0	4.9994198	4.99916	4.9994182	4.9994170	4.999417545
2000.0	13.38844178	13.38834	13.388441696	13.388441635	13.388441701

Table 18: $|log_{10}(\text{absolute error})|$ for quartic, sextic and octic oscillators ($m =$ 2, 3, 4 respectively) obtained from two-point approximants. Expansion about $\kappa = 1$ furnishes two coefficients and that about $\kappa = 0$ (excluding $c_0^{(m)} = 1$) gives the others.

γ	$m = 2$				$m = 3$				$m = 4$	
	τ_2	[1/1]	τ_3	[1/2]	τ_2	[1/1]	τ_3	[1/2]	τ_2	[1/1]
0.2	4.1	4.0	5.0	4.9	3.2	2.5	3.8	2.9	2.9	1.9
1.0	4.1	3.4	4.8	4.8	3.4	2.4	4.0	3.2	3.2	1.9
4.0	4.4	3.3	5.0	5.1	3.8	2.4	4.3	3.5	3.5	2.0
100.0	5.6	3.6	6.2	6.3	4.7	2.7	5.1	4.4	4.4	2.2
2000.0	7.1	4.0	8.3	7.2	5.6	3.0	6.0	4.9	4.9	2.4

Table 19: Values of $K_0^{(m,n)}$ for different values of m and n

n	$K_0^{(2,n)}$	$K_0^{(3,n)}$	$K_0^{(4,n)}$
0	1.0604	1.1448	1.2258
1	1.2666	1.4516	1.5853
2	1.4911	1.8187	2.0627
3	1.6634	2.1370	2.4886
4	1.8068	2.4157	2.8771
5	1.9307	2.6663	3.2355

()

excited states. However, it is tempting to mention that there are remarkable systematic in the energy eigenvalues of the quantum an-harmonic oscillators [93,94]. If $E^{(m,n)}$ be the nth excited state energy of the Hamiltonian given by equation- 114, then the energy predicted by the equation

$$\left(\frac{E^{(m,n)}}{2n+1}\right)^{(m+1)} - \left(\frac{E^{(m,n)}}{2n+1}\right)^{(m-1)} = \left(K_0^{(m,n)}\right)^{(m+1)} \gamma, \qquad (123)$$

where $K_0^{(m,n)}$ are constants. The values of $K_0^{(m,n)}$for for different m and n are shown in table- For the ground state $K_0^{(m,0)} has$ been evaluated by different authors [95, 96] for $m = 2$, 3, 4, 5. For the quartic oscillator, $K_0^{(2.n)}$has been evaluated by Skăla *et al* [95] for $n = 1\,2, \cdots 10$. It can be shown that for very large coupling constant $K_0^{(m,n)}$ is re related to $E^{(m,n)}$, *i.e.*,$E^{(m,n)} \cong \gamma^{\frac{1}{m+1}} K_0^{(m,n)}$. For the sextic and octic oscillators, the values of $K_0^{(m,n)}$ for the excited states were estimated by evaluating the energy for very large γ (=10^6). We then made rational interpolation to obtain n-dependence of $K_0^{(m,n)}$and these are as follows:

$$K_0^{(2,n)} = \left(\frac{1.1924+33.2383\,n=56.2169\,n^2}{1+43.6106\,n}\right)^{1/3}$$

$$K_0^{(3,n)} = \left(\frac{1.7176+1.3224\,n+2.6933\,n^2+0.7092\,n^3}{1+0.4510\,n}\right)^{1/4}$$

$$K_0^{(4,n)} = \left(\frac{2.7676+12.6576\,n+9.2212\,n^2+13.3678\,n^3+6.4509\,n^4}{1+3.1840\,n}\right)^{1/5}$$

Some values of $K_0^{(m,n)}$ for $m = 2$, 3, 4 are shown in table-19

The authors [94] calculated the energy eigenvalues of 25 excited sates for the quartic oscillator, 19 excited states for the sextic oscillator and for different values of the coupling parameter. It was found that the simple formula reproduces the energy eigenvalues with an accuracy of 1% over the wide range of the coupling parameter.

A global Padé approximant was also made for $K_0^{(m,0)}$ as follows:

$$K_0^{(m,0)} = \frac{1 + 0.7961\,(m-1) - 0.05129\,(m-1)^2 - 0.04694\,(m-1)^3}{1 + 0.7858\,(m-1) - 0.1655\,(m-1)^2 + 0.01902\,(m-1)^3}$$

To test the above, the values calculated for $m = 250$ and $m = 500$ are respectively 2.3954 and 2.4307 which compares well with the values 2.400235 and 2.433557 reported by Farandez and Guardiola [96].

6 Other Applications and Conclusion

In a subsequent article Roy and Bhattacharya [97] used the Levin and Weniger transforms to predict the unknown terms of a series.. One advantage of the Levin-like transforms is that these transforms have a free parameter β and one can exploit it for prediction of the subsequent terms. The Levin and Weniger transforms k, which requires $k+1$ terms of the original series, we can adjust the value of β so that the $(k+2)$-th term is predicted exactly. One can then include one more term of the series, obtained by expanding the k-th order transform, and form a transform of order $k+1$ with the same value of β. We iterate the procedure to predict the subsequent terms of the series and the procedure may be termed as the method of successive expansion. Using this method it is possible to predict the subsequent terms of the series even when the coefficients themselves form a sequence of functions of some other variable. Such situations arise in some Ising problems and in some problems in QCD .

The authors applied the method to a number of physical problems, namely, the perturbation series for the hydrogen atom in a magnetic field, the quartic anharmonic oscillator, the sequences encountered in Ising problems, some series encountered in quantum electrodynamic (QED) and quantum chromodynamics (QCD) and the excluded volume problem in polymers. It is observed that in almost all these diverse physical problems the relevant physical parameters can then be evaluated with an accuracy higher than that obtainable by summing the original input series. Thus it is possible to obviate, to some extent, the necessity as well as the labour of evaluating more terms of the divergent series encountered in many physical problems.

Das and Roy [98] used these transforms to solve the motion of a projectile with quadratic damping in a constant gravitational field. It was demonstrated that it is possible to obtain the path with a few terms of the divergent series for $x(t)$ and $y(t)$ by using these transforms.

There exists the possibility of extending these transforms to sequences of vectors and sequences of matrices.

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Modeling of blood flow through a deformable artery

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ABSTRACT

The application of drug targeting delivery using magnetic nanoparticles to treat various medical conditions is of significant interest, particularly in the context of controlling tumor growth and addressing cardiovascular diseases like atherosclerosis and aneurysms. This paper aims to develop a mathematical model describing blood flow and magnetic nanoparticles injected into the bloodstream. These nanoparticles are directed to specific locations within the body by utilizing an external magnetic field applied to the flowing blood. The analytical solutions obtained from this model to examine how wall deformation influences the motion of nanoparticles within the bloodstream and the overall dynamics of blood flow. The validity of our findings has been substantiated by comparing them with previous research concerning the velocity profile.

Keywords: Deformable artery, Magnetic nanoparticles, Drug delivery, Pressure wave propagation

NOMENCREATURE

Quantity	Symbol	Value		
Radius of the vessel (m)	R_0	0.01	Induced electric field (V/m)	$\boldsymbol{E}$
Circular frequency (rd/s)	ω	7.854	Magnetic flux intensity (T)	**B**
Young modulus of aortic (Pa)	E	10^6	Induced current density (A/m^2)	$\boldsymbol{J}$
Thickness ofthe wall (m)	h	0.002	Electric permittivity (F/m)	ϵ
Wall density (kg/m^3)	ρ_s	1100	Charge density (C/m^3)	ρ_e
Blood density (kg/m^3)	ρ	1050	Magnetic permeability (H/m)	μ
Blood viscosity (Pa s)	η	4×10^{-3}	Electricalconductivity of blood (S/m)	σ
Stokes constant	K_s	3.17×10^{-17}	Uniform magnetic field strength (T)	B_0
Mass of nanoparticle (kg)	m	26.2×10^{-20}	Magnetic flux intensity (T)	**B**
Poisson's ratio	σ_p	0.5		

INTRODUCTION

Delivering the precise dosage of a drug to a specific location in the human body is a challenging task aimed at avoiding excessive drug exposure to healthy tissues, which can lead to side effects and affect other organs [1,2]. Ciofani et al. [3] introduced a nanotechnology platform that utilizes magnetic nanoparticles for drug delivery applications, particularly in the realms of chemotherapy and thermotherapy. Magnetic drug targeting has emerged as a valuable technique for directing drugs to precise locations within the body by imposing an externally applied magnetic field. Several numerical and analytical studies [4, 5, 6,7] have investigated the flow of blood containing magnetic nanoparticles within arteries. The impact of a magnetic field on blood flow has been examined both analytically and numerically by Abi-Abdallah [8,9] in a straight tube, while Drochon [10] examined the blood flowin a vessel with wall deformation. However, these studies did not specifically account for the motion of magnetic nanoparticles in the context of targeted drug delivery applications. Moreover, it is crucial to emphasize the drug delivery with magnetic nanoparticles for the deformable characteristics of the vessel wall.

2 PROBLEM FORMULATION

The following Maxwell's equations of electromagnetism are employed to represent the magnetohydrodynamic flow of blood in an arterial segment:

$$\nabla . \boldsymbol{E} = \frac{\rho_e}{\epsilon},$$

$$\nabla \times \boldsymbol{E} = -\frac{\partial \vec{B}}{\partial t}, \quad (1)$$

$$\nabla . \mathbf{B} = 0,$$

$$\nabla \times \mathbf{B} = \mu.$$

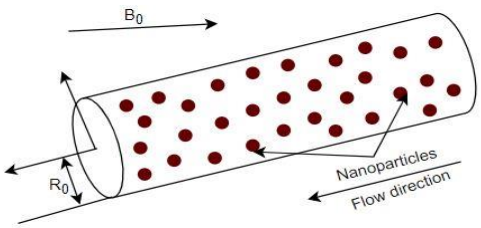

Fig. 1: Geometry of the model

In this model (cf. Fig. 1), it is important to consider the direction of the externally applied magnetic field and the direction of blood flow at an angle θ. As a consequence of this configuration, the magnetic flux intensity is represented as $\boldsymbol{B} = (B_0 cos\theta, -B_0 sin\theta, b_z(r,\theta,t))$. The angle between the direction of flow and the applied magnetic field is assumed to be $\theta = \frac{\pi}{2}$. The induced current density $\boldsymbol{J}$ can be obtained from Ohm's law ,$\boldsymbol{J} = \sigma(\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B})$. (2)

2.1 Equations of Motion

The continuity equation with fluid velocity components $(u_r, 0, u_z)$ and the nanoparticle velocity components $(v_{rp}, 0, v_{zp})$ can be written as:

$$\frac{\partial u_r}{\partial r} + \frac{u_r}{r} + \frac{\partial u_z}{\partial z} = 0. \qquad (3)$$

The Navier-Stokes equation can be projected onto the radial and axial directions as follows:

$$\frac{\partial u_r}{\partial t} = -\frac{1}{\rho}\left(\frac{\partial P}{\partial r}\right) + \nu\left(\frac{\partial^2 u_r}{\partial r^2} + \frac{1}{r}\frac{\partial u_r}{\partial r} + \frac{\partial^2 u_r}{\partial z^2} - \frac{u_r}{r^2}\right) - \frac{\sigma u_r B_0}{\rho} + \frac{K_s N}{\rho}(v_{rp} - u_r), \qquad (4)$$

$$\frac{\partial u_z}{\partial t} = -\frac{1}{\rho}\left(\frac{\partial P}{\partial z}\right) + \nu\left(\frac{\partial^2 u_z}{\partial r^2} + \frac{1}{r}\frac{\partial u_z}{\partial r} + \frac{\partial^2 u_z}{\partial z^2}\right) - \frac{\sigma u_z B_0}{\rho} + \frac{K_s N}{\rho}(v_{zp} - u_z). \qquad (5)$$

The amplitude of the pressure disturbance is sufficiently small to the extent that the nonlinear terms related to the inertial term of fluid flow can be regarded as negligible when compared to the linear terms.

2.2 Boundary conditions

It is assumed that the velocity of blood at the vessel wall is the same as the wall motion. The mathematical form is provided as follows:

$$u_r = \frac{\partial \zeta_r}{\partial t}, \quad u_z = \frac{\partial \zeta_z}{\partial t}, \qquad \text{at } r = R_0,$$

$$\text{and} \quad u_r = 0, \ \frac{\partial u_z}{\partial r} = 0, \qquad \text{at } r = 0. \qquad (6)$$

2.3 Deformation of the vessel wall

We assume that $\zeta = (\zeta_r(z,t), 0, \zeta_z(z,t))$ be the radial and longitudinal displacements of an arbitrary point at the wall after deformation. The equations of motion of the interaction of deformed vessel wall and blood flow are taken in components as

$$\rho_s h \frac{\partial^2 \zeta_r}{\partial t^2} = \left[P - 2\eta \frac{\partial u_r}{\partial r}\right]_{r=R_0} - \frac{Eh}{R_0(1-\sigma_p^2)}\left(\frac{\zeta_r}{R_0} + \sigma_p \frac{\partial \zeta_z}{\partial z}\right), \qquad (7)$$

$$\rho_s h \frac{\partial^2 \zeta_z}{\partial t^2} = -\eta \left[\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}\right]_{r=R_0} + \frac{Eh}{(1-\sigma_p^2)}\left(\frac{\partial^2 \zeta_r}{\partial z^2} + \frac{\sigma_p}{R_0}\frac{\partial \zeta_r}{\partial z}\right). \qquad (8)$$

3 ANALYTICAL SOLUTION

By utilizing the Navier-Stokes Eqs. (3), (4) and the continuity equation (2), we obtain,

$$\nabla^2 P - div(\boldsymbol{J} \times \boldsymbol{B}) = 0. \qquad (9)$$

We assume that the solution of the unknown variables takes in the form

$$\left[\boldsymbol{u}, \boldsymbol{v}_p, P\right] = \left[\boldsymbol{u}^*, \boldsymbol{v}_p^*, P^*\right] \exp\left[i\omega\left(t - \frac{z}{c}\right)\right]. \qquad (10)$$

We obtain the solution P^* by using equations (9) and (10) as

$$P^*(r) = \frac{\eta c}{\omega}\frac{\alpha_m^2}{R_0^2} A_1 J_0\left(\frac{i\omega}{c} r\right), \qquad (11)$$

where the dimensionless parameter α_m is defined as $\alpha_m = R_0\sqrt{\frac{\omega}{\nu} - \frac{iK_s N}{\eta} + \frac{iK_s^2 N}{\eta(mi\omega + K_s)} - i\frac{Ha^2}{R_0^2}}$

and Hartmann number Ha defined as $Ha = R_0 B_0 \sqrt{\frac{\sigma}{\eta}}$.

Using the boundary condition (5), axial velocity can be obtained as

$$u_z^*(r) = A_1 J_0\left(i\frac{\omega}{c} r\right) + A_2 \frac{J_0\left(\frac{\delta r}{R_0} i^{\frac{3}{2}}\right)}{J_0\left(\delta i^{\frac{3}{2}}\right)}, \qquad (12)$$

where $\delta = \sqrt{\alpha_m^2 - i\frac{\omega^2}{c^2} R_0^2}$.

The radial velocity of the blood can be obtain as

$$u_r^*(r) = A_1 J_0\left(i\frac{\omega}{c} r\right) + \frac{R_0 i\omega}{c\delta i^{\frac{3}{2}}} A_2 \frac{J_1\left(\frac{\delta r}{R_0} i^{\frac{3}{2}}\right)}{J_0\left(\delta i^{\frac{3}{2}}\right)}. \qquad (13)$$

The displacement of the vessel wall can be taken in the form

$$\zeta_r(t,z) = A_3 \exp\left[i\omega\left(t - \frac{z}{c}\right)\right],$$

$$\zeta_z(t,z) = A_z \exp\left[i\omega\left(t - \frac{z}{c}\right)\right]. \qquad (14)$$

In order to determine the integration constants A_1, A_2, A_3 and A_4, the following assumptions are made:

(i) The radius of the vessel is smaller than the wavelength of oscillation, ensuring that $\frac{\omega R_0}{c} \ll 1$.

(ii) $J_0\left(i\frac{\omega}{c}R_0\right) \approx 1,\ J_1\left(i\frac{\omega}{c}R_0\right) = \frac{i\omega R_0}{2c}.$

Let us define $F = \frac{2J_1\left(\delta i^{\frac{3}{2}}\right)}{\delta i^{\frac{3}{2}} J_1\left(\delta i^{\frac{3}{2}}\right)}.$

A homogeneous linear system of equations represented by $BA = 0$ is obtained using the boundary conditions (6) into the Eqs. (7), (8), (12) and (13), yields

$$B=[b_{ij}]_{4\times4}=\begin{pmatrix} \frac{i\omega R_0}{2c} & \frac{i\omega R_0}{2c}F & -i\omega & 0 \\ 1 & 1 & 0 & -i\omega \\ b_{31} & -\eta i\omega(2-F) & -\frac{4Eh}{R_0^2} & \frac{2Ehi\omega}{3R_0c} \\ -\frac{\eta\omega^2}{c^2}R_0 & \frac{\eta}{2}\left[\frac{\delta^2 i^3}{R_0^2}-\frac{\omega^2}{c^2}\right]R_0F & -\frac{2Ehi\omega}{3R_0c} & \frac{\rho_s h\omega^2}{3c^2} \end{pmatrix},$$

Where the unknowns $A = [A_1 A_2\ A_3\ A_4]^T$, and

$$b_{31} = \rho c - \frac{\eta c}{\omega}\frac{iM^2}{R_0^2} - \frac{\eta i\omega}{c} - \frac{iK_s Nc}{\omega} + \frac{iK_s^2 Nc}{\omega(mi\omega+K_s)}.$$

Using the row and column operations, and the method adopted by Atabek and Lew [11], we obtain the frequency equation in $\frac{c}{c_0}$ as

$$\frac{16}{3}(1-F)\left(\frac{c_0}{c}\right)^2 + \left[-\frac{8}{3}(1-F)k + \frac{4}{3}\left(K + \frac{iNK_s}{\rho\omega}\left(\frac{K_s}{im\omega+K_s}-1\right)(F-4)\right]\left(\frac{c}{c_0}\right)^2 + \left(\frac{\delta^2\nu}{R_0^2\omega}F + 2k\right)\left(K + \frac{iNK_s}{\rho\omega}\left(\frac{iNK_s}{im\omega+K_s}-1\right)\right) = 0. \qquad (15)$$

In the above equations, two non-dimensional numbers, denoted as k and K are defined as

$$k = \frac{\rho_s h}{\rho R_0}, \qquad K = 1 - i\frac{Ha^2\nu}{R_0^2\omega}.$$

Table 2: The roots of the frequency equation, represented by Young mode solution $(\frac{c_1}{c_0})$ and the Lamb mode solution $(\frac{c_2}{c_0})$, when $N = 3.78 \times 10^{20}$.

Ha	**0**	**1**	**2**
$\frac{c_1}{c_0}$	0.920+ 0.02818 i	0.9207+ 0.0302 i	0.920+ 0.0359i
$\frac{c_2}{c_0}$	3.11687+0.3587i	3.1171+ 0.35955i	3.1179+ 0.3620 i

Mod(c_1) (m/s)	8.99122	8.99073	8.9882
Mod(c_2) (m/s)	30.6214	30.6251	30.6351

Ha	**4**	**10**	**20**
$\frac{c_1}{c_0}$	0.9172+0.05904 i	0.85536 + 0.19855 i	0.5602 + 0.3299 i
$\frac{c_2}{c_0}$	3.12097+0.3719 i	3.1337 + 0.4405 i	3.1082 + 0.6519 i
Mod(c_1) (m/s)	8.9704	8.57027	6.3452
Mod(c_2) (m/s)	30.6762	30.8856	30.9961

Calculating the celerities$c$, we solve the constants $A_1, A_2, A_3$and A_4, such that the system expresses in terms of the free variable A_1as follows

$$\frac{A_2}{A_1} = -\frac{\left(K-\frac{\omega\nu i}{c^2}+\frac{iK_S N}{\rho\omega}\left(\frac{K_S}{mi\omega+K_S}-1\right)\right)}{-\frac{\nu i\omega}{c^2}(2-F)+\frac{2Eh}{3R_0\rho c^2}(1-F)}, \tag{16}$$

$$\frac{A_3}{A_1} = \frac{R_0}{2c} + \frac{R_0}{2c} F \frac{A_2}{A_1}, \tag{17}$$

$$\frac{A_4}{A_1} = \frac{1}{i\omega}(1 + \frac{A_2}{A_1}). \tag{18}$$

The non-dimensional equations for fluid velocities and the behavior of nanoparticles are obtained as

$$\frac{u_Z^*(r)}{A_1} = 1 + \frac{A_2}{A_1}\frac{J_0\left(\frac{\delta r}{R_0} i^{\frac{3}{2}}\right)}{J_0\left(\delta i^{\frac{3}{2}}\right)}, \quad \text{since } J_0\left(\frac{i\omega r}{c}\right) = 1. \tag{19}$$

$$\frac{u_r^*(r)}{A_1} = \frac{i\omega R_0}{c}\left[\frac{r}{2R_0} + \frac{A_2}{A_1}\frac{1}{\delta i^{\frac{3}{2}}}\frac{J_1\left(\frac{\delta r}{R_0} i^{\frac{3}{2}}\right)}{J_0\left(\delta i^{\frac{3}{2}}\right)}\right], \text{as } J_0\left(\frac{i\omega r}{c}\right) = \frac{i\omega r}{2c}, \tag{20}$$

$$\frac{v_{rp}^*}{A_1} = \frac{K_s}{mi\omega+K_s}\frac{i\omega R_0}{c}\left[\frac{r}{2R_0} + \frac{A_2}{A_1}\frac{1}{\delta i^{\frac{3}{2}}}\frac{J_1\left(\frac{\delta r}{R_0} i^{\frac{3}{2}}\right)}{J_0\left(\delta i^{\frac{3}{2}}\right)}\right], \tag{21}$$

$$\frac{v_{zp}^*}{A_1} = \frac{K_s}{mi\omega + K_s}\left[1 + \frac{A_2}{A_1}\frac{J_0\left(\frac{\delta r}{R_0} i^{\frac{3}{2}}\right)}{J_0\left(\delta i^{\frac{3}{2}}\right)}\right]. \qquad (22)$$

4 RESULTS AND DISCUSSION

The wave celerities, are the roots of Eq. (15), provided in Table 2. It is worth noting that the values obtained in the case of $Ha = 0$ and $N = 0$ are consistent with the results of Atabek and Lew [11] while considering the propagation of pressure pulses in elastic vessels without a magnetic field.

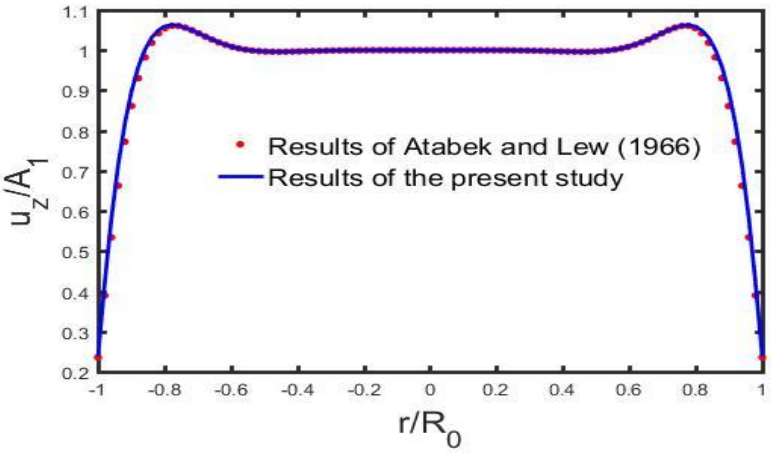

Fig. 2: Comparison of the axial component of velocity u_z/A_1 for the Young wave with the solution of Atabek and Lew, when Ha = 0, Ks = 0.

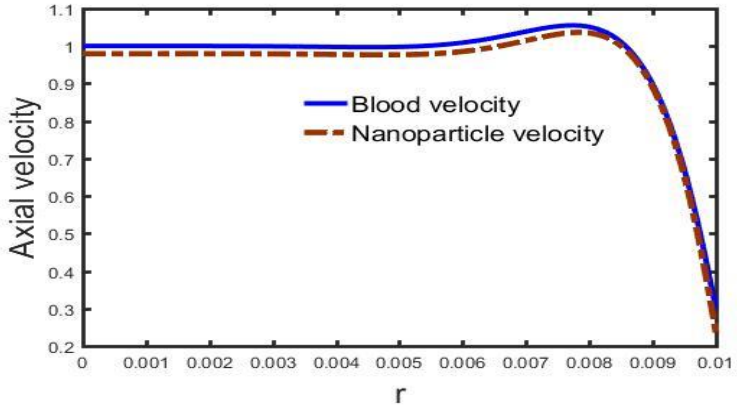

Fig. 3: The moduli (absolute values) of the amplitudes of the non-dimensional axial velocity, $\left|\frac{u_z^*}{A_1}\right|$ and $|\frac{v_{zp}^*}{A_1}|$ for Hartmann number, $Ha = 2$.

The absolute values (moduli) of the amplitudes of the non-dimensional axial and radial velocities $\left|\frac{u_z^*}{A_1}\right|$, $\left|\frac{v_{zp}^*}{A_1}\right|$, $\left|\frac{u_r^*}{A_1}\frac{c}{\omega R_0}\right|$ and $\left|\frac{v_{pr}^*}{A_1}\frac{c}{\omega R_0}\right|$ have been computed using the Eqs. (19), (20), (21) and (22) for both types of waves, namely Young waves ($c = c_1$) and Lamb waves ($c = c_2$).

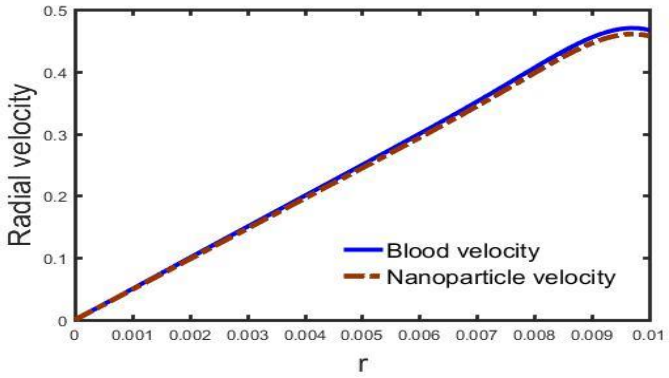

Fig. 4: The moduli (absolute values) of the amplitudes of the non-dimensional radial velocity, $\left|\frac{u_r^*}{A_1}\frac{c}{\omega R_0}\right|$ and $\left|\frac{v_{pr}^*}{A_1}\frac{c}{\omega R_0}\right|$ for Hartmann number, $Ha = 2$.

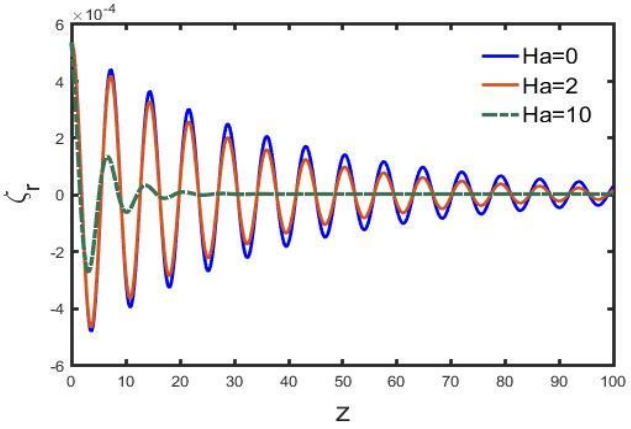

Fig. 5: The radial displacement, $\frac{\zeta_r}{A_1}$, of the wall is plotted for various values of the Hartmann number, Ha, in the case of Young waves at $t = 0$.

In this context, the velocity profiles of both the fluid and nanoparticles are plotted in Fig. 2 and Fig. 3 for the case with a Hartmann number, $Ha = 2$, and under the influence of Young waves. It is evident that the external magnetic field exerts an influence on the wave celerities within the fluid and the vessel wall, as well as on the fluid velocity profiles. Specifically, it tends to

decrease blood flow and flatten the velocity profile.The graph illustrates that the absolute value of fluid velocity is higher than that of nanoparticle velocity.Fig. 4 depicts that the radial displacement of the wall (Eq. 14) decreases as the Hartmann number increases.

CONCLUSION

The influence of the external magnetic field is evident in various aspects, including its impact on the wave celerities within the fluid and the vessel wall, fluid velocity profiles, and wall displacements. Regarding wall displacement, it is important to note that the axial velocity is not zero at the vessel wall. The flow of nanoparticles is equal to $\frac{K_s}{mi\omega+K_s}$ times the flow of blood with $|\frac{K_s}{mi\omega+K_s}| < 1$.

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