Topologically related quantities in turbulent flows

Cassidy, William Alfred, Ph.D.

City University of New York, 1987

U·M·I
300 N. Zeeb Rd.
Ann Arbor, MI 48106

PLEASE NOTE:

In all cases this material has been filmed in the best possible way from the available copy. Problems encountered with this document have been identified here with a check mark __√__.

1. Glossy photographs or pages _____
2. Colored illustrations, paper or print _____
3. Photographs with dark background _____
4. Illustrations are poor copy _____
5. Pages with black marks, not original copy _____
6. Print shows through as there is text on both sides of page _____
7. Indistinct, broken or small print on several pages __√__
8. Print exceeds margin requirements _____
9. Tightly bound copy with print lost in spine _____
10. Computer printout pages with indistinct print _____
11. Page(s) _____ lacking when material received, and not available from school or author.
12. Page(s) _____ seem to be missing in numbering only as text follows.
13. Two pages numbered _____. Text follows.
14. Curling and wrinkled pages _____
15. Dissertation contains pages with print at a slant, filmed as received __√__
16. Other _____

TOPOLOGICALLY RELATED QUANTITIES IN TURBULENT FLOWS

by

WILLIAM ALFRED CASSIDY

A dissertation submitted to the Graduate Faculty in Engineering in partial fulfillment of the requirements for the degree of Doctor of Philosophy, The City University of New York.

1987

This manuscript has been read and accepted by the Graduate Faculty in Engineering in satisfaction of the dissertation requirement for the degree of Doctor of Philosophy.

6/22/87
Date

Chair of the Examining Committee

6/22/87
Date

Paul R Karmel
Executive Officer

Dr. H. Weinstein

Dr. D. Rumschitzki

Dr. R. Pelz
Supervisory Committee

The City University of New York

Abstract

TOPOLOGICALLY RELATED QUANTITIES IN TURBULENT FLOW

by

William A. Cassidy

Advisors: Professor Benjamin G. Levich
Professor Evgeny V. Levich

The purpose of this work is to study the role of changes in the topology of the vortex field in the development of turbulence. Analytical work on helicity and representability in terms of Clebsch variables is presented relating both to the instantaneous topology of the vortex field and to the dynamics of the time development of the fields in the case of incompressible, Newtonian flows. It is found that, at a given point, the topological changes relating to helicity and Clebsch representability are due to only one component of the viscosity term in the Navier-Stokes, that component which is parallel to the vorticity at the point. When this component of the viscosity term is subtracted a modified Navier-Stokes equation results which conserves helicity and Clebsch representability. Some analytical properties of the resulting equation are discussed.

The simulation of the resulting equation is discussed and the results are presented. The usual statistics of the resulting flow fields are presented as well as some more novel ones. Comparing the simulation results of the usual and modified Navier-Stokes equations, the most remarkable differences that emerge are related to the non-linearity of the modified viscosity term rather than the conservation of helicity and Clebsch representability. The growth of helicity spectral density is observed for the lowest wave-number modes, and appears insensitive to the preservation of Clebsch representability and conservation of total helicity as well. It is concluded that conservation in time of total helicity and preservation of Clebsch representability do not prevent the development of turbulence. Suggestions of the implications of this to possible further research are given.

We would like to thank the following people for thier indispensible help in the preparation of this thesis:

Dr. A. Frenkel
Dr. R Pelz
Dr. L. Shtilman

This work was preformed under the auspices of the Deparment of Energy, Grant #DE-AC02-80ER10559 (RF 447805)

'And it is also said,' answered Frodo: 'Go not to the Elves for counsel, for they will say both no and yes.'

'It is indeed?' laughed Gildor. 'Elves seldom give unguarded advice, for advice is a dangerous gift, even from the wise to the wise, and all courses may run ill.'

J.R.R. Tolkien
The Fellowship of the Ring

TABLE OF CONTENTS

LIST OF GRAPHS

CHAPTER I

INTRODUCTION:

1. ABOUT THIS WORK

The purpose of this work is to elucidate the role of the topology of the vortex lines in the development of turbulence. The starting point of this work is the observation that Euler flows (flows with zero viscosity) preserve the topology of the vortex lines. As a result, Euler flows preserve a number of topologically related properties. Here we look at two of these, conservation of total helicity and Clebsch representability. These properties are not conserved in the Navier-Stokes equation, because of the non-zero viscosity in this case. Because real turbulence is described by the Navier-Stokes, but in many ways seems to behave in an almost Eulerian manner, it makes sense to wonder whether the development of real turbulence depends in some essential way on the non-conservation of the aforementioned properties.

Some results of original analytical work on Clebsch variables and helicity is presented, with the intention of clarifying the link between Clebsch variables, helicity, and the Navier-Stokes equation. This work motivates a modification of the viscosity term in the Navier-Stokes which results in an equation which preserves Clebsch representability and total helicity. Some analytical results are presented for the resulting, modified Navier-Stokes equation. The resulting equation is simulated as described in a later chapter, and various quantities, some of them not usually computed in numerical simulations, are computed from the resulting flow fields. The results are presented and discussed, both to verify the accuracy of the simulation, and to show how the modification of the viscosity term affects the development of turbulence. Finally, the conclusions that can be drawn from this study relevent to the theory of turbulence are presented.

2. THE PROBLEM OF TURBULENCE

Turbulence is the chaotic flow of fluids subjected to macroscopically non-chaotic boundary conditions. It typically occurs at large Reynolds numbers for flows which at small Reynolds numbers are laminar (non-chaotic). For flow in a pipe, below Reynolds numbers of 1000 flow is generally laminar; for Reynolds numbers over 3000 flow is usually turbulent. The regime of laminar flow can be extended by keeping the pipe extremely smooth and avoiding all perturbations in the system.

One important distinction between laminar and turbulent flow is that for steady boundary conditions, the laminar flow field is steady; it looks exactly the same from instant to instant. In turbulence, the flow field is never steady. In fact, the time evolution of a turbulent flow field probably never begins to repeat itself. Another difference is that a turbulent field has greater dissipation than the corresponding laminar field. This can be seen in the case of flow fields with borderline Reynolds numbers in which the flow can be either laminar or turbulent, depending on the perturbations in either spatial boundary conditions or initial conditions. This is also seen in numerical simulations. When the initial condition is a randomly generated velocity field, the first stage of the simulation always shows a noticeable increase in dissipation for a length of time on the order of one turnover time (in the simulations presented here one turnover time is about one time unit in the units of the simulation).

Here we will consider flow fields that are incompressible and follow Newton's law of viscosity with constant viscosity. This is typical of many flows of interest, such as the isothermal flow of wind on the earth, water in rivers or oil in pipelines. Of course, no known flow is absolutely incompressible or Newtonian, but many follow the model so closely that it seems to make no difference if the above assumptions are taken as absolute.

There is some possibility that the miniscule compression and non-Newtonian properties of all real fluids are actually essential to the development of turbulence, but in the literature considered here this proposition is universally disbelieved. Similar agreement seems to exist that the incompressible Navier-Stokes equation, which is just a force balance on the fluid with Newton's law of viscosity taken as a constitutive relation, has a unique solution for well determined boundary conditions. But there are many turbulent flow fields that result from a given set of initial and boundary conditions. The reason for this is that for a given set of macroscopic experimental conditions there exist many different sets of microscopic perturbations of the system. In laminar flow these perturbations quickly die out and have no discernible effect. In turbulence they do not die out, but cause deviation from the single laminar solution into the chaotic paths in phase space characteristic of turbulence.

The chaotic nature of turbulent flow fields leads to some difficulty in asking the correct questions in formulating a model of turbulence. In laminar flow, one usually finds the entire flow field. All other questions are answered starting from the known flow field. In turbulence, no one flow field or even sequence of flow fields can be the answer. A minimum solution to the problem of turbulence must at least include a way to find statistics such as heat transfer rates, flow rates, average pressure drops and diffusion rates. Exactly what kind of model is to be used to answer these questions is unclear. A computation of average velocities, and all other moments of velocities is one possibility. A probability distribution function of velocity fields classified according to some as yet unknown scheme is another. Even a method of simulating turbulence for practical situations in a reasonable amount of computer time and memory might be considered a solution. Besides not knowing how to accomplish these goals, nobody even knows which of these goals can be accomplished in the immediate future.

In spite of this, some descriptions of turbulence exist already. Kolmogorov used the idea of describing the turbulent flow field as a spectrum in Fourier space, as a distribution of superimposed sinusoidal motions of different length scales. He used this model with dimensional considerations and further assumptions to deduce some aspects of fully developed turbulence. Kolmogorov's approach is the most notably successful theory of turbulence so far. There has been successful description of the length and time scales involved in various turbulent flow fields which are of great practical importance. Ideas such as eddy viscosity and turbulent diffusivity started as practical methods for dealing with turbulence in semi-empirical models, and are sometimes used also in more theoretical discussions.

Statistical mechanical approaches to turbulence enjoy some popularity. In the computational approaches, large eddy simulation and direct spectral simulation of turbulence both have had some success. Practical application of these techniques at high Reynolds numbers does not seem to be a prospect for the immediate future without some breakthrough in either the theory of turbulence simulation or computational machinery.

In the theoretical work that has been done so far, one idea that has been accepted is the distinction between shear flow turbulence and homogeneous, isotropic turbulence. Shear flow turbulence arises from flow which is on the average a shear flow, such as flow in a pipe or flow between two planes. Some aspects of shear flow turbulence can be studied as perturbations from a basic laminar type shear flow. Shear flow is not isotropic since the direction of overall shear destroys isotropy, and it is not generally homogeneous because there is usually a solid body in the vicinity which causes inhomogeneities, such as the buffer zone and viscous sublayer. Isotropic, homogeneous turbulence is somewhat of an idealization, but it can be approximated for limited amounts of time by rapidly passing a large grid through a large, initially quiescent body of water. Far from the edges of the grid, a moderate amount of time after the grid has been passed, the turbulence that exists will be approximately homogeneous and isotropic.

CHAPTER II

SCOPE OF RESEARCH

There are two parts to the work done for this doctorate. The first part is theoretical work done on the Clebsch variables and helicity. It is known that these are related to the topology of the vortex field. It is felt that changes in the topology of the vortex field are crucial to the phenomenon of turbulence. The theoretical work done on these topics is meant to elucidate the relationships between Clebsch variables, helicity and the topology of the vortex field. The results suggest a simulation to clarify the role of changes in topology of the flow field in the development of turbulence.

The work on Clebsch variables includes three instantaneous constraints that apply if any vector field is to be described in terms of Clebsch variables at one instant. One of these, the (integral) helicity constraint, is well known from the literature. Another, the first integrals constraint, most directly elucidates the significance of Clebsch variables in relation to the structure of the vorticity field. The third, the helicity density constraint, is most useful in actually determining whether a field is describable in terms of Clebsch variables. These last two are, as far as I know, original in this work.

A further constraint is introduced if the Clebsch variable representation is to hold for some amount of time. Even if the velocity field at one moment is representable in terms of Clebsch variables, the time derivative of the velocity might not be. Whether or not this is true depends on the time evolution equation used. The initial analysis is done for the Navier-Stokes equation. The results suggest a modification of the equation so that the time derivative is always representable in terms of Clebsch variables if the instantaneous field is itself representable in terms of Clebsch variables, except at certain types of singularities of the vorticity field.

In most of the work already done on helicity, only the topological meaning of helicity in a magnetic volume (a volume for which the normal component of vorticity is zero on the surface) is discussed. The helicity balance over a magnetic volume is already treated in the literature. More recently, Berger and Field have shown that the helicity of an arbitrary volume also has topological meaning. So, a helicity balance in an arbitrary volume is done for the case of the Navier-Stokes equation. The change of helicity in an arbitrary volume is divided into flux terms and a source term the latter of which is independent of the inertial frame chosen (helicity itself is not independent of the inertial frame for an arbitrary volume).

It is found that, if the source term in the helicity balance is equal to zero, the time evolution equation is always algebraically solvable in terms of the Clebsch variables. This suggests a modification of the viscosity term in the Navier-Stokes which preserves both of these properties, but is still, in some sense, close to the original Navier-Stokes. It is possible that this equation describes the behavior of some non-Newtonian flow, but I am unaware of any fluid matching this description.

The second part of the project is the simulation of the modified equation and comparison of the results with simulation results for the unmodified Navier-Stokes. A spectral method using a Fourier series has been used, similar to S. Orszag's BIGBOX. This method has been chosen because it has successfully been used for simulation of homogeneous, isotropic turbulence before. The fast Fourier transform methods are especially advantageous because high accuracy with a reasonable amount of computation time and computer memory is needed. One of the main drawbacks of this method, the necessity of using periodic boundary conditions, is unimportant here, because it is not necessary to fit any particular boundary conditions.

The calculations have been carried out on a CRAY computer. This is desirable mainly because of the large memory of the CRAYs, although the high speed of calculation is no drawback either. The maximum resolution possible on the CRAY-XMP, if the entire computation is to be done relying on the active memory (an "in core" code), is between 32 and 64 gridpoints in each direction. The alternative, to continually read data into and out of the active memory, is prohibitively expensive. The resolution of 32^3 is nearly the minimum to get any significance is the results, but this is always a problem in the full spectrum simulation of turbulent flow.

To interpret the results, more programs have been written. The Fourier spectra of the energy, enstrophy and H(k) at various times are calculated, as well as the distribution of the angle between velocity and vorticity. H(k) is the dot product of the Fourier transform of velocity and the Fourier tranform of vorticity for a given wavenumber, k. Two quantities that have not been calculated yet in any other numerical simulations (to my knowledge) are also calculated. These are alpha, the integral of H(k) squared, and beta, the integral of H(k) squared divided by the maximum possible H(k) for the given magnitude of v(k). These quantities are discussed further in chapter VII.

One question that is addressed is: does this modification prevent the development of the usual behavior that is characteristic of turbulence? If the answer is yes, this would be an indication that the development of helicity density fluctuations and the tangling of vortex lines is indeed crucial to the development of turbulence. We also look at the growth of the "horns of cosine theta" (discussed in chapter III and in Pelz et al. 1986) to see whether these result from helical fluctuations in time, as has been postulated. The parameters alpha and beta are used to investigate whether the fluctuations of H(k) tend to become very large as has also been postulated.

CHAPTER III

LITERATURE REVIEW

1. THEORETICAL WORK

The Clebsch variable representation of the velocity field in hydrodynamics is first given, naturally enough, by A. Clebsch in an article entitled "Ueber die Integration der hydrodynamischen Gleichungen" ("On the integration of the hydrodynamic equations").(Clebsch 1858) In this article, and an earlier one (Clebsch 1857), Clebsch attempts a variational formulation of the Euler equation. It is this same attempt that has attracted much of the current interest in Clebsch variables. This work is reported in Lamb's "Hydrodynamics" (Lamb 1932), the earliest reference in English that I have found for this formulation. In this work, the necessary and sufficient condition of the representability of the velocity field in terms of the representability of the vortex field is given, and the indeterminacy of λ and μ is described. The mistake sometimes made later in saying that a velocity field is always representable locally in terms of Clebsch variables is not made in this reference.

In recent times, interest in Clebsch variables seems to have been reawakened by an article by R.L. Seliger and G.B. Whitham (Seliger and Whitham 1967) entitled "Variational principles in continuum mechanics." This work derives the equations of inviscid incompressible isentropic flow from a variation of the integral of a Lagrangian density written in terms of mass density and the three Clebsch variables. This work attributes to Clebsch and seems to agree with the idea that any velocity field can be written in terms of Clebsch variables. Some later works corrected the idea of global representability of velocity fields in terms of Clebsch variables. But none that I have seen has considered the idea that some fields are not representable even locally in terms of Clebsch variables. I know of no works that discuss the possible implications of the fact that the variational principles that have been found for Euler's equation lack global and even local validity in some cases.

The use of Clebsch potentials to formulate Euler's equation is discussed in a book by E.C.G. Sudarshan and N. MuKunda on classical dynamics (Sudarshan 1974). There the claim that any velocity field is representable in terms of Clebsch variables is repeated, and a spurious proof is given. (The proof assumes that the representation of the vortex field in terms of Clebsch variables always exists, which is false.)

More interest in Clebsch variables seems to have stirred up with an article by E.A. Kuznetsov and A.V. Mikhailov in "Physics Letters" (Kuznetsov et al. 1980). This article introduces the idea of topological constraints introduced by single valued Clebsch variables. It claims a constraint that single valued Clebsch variables cannot describe any knots in the vortex field. This article also connects single valued Clebsch variables to helicity, stating what is called in this paper the (integral) helicity constraint. This paper, like most others discussed here, limits itself to the case of ideal fluids.

The use of Clebsch variables to formulate Poisson bracket representations and Hamiltonian representations of the Euler equations became very popular after the paper by Kuznetsov and Mikhailov. Some authors (Marsden et al. 1983 ; Heyney 1983) use them for incompressible non-magnetohydrodynamic fluids. More authors use two sets of Clebsch variables, one for magnetic effects and one for Euler flow effects in formulating variational, Hamiltonian and Poisson bracket representations of ideal magnetohydrodynamics (Holm et al. 1982 ; Holm et al. 1983 ; Oppeneer 1984 ; Nassar et al. 1984 ; Frenkel et al. 1982). Some of these seem to be unaware of the constraints, local and global, on the flow field introduced by the use of Clebsch variables.

Interesting in this respect is the work of S. Grossmann. No mention is made in his works that I have seen of the constraints introduced on flow fields by the use of Clebsch variables. In the two articles cited here Dr. Grossmann is interested in extending the use of Clebsch variables to viscous fluids. He substitutes them into the incompressible Navier-Stokes equation, and derives a system of three scalar equations for the time derivatives which, if solvable, give the same time evolution as the Navier-Stokes. But then, talking about the gauge freedom of the choice of Clebsch variables, he claims that this system of equations is underdetermined, when in fact it is overdetermined. He then adds further constraints on the equations, claiming that this is allowable because the equations are underdetermined (Grossmann 1974). He uses these equations in computer simulations and claims greater accuracy for the results with Clebsch variables than for simulations using the ordinary velocity variables.

He continues in a later paper (Grossmann 1976) to claim that these equations are valid, and uses them in further simulations, this time using renormalization group methods, to calculate the exponent in the Kolmogorov inertial range. Once again he arrives at accurate results using an inaccurate equation. Perhaps there is a moral here about the believablity of computer results. But whatever mistakes might have been made, I do not wish to criticize the work too strongly, since the overdetermined equations given in his paper were the starting point for my investigations.

In works by Levich, the Clebsch variables are discussed in conjunction with helicity and used to formulate various constraints on Euler flows. The integral helicity constraint is cited as a necessary condition for the representability of a velocity field in terms of Clebsch variables. Euler's equation is shown to have an infinite number of invariants and the constraints introduced by these are discussed (Levich 1981 ; Levich 1982). The role of helicity in the formation of coherent structures is discussed further using Clebsch variables and the related **n** variables (as described in the paper (Kuznetov 1980)) in two more articles (Levich et al. 1983a and Levich et al. 1983b). Much of the arguments in these papers is related to subtleties of the idea that, although there is no preferred sense of rotation and hence no net helicity in many flows as a whole, the local existence of fluctuations in helicity in parts of the flow can have an important effect on the overall flow properties.

H.K. Moffatt has worked on the topology of the vortex field, relating it to the helicity computed over a magnetic volume. The topology of the vortex field is conserved in Eulerian flow. In turbulent flows the Reynolds number is typically high, and so the magnitude of the convective term is much greater than the magnitude of the viscous term. Because of this, Moffatt considers Euler's equation a good approximation of the short time behavior of the Navier-Stokes equation for the purposes of describing some characteristics of the time evolution of the vortex field. Since Euler's equation also conserves helicity, he uses helicity conservation in describing the short time behavior of various vortex structures (Moffatt 1968). The effects of non-zero helicity on the cascade of energy in the Kolmogorov spectrum is discussed (Moffatt 1978). The connections with topology are discussed by Moffatt (Moffatt 1981) referring to work by Arnold (Arnold 1974). Moffatt also connects kinematic helicity with magnetic helicity in the non-linear dynamics of fluid flow (Moffatt 1983).

Most of these works concentrate on the helicity in a magnetic volume (i.e. a volume bounded by a surface which has no non-zero component of vorticity anywhere on its surface), often one which is assumed to go to zero quickly enough as the position coordinate related to a fixed coordinate system goes to infinity. But it is useful to have an idea of the importance of the helicity integral in an arbitrary volume. This question is researched in an article by Berger and Field mainly in the context of magnetic helicity (Berger et al. 1984). They show analytically that the difference in helicities for two fields in an arbitrary simply connected volume is independent of the connection of the field lines outside the volume and independent of the choice of gauge, given only that the two fields meet the same boundary conditions on the surface of the volume. In the case of the vortex field, the gauge invariance implies an invariance with respect to any irrotational velocity field. This is important because the vortex field determines only the rotational part of the velocity field. As a special case, this implies that differences in helicities are Galilean invariants, even though the helicity of an arbitrary volume itself is dependent on the choice of inertial reference frame. (In a magnetic volume the helicity is independent of the choice of inertial reference frame.) Other details of helicity, such as the division of helicity into writhing and kinking components is also discussed.

Another quantity, related to helicity, that has been the topic of recent discussion, is the distribution of the angle between the velocity and vorticity over the whole flow field in question. This is often referred to as "the distribution of cosine theta" or "the probability of cosine theta" or $P(\cos\theta)$.

First we define the cumulative distribution function of cosine theta for the case of a finite volume. This is the quotient of the volume of the field that has values of cosine theta less than or equal to the given value of cosine theta and by the total volume. The probability density of cosine theta is then just the derivative of the cumulative distribution function of cosine theta with respect to cosine theta. This is the standard way of defining a probability density function. More casually, we can say, using $P(\cos(\theta))$ for the probability of cosine theta that the volume of points having values between $\cos(\theta)$ and $\cos(\theta)+d(\cos(\theta))$ is $P(\cos(\theta))d(\cos(\theta))$. In practice the normalization (division by the total volume) is often not done, and then this quantity is often referred to as the "distribution of cosine theta." (distinct from the "cumulative distribution function of cosine theta") In the case of computer simulations, the number of of points replaces the volume in the definitions.

If velocity and vorticity were independent, isotropically distributed quantities, the distribution of cosine theta would be flat, that is it would be a constant independent of theta. It is found in the results of numerical simulations that, as turbulence develops in time, the initial distribution of cosine theta gives way to a concave distribution with pronounced peaks at ± 1 (Pelz et al. 1986). This effect was observed for initial conditions including: the Taylor-Green vortex, a zero helicity initial condition, a low helicity initial condition, and a high helicity initial condition. The severity of the peaks eventually formed was found to be a function of the Reynolds number, high Reynolds numbers leading to more pronounced peaks. In the case of initial conditions set by randomly generating Clebsch variables in Fourier space, the initial distribution was found to be strongly convex, but the concave shape still developed with time.

For compressible inviscid flow the Clebsch variables have proved computationally useful for numerical simulations using central difference approximations. They have been used successfully for computer simulations by Buneman (Buneman 1980). This turns out to be closely related to the Hamiltonian formulation of flows discussed by authors mentioned above.

2. SPECTRAL SIMULATION OF THE NAVIER-STOKES EQUATION

The spectral simulation of turbulent flow has been pursued actively for more than twenty years. The advantages of spectral methods include the infinite order approximation of infinitely smooth periodic functions, and the efficiency of calculation allowed by the use of the Cooley-Tukey algorithm in the fast Fourier transform. Orszag gives an thorough discussion of various aspects of the accuracy of spectral approximations in his 1971 paper (Orszag 1971b). This article includes experimental comparisons with various finite difference schemes, theoretical discussions of the reasons for the great accuracy of spectral methods and the efficiency of calculation is discussed. The aliasing interactions in spectral computations is further discussed, and a new way of dealiasing in certain computations is introduced. More calculational details are given in an article written that same year (Patterson 1971). In this work the problems of dealiasing and boundary conditions are given special attention. In an earlier article, discrete Fourier transform methods are discussed in terms of both theory and experimental results, and comparisons are made between the spectral simulation of turbulence and a real space finite difference method in which the Fourier transform is used only in enforcing incompressibility (Orszag 1969).

In the book "Numerical Analysis of Spectral Methods: Theory and Applications" (Gottlieb et al. 1977) Gottlieb and Orszag give a very wide review of spectral methods including mathematical formalism of different numerical methods, analysis of their uses in a wide range of the equations of physics, and experimental results illustrating the ideas described. Unfortunately, many of the analytical results of this work are not immediately applicable to the simulation of the Navier-Stokes equation, because it is non-linear.

In some ways the most instructive exercise is to look at an actual existing program. This is especially helpful in conjunction with information on the problems encountered in the use of that program and methods of evaluating the results. This opportunity was afforded me by Orszag's program "BIGBOX" and discussions with people associated with his group in Princeton, especially Pelz and Shtilman. It was especially helpful to me to be able to hear about the difficulties that were encountered before the work was completed, many of which are never fully reported in articles. (The discarded simulations are not very interesting to the general scientific public, but useful to someone about to start a similar project).

Also of great help to me has been the receipt of a program modelled on BIGBOX called "INCORE". This code, prepared by Pelz, simulates the incompressible Navier-Stokes equation without the need to constantly read data into and out of the active memory. In fact, many subroutines and part of the main program used in the simulation that I have written were taken from INCORE with very little or no modifications.

Besides the invaluable help given to me in discussions with the above mentioned members of Orszag's group, an article by Kerr has been helpful in forming criteria for whether the results of a simulation can be taken as credible (Kerr 1985). Since the complete analytical evaluation of the errors in the spectral approximation of the Navier-Stokes is unavailable and perhaps even impossible using present methods, it is important to have empirical criteria for whether a certain Reynolds number is too high to use with a given resolution, whether aliasing error are accumulating quickly, and similar problems. These criteria can only be found through experience in actually performing simulations. Because of this, the accumulated experience of others, sometimes communicated by word of mouth, has been invaluable to me. In this connection I would like to thank especially Shtilman and Pelz who have been generous with their experience and advice.

CHAPTER IV

THE CLEBSCH VARIABLES

1. INSTANTANEOUS CONSTRAINTS

The new results presented in this section were obtained in collaboration with Dr. Frenkel (Cassidy and Frenkel, 1987).

Various equivalent representations are used for Clebsch variables, here the form used will be:

$$\mathbf{v} = \lambda\nabla\mu + \nabla\phi$$

The variables λ, μ, ϕ are taken to be single valued functions of position throughout this thesis. It will be assumed unless stated otherwise that the domain in question is simply connected. Some writers prefer to emphasize the symmetry of λ and μ by substituting:

$$\mu' = 1/2\bullet\lambda \qquad \mu' = \mu \qquad \phi' = \phi + 1/2\bullet\lambda\mu$$

Which results in the equivalent form:

$$\mathbf{v} = \lambda'\nabla\mu' - \mu'\nabla\lambda' + \nabla\phi'$$

Obviously the Clebsch variable representation is not unique. Addition of constants to μ, or multiplication of λ by a non-zero constant and multiplication of μ by its reciprocal, or gauge transformations between the two terms all leave the velocity field unchanged.

Not all velocity fields can be represented by Clebsch variables. It is sometimes said that any velocity field can be represented locally by Clebsch variables, but this is not true at some singular points, for instance at the points where the zero velocity, non-zero vorticity axes meet the the zero velocity planes in the Taylor-Green vortex.

Another example of a case where the velocity field is not locally representable in terms of Clebsch variables is any velocity field for which the associated vorticity field is given by:

$$\omega_x = x, \ \omega_y = y, \ \omega_z = -2z$$

Any first integral passing through the origin must have all the vorticity lines that run to the origin lying entirely on it. But the first integrals that run to the origin include the vortex lines x=cy,z=0 for any constant, c. These lines cover the entire z=0 plane, so that there can be only one possible first integral through any point on the z=0 plane. Hence, the Clebsch variable representation is not possible even locally at this point.

A velocity field can be represented in Clebsch variables if and only if the associated vorticity field can be represented in the form:

$$\omega = \nabla\lambda \times \nabla\mu$$

The necessity of this condition can be seen immediately by taking the curl of the defining equation for Clebsch variables. To see the sufficiency recall that any irrotational, continuous vector field can be written as the gradient of a scalar. Since the curl of $\underline{v}$ equals the curl of $\lambda\nabla\mu$, the curl of $\mathbf{v} - \lambda\nabla\mu$ equals zero and so the equation:

$$\nabla\phi = \mathbf{v} - \lambda\nabla\mu$$

has a solution determined up to an additive, physically insignificant constant. If the region in question is simply connected (i.e. if it has no holes), ϕ will be single valued.

The variables λ and μ are determined to within any transformation for which the Jacobian is exactly one at all points of non-zero vorticity. For a new pair of variables, call them λ' and μ', the condition that they give the same vorticity field is:

$$\frac{\partial(\lambda',\mu')}{\partial(\lambda,\mu)} = 1$$

This can be seen from the fact that, for example, the x component of the vorticity field at a given point is:

$$\frac{\partial(\lambda,\mu)}{\partial(y,z)} = \frac{\partial(\lambda',\mu')}{\partial(y,z)} \times \frac{\partial(\lambda,\mu)}{\partial(\lambda',\mu')} = \frac{\partial(\lambda',\mu')}{\partial(y,z)}$$

There are two other criteria for whether a velocity field can be written in terms of Clebsch variables. I will call them the "first integrals constraint" and "the helicity density constraint".

The first integrals constraint is that in a simply connected region, for a differentiable velocity field the Clebsch variable representation exists if and only if there exist two first integrals of the vorticity field which have linearly independent gradients at all points where the vorticity field is non-zero. If there are surfaces of discontinuity in the first integrals or the Clebsch variables, there the derivatives at these points are defined to be the limiting value of the derivatives as that surface is approached. Of course the limits must exist if the Clebsch variable representation is to exist at that point). By first integrals I mean differentiable scalar functions of position whose derivatives in the direction of the vorticity field are zero i.e.

I^1 and I^2, scalar functions of positions such that:

$$\nabla I^1(\mathbf{x}) \cdot \omega(\mathbf{x}) = 0 \qquad \text{and} \qquad \nabla I^2(\mathbf{x}) \cdot \omega(\mathbf{x}) = 0$$

everywhere.

Linearly independent gradients at non-zero vorticity points implies that the rank of the matrix:

$$\frac{\partial(I^1, I^2)}{\partial(x,y,z)}$$

is two at all non-zero vorticity points.

In geometrical terms, a function is a first integral of the vorticity field if the vorticity lines lie entirely on the function equals constant surfaces. This can be seen from the fact that if a vorticity line leaves or passes through an I=constant surface, it must have some component in the direction of ∇I, which is the normal to the surface. The gradients of the first integrals are linearly independent only if they are non-parallel. So the independence condition is the same as the condition that the I=constant surfaces passing through a given point are not parallel at any point where the vorticity is non-zero.

To see the sufficiency of this condition, consider that, since the gradients of I^1 and I^2 are both perpendicular to the vorticity field and both non-zero and are non-parallel at non-zero vorticity points,

$$\omega = C(\nabla I^1 \times \nabla I^2)$$

For some scalar function of position, C. Since the vorticity, ω, is the curl of the velocity:

$$\nabla \cdot \omega = \nabla C \cdot \nabla I^1 \times \nabla I^2 = 0$$

And so C is a function only of λ, μ, and an arbitrary additive constant. At points where the vorticity is non-zero the value of C is determined by:

$$C = |\omega| / |\nabla I^1 \times \nabla I^2|$$

At points of zero vorticity C must be zero unless the gradients of the first integrals are not linearly independent, when this occurs C may assume any value.

Now we construct a Clebsch variable representaion for which $I^2=\mu$. To construct the representation choose an integral surface, $I^1=I^{10}$, and assign along that surface any continuous values for λ. (Even after choosing μ there is still some gauge freedom for λ). The family of I^2=constant surfaces which intersect the given $I^1=I^{10}$ surface fills a volume. Define for each $I=I^{20}$ surface in that volume:

$$\lambda(I^{20},I^1) = \int_{I^{10}}^{I^1} C(I^{20},I^{1\prime})dI^{1\prime} + \lambda^0$$

The simplest is choice of λ^0 is to chose $\lambda^0 = 0$. The variable λ^0 can be assigned in any manner along the $I^1=I^{10}$ surface which has only a finite number of discontinuities. Of course, any discontinuities in λ^0 will cause a discontinuity in λ throughout the volume.

If the entire region of interest is not covered by one choice of λ^0 it is necessary to chose a second point, λ^{00}, and repeat the process to cover the entire region of interest. Since μ equals I^2 we get:

$$\nabla\lambda\times\nabla\mu = [\frac{\partial\lambda}{\partial I^1}\ \nabla I^1 + \frac{\partial\lambda}{\partial I^2}\ \nabla I^2] \times \nabla I^2$$

$$= C\cdot\nabla I^1 \times \nabla I^2$$

$$= \omega$$

And, as mentioned above, an appropriate ϕ can always be constructed.

Conversely, suppose the Clebsch variable representation exists for some velocity field, then since the vorticity is the cross product of the gradients of λ and μ, it is everywhere perpendicular to their gradients, and so they are first integrals. They are independent wherever the vorticity is non-zero since otherwise their cross product, and so the vorticity, would be zero.

The above formula for vorticity also shows that λ and μ are constant along vorticity lines. So the Clebsch variables label the vorticity lines. This implies that the Clebsch variable representation is impossible for any flow field with a region of non-zero vorticity in which the vorticity lines are ergodic since, in any such region, λ and μ would have only one value each, i.e. the one value for the one vorticity line. In fact, if a vorticity line is merely dense in some volume of non-zero vorticity, then the Clebsch variable representation is impossible there since, by continuity, if λ and μ have some value on a set dense in a volume, they have that value throughout the volume.

Note that an r times differentiable Clebsch variable representation is always possible locally at a non-singular (non-zero) point of an r times differentiable vorticity field by the basic theorem of ordinary differential equations, (Arnold 1973). By this theorem any vector field in the neighborhood of a non-singular point is diffeomorphic to the field:

$$dx/dt=1, \ dy/dt=0, \ dz/dt=0$$

The maps of the diffeomorphism are differentiable as many times as the field in question. Two locally independent, r times differentiable first integrals exist for the standard equation, for example:

$$y=I^1 \text{ and } z=I^2$$

for any constants I^1 and I^2. Simply applying the r times differentiable inverse map from the standard field to the field containing the non-singular point in question produces two, r times differentiable, linearly independent first integrals. This same mapping also implies that the existence of Clebsch variable representation is a property of a differentiable manifold rather than of a single vector field.

Since the vortex lines are defined by the intersections of independent first integrals, and these must be surfaces in space, the topology of the vortex lines must be trivial if they are to be representable in terms of Clebsch variables. The helicity constraints related to this are discussed by Moffatt (Moffatt 1969).

A necessary condition for Clebsch representability given by the helicity density constraint is that a function, ϕ, must exist such that a derived field $\mathbf{q}=\lambda\nabla\mu$ defined by:

$$\mathbf{q} = \mathbf{v} - \nabla\phi$$

has zero abnormality, i.e.

$$(\nabla\times\mathbf{q})\cdot\mathbf{q} = 0$$

This ϕ is indeterminate to within any additive function which is a first integral of the vorticity field.

The necessity follows immediately from the fact that $\nabla\lambda\times\nabla\mu\cdot(\lambda\nabla\mu)=0$. To actually construct ϕ it is necessary to globally solve the the equation:

$$\omega\cdot\nabla\phi = \omega\cdot\mathbf{v}$$

The solution of this equation can be constructed by choosing a surface intersecting the vorticity lines just once. Continuous values are assigned to ϕ on this surface. The value of ϕ along the rest of each vorticity line is found by integrating along each vorticity line, starting with the plane where $\phi=\phi^0$ and using arc length (ds) as the variable of integration:

$$\phi = \phi^0 + \int \frac{\omega\cdot\mathbf{v}}{|\omega|}\, ds = \phi^0 + \int \mathbf{v}\cdot d\mathbf{l}$$

This shows that for the Clebsch variable representation to hold with a continuous ϕ, the circulation (of velocity) about any closed vortex line must be zero. (Note that the integral given is just the circulation about the vortex line.) Otherwise the value of ϕ at the end of the circuit will not match its value at the beginning, contrary to hypothesis. Note that this does not mean that the velocity must be the gradient of a scalar. This is a much stronger constraint that would be implied only if the circulation around any line would be required to be zero.

The quantity in the numerator of the integrand is the (velocity) helicity density. Helicity density equal to zero is a necessary and sufficient condition for the existence of planes normal to the velocity field (Truesdel 1954). The integral of the helicity density, helicity, has been directly related to the Hopf invariant, a topological property of a vector field (Moffatt 1969).

If the derived field, q, has no singularities (sets where q=0), the existence of an appropriate ϕ is also sufficient for the existence of the Clebsch Variable representation. If there are singularities in the derived field, then the Clebsch variable representation will still exist if the μ=constant planes do not intersect there. This is so because the derived field has zero helicity, and so planes exist which are normal to the q field. In any region of non-zero q these planes are unique. Taking these planes to be the μ=constant planes, and assigning them any strictly monotonic values along q lines gives a proper μ for the representation. (q lines are lines everywhere tangent to the q field. Such lines always exist and are unique at all non-singular points by the basic theorem of ordinary differential equations). Finally λ is set equal to the quotient of the moduli of q and the gradient of μ. This completes the construction of the Clebsch variables throughout the region of non-zero q. The only remaining question is whether the representation can be continued in regions containing singular sets. This is impossible for a given ϕ only if the normal planes intersect at these sets. In this case it may still be possible to represent the field in terms of Clebsch variables by choosing a different ϕ.

Considering both of the above constraints together, it is seen that, in order for the Clebsch variable representation to fail to exist locally, it is necessary both that any derived field, q, be zero at the point in question, and that the vorticity be zero there.

The discussions in the proofs of the two constraints give a round-about way of constructing first integrals of a vector field in terms of a vector potential field. If the first integrals do not exist for the given field, the following method gives a recipe for excluding parts of the original so that the two first integrals can be constructed.

Any vector potential for the given vector field can be chosen. The appropriate ϕ can be computed (by integrating along vorticity lines) to make the potential a zero helicity density one. If this construction fails, then the set of vorticity lines where it fails can be found. A sort of branch cut (i.e. a surface through which the construction is not carried out) must be made through these vorticity lines to continue the construction. Next the singular sets of the derived potential field can be inspected to see whether the normal planes intersect on these sets. Wherever they do intersect, these sets can also be excluded. Then the construction on the reduced domain can be completed as described in the helicity density constraint. In the usual case one would want to exclude open regions from the original domain, leaving the remaining part of the domain a closed set. One advantage of this method of construction is that when construction cannot be done globally, the parts of the domain that must be excluded are clearly indicated.

There is another, weaker constraint on the possible velocity fields representable by Clebsch variables, which will be called the "helicity constraint". Consider a volume, V, enclosed by a surface, S, for which over the entire surface the component of vorticity normal to S is zero (i.e. a "magnetic volume"). If the velocity field in the volume is representable in terms of Clebsch variables, the integral of helicity over the entire volume must be zero. This is easily seen by direct computation of the integral of helicity over the volume.

$$\int_V \mathbf{v}\cdot\omega = \int_V \nabla\phi\cdot\nabla\lambda\times\nabla\mu = \int_V \nabla\phi\cdot\omega = \int_V [\nabla\cdot(\phi\omega)-\phi\nabla\cdot\omega] =$$

$$= \int_S \nabla\cdot(\phi\omega) = \int_S \phi\omega\cdot\mathbf{n} = \int_S 0 = 0$$

Where $\mathbf{n}$ is the unit normal on the surface.

It is a necessary condition for the existence of the Clebsch Variable constraint, that the total helicity over any periodic box (such as the one used for spectral simulations) must be zero. This can be shown by recalling that for any periodic box the quantity $\omega\cdot\mathbf{n}$

has equal magnitude, but opposite sign on opposing faces of the box, so that each part of the surface integral: $\int \phi \omega \cdot \mathbf{n}$ cancels with the integral over the opposing face.

Note that the first integrals of the vorticity field are tangential to the vorticity lines, so any surface made up of pieces of first integrals, such as λ=constant and μ=constant surfaces, which form the complete boundary of a region is a magnetic surface.

2. DYNAMIC CONSTRAINTS

Besides the constraints introduced by the Clebsch variables on the velocity field at any one moment in time, there are further constraints introduced by demanding that the time evolution of the field be representable in terms of a continuous time evolution of Clebsch variables. The time representation could fail in two different ways. It might be that the representation exists at one moment for the field, but not at a moment soon after. Or it could be that the representation exists at all moments, but that the representations are not continuous or differentiable in time.

To consider this possibility, we will recast (following Grossmann) the Navier-Stokes equation in terms of Clebsch variables. If the resulting equation is solvable then the representation can exist continuously for some amount of time. Otherwise the representation will fail because of the dynamic constraints.

First consider the total derivative of velocity. Subscripts after slashes on vectors indicate differentiation and subscipts on scalars indicate differentiation throughout this work. Using the operator identity:

$$D_t\partial_i = \partial_i D_t - v_{j/i}\partial_j$$

we find:

$$D_t v_i = D_t(\phi_i + \lambda\mu_i) = D_t\phi_i + \mu_i D_t\lambda + \lambda D_t\mu_i =$$

$$= (D_t\phi)_i - v_{j/i}\phi_j + \mu_i D_t\lambda + \lambda(D_t\mu)_i - v_{j/i}\lambda\mu_j =$$

$$= (D_t\phi)_i - v_{j/i}(\phi_j + \lambda\mu_j) + (\lambda D_t\mu)_i - \lambda_i D_t\mu + \mu_i D_t\lambda =$$

$$= (D_t\phi - v^2/2 + \lambda D_t\mu)_i + \mu_i D_t\lambda - \lambda_i D_t\mu$$

Subscripts on scalars indicate differentiation in space throughout this paper. For the viscosity term we first derive the incompressibility condition:

$$(\lambda\mu_j + \phi_j)_j = \lambda_j\mu_j + \lambda\mu_{jj} + \phi_{jj} = 0$$

Differentiating again gives:

$$\phi_{jji} = - \lambda_{ji}\mu_j - \lambda_j\mu_{ji} - \lambda\mu_{jji} - \lambda_i\mu_{jj}$$

Using this to calculate the viscosity term:

$$(\nabla^2 v)_i = (\lambda\mu_i - \phi_i)_{jj} = \lambda\mu_{ijj} + 2\lambda_j\mu_{ij} + \lambda_{jj}\mu_i + \phi_{ijj}$$

$$= \lambda_j\mu_{ij} - \lambda_{ij}\mu_j + \lambda_{jj}\mu_i - \lambda_i\mu_{jj}$$

Substituting this into the incompressible Navier-Stokes and rearranging gives:

$$\mu_i D_t\lambda - \lambda_i D_t\mu = -(p/\rho - v^2/2 + D_t\phi + \lambda D_t\mu)_i + \nu(\lambda_j\mu_{ij} - \lambda_{ij}\mu_j + \lambda_{jj}\mu_i - \lambda_i\mu_{jj})$$

This equation has three free variables, the partial time derivatives of λ, μ and ϕ. Everything else is specified by the instantaneous flow situation. Any combination of these three variables that satisfies this equation is a solution of the algebraic constraints introduced by the use of Clebsch variables. There is no need to separately satisfy the incompressibility constraint. If the pressure field is correctly specified, the incompressibility constraint will be fulfilled. The incompressibility constraint on the partial time derivative of velocity does not have to to be enforced separately, but is satisfied automatically when it is calculated from a Navier-Stokes with a correct pressure field.

One might think "three variables and three equations, no problem", but there is a problem. The partial time derivative of ϕ is not just multiplied by coefficients, but instead a gradient is taken. The equation above has been arranged in this way to separate the free variables that are multiplied by vectors from everything else. These two free variables are the partial time derivatives of λ and μ or equivalently the two total time derivatives of λ and μ. (If the total derivative is solved for then the partial can be always be found by subtraction of the convective term, and if the partial derivative is known adding the convective term will yield the total derivative).

The freedom in the time derivative of ϕ amounts to a freedom to add to the right hand side of the equation the gradient of any scalar needed to make the equation solvable. After ϕ is chosen the equation is algebraically solvable if it is solvable by the Fundamental Theorem of linear equations (Kreyzig 1979 p.313). Writing the equation:

$$\mu_i D_t \lambda - \lambda_i D_t \mu = W_i$$

one sees that the equation is solvable if the rank of the matrix $[\nabla\mu \ \nabla\lambda]$ equals the rank of the matrix $[\nabla\mu \ \nabla\lambda \ \mathbf{W}]$ for some allowable choice of W. The allowable choice is any W satisfying:

$$W_i = \nu(\nabla^2 \mathbf{v})_i - (\nabla S)_i$$

for any scalar function of position S.

First we consider points of non-zero vorticity. At points of non-zero vorticity, the gradients of λ and μ are always non-zero and non-parallel. The rank of the first matrix is always two at non-zero vorticity points. The rank of the second (augmented) matrix must then be two or three. So at points of non-zero vorticity the equation is algebraically solvable if and only if the determinant of the augmented matrix is zero:

$$\epsilon_{ijk}\mu_i \lambda_j W_k = 0$$

Recalling that $\omega = -\epsilon_{ijk}\mu_i\lambda_j$ and the definition of W, this condition can be written in physical terms. The system is algebraically solvable iff:

$$\omega \cdot \nabla^2 \mathbf{v} = \omega \cdot \nabla S$$

for some scalar S.

The scalar S can be calculated by a method analogous to that for calculating ϕ. Assign continuous values for S on some set of surfaces intersecting the vorticity lines just once. Then extend the values of S to all space by integrating along vortex lines:

$$S = S^0 + \int \frac{\omega \cdot \nabla^2 \mathbf{v}}{|\omega|} \, ds$$

where s is arc length. This implies that the circulation of the viscosity term about any closed vorticity line must be zero if the scalar S is to be continuous.

At points of zero vorticity the situation is somewhat more complicated. Since one would expect that all sets of zero vorticity would be of measure zero, that is, not occupy any volume, one could state that if the time derivatives of the Clebsch variables can be continued continuously across all sets of zero vorticity, then the representation can be extended to the entire volume. But it is interesting to consider the sets of zero vorticity separately, since these sets can be important for organizing the topology of the entire space.

If vorticity is zero at some point, then either one or both of the gradients of λ or μ is zero at that point, or the gradients are non-zero but parallel. If the gradients are both zero, then the entire left hand side of the time evolution equation for Clebsch variables is zero and so the right hand side must equal zero independently. In this case, ∇S must exactly cancel out $\nu\nabla^2\mathbf{v}$, and both time derivatives are left entirely unspecified. If the two gradients are parallel or only one is zero, the rank of the left hand side is one and so the right hand side must be exactly proportional to the left. In this case either one time derivative is unspecified or only the sum of the derivatives is specified when the equation is solved.

Obviously, any steady flow that is representable in terms of Clebsch variables at one instant is representable for all time simply by setting the partial time derivatives of the Clebsch variables equal to zero.

If an appropriate scalar S can be found to make the equation solvable then the solution will be:

$$D_t\lambda = \frac{\omega \times (\nu\nabla\times\omega + \nabla S)}{\omega\cdot\omega}\cdot\nabla\lambda \quad \text{and} \quad D_t\mu = \frac{\omega \times (\nu\nabla\times\omega + \nabla S)}{\omega\cdot\omega}\cdot\nabla\mu$$

This gives further hints of possible trouble at zero vorticity points. If the numerators of the above fractions do not approach zero sufficiently quickly as the zero vorticity points are approached, then the time derivatives will become infinite in the neighborhood of the zero vorticity point and the representation will fail.

It is interesting to note that one can define a potential convection velocity:

$$\bar{\mathbf{v}} = \mathbf{v} - \frac{\omega \times (\nu\nabla\times\omega + \nabla S)}{\omega\cdot\omega}$$

and using this velocity one can define a total derivative:

$$\bar{D}_t = \partial_t + \bar{\mathbf{v}}\cdot\nabla$$

so that the evolution equations become:

$$\bar{D}_t\lambda = \bar{D}_t\mu = 0.$$

Before finishing this section, it is desirable to give at least one example of a velocity field for which the Clebsch representability holds instantaneously, but not dynamically. It might otherwise be argued that the instantaneous constraints imply the dynamic constraints in some as yet undiscovered fashion. Since I have already shown that Clebsch representability implies zero helicity in a periodic volume, it is sufficient to show that there is a field representable in terms of Clebsch variables which has a nonzero helicity generation. One such field is given by:

$$\lambda = \cos(-x+2y-z) + \sin z \qquad \text{and} \qquad \mu = \cos x + \cos 2y$$

It is easiest to show that this leads to nonzero helicity after separating the helicity evolution equation into flux and source terms. This counterexample will be completed at the end of the next section.

3. HELICITY BALANCE

In the last section the instantaneous constraints introduced by the Clebsch variable representation showed one relation between helicity and the integrability of the vorticity field. The dynamic constraint also involves helicity, but this is easiest to see after doing a helicity balance on an arbitrary fluid element.

The total helicity in a magnetic volume is known to be related to the topology of the vortex field. The helicity of an arbitrary fluid element also has topological meaning; it is related to the amount of tangling or untangling of vortex lines (Berger and Field 1984). Although the helicity of an arbitrary volume element is not gauge invariant (e.g. Galileian invariant) the difference in helicity between two flow fields is both gauge invariant and independent of the flow field outside the element. This is similar to saying that a short length of string can be said to be twisted or knotted, even though the topological property of the strands being linked or knotted is not definite until the rest of the string is considered.

Using the Navier-Stokes and vorticity equations to directly compute the derivative of helicity, using incompressability and the divergence theorem yields:

$$\frac{\partial}{\partial t}\int_V \omega\cdot\mathbf{v} = \int_S \{(\frac{v^2}{2} - \frac{p}{\rho})\omega + (\mathbf{v}\cdot\omega)\mathbf{v} + \nu[\mathbf{v}\cdot(\nabla\omega) - \omega\cdot(\nabla\mathbf{v})]\}\cdot\mathbf{n} - 2\nu\int_V \omega\cdot\nabla\times\omega$$

Where $\mathbf{n}$ is the unit normal vector.

The last term on the right is a source term. It can be written in different ways by combining it with parts of the surface term, but when written this way it is a Galilean invariant. It is maximized for a given modulus of vorticity and curl of vorticity by a Beltrami flow. (A Beltrami flow is one in which velocity is parallel to vorticity. It is called a strong Beltrami flow if the scalar of proportionality is a constant rather than a function of position.)

On the other hand, the viscosity term in the surface integral is zero for a flow with the strong Beltrami property. This is seen most easily by writing the term in Einstein notation. In this notation the term is:

$$v_i \omega_{i/j} - \omega_i v_{i/j} = v_i v_i (\omega_i / v_i)_{/j}$$

And since the ratio of the components of vorticity to the components of velocity is just a constant for a flow with the strong Beltrami property, the derivative is zero and the whole term is zero. For a flow with a weak Beltrami property this term is entirely determined by the derivative of the scalar of proportion between the vorticity and the velocity.

The first term in the surface integral is the convection of helicity by the exchange of pressure energy for flow energy along vorticity lines. One might expect a plus sign instead of the negative sign, but note that in the solution of the Clebsch variable equation one also see a negative sign in this term.

The remaining term is the convection of helicity by fluid motion. Both of these terms are from Euler's equation.

Now it is easy to complete the example of a flow field which is instantaneously Clebsch representable but not dynamically Clebsch representable. The term $\omega \cdot \nabla \times \omega$ can be written directly in terms of λ and μ without the need to compute ϕ. We find that:

$$\omega \cdot \nabla \times \omega = \nabla\lambda \times \nabla\mu \cdot \nabla\nabla\lambda \cdot \nabla\mu$$

Which for the above stated counterexample is:

$$\cos(-x+2y-z)[\sin x - 2\sin(2y)][2\sin(2y)\cos z + 2 \sin x \cdot \sin y]$$

which, when integrated of the periodic volume, reduces to:

$$\int_V \sin^2 x \cdot \sin^2(2y) \cdot \cos^2 z = \pi^3$$

which is not zero.

CHAPTER V

THE MODIFIED EQUATION

In the Navier-Stokes equation, it is only the viscosity term that sometimes makes it impossible to represent the time evolution of a velocity field in terms of Clebsch variables when the instantaneous field does have a Clebsch variable representation. This same term is the only source term in the helicity balance. Let us modify the viscosity term so that the helicity is conserved, and the Clebsch variable evolution equation is always solvable. Of course, there are different modifications of the viscosity term that will achieve this. One modification is to drop the viscosity term altogether and to study Euler's equation. Another possibility would be to approximate the viscosity with the gradient of a scalar, which would, however, lead to zero dissipation in the periodic case.

It would be desirable to change the viscosity term as little as possible, to stay as close as possible to the Navier-Stokes equation. In both the solution of the dynamic equation for Clebsch variables and in the helicity balance it is only the component of the viscosity term which is parallel to the vorticity that gives us these effects.

The Clebsch variable evolution equation is algebraically solvable if the dot product of vorticity and the right hand side, which consists of the viscosity term and the divergence of an arbitrary scalar, is zero. If the viscosity term has no component parallel to vorticity, then setting the scalar equal to a constant gives a right hand side that is identically zero. Then the system is algebraically solvable. In the helicity balance the component of the viscosity term parallel to the vorticity is the only source term. If this term is eliminated, then the helicity will never change. Fluctuations in the helicity density will move around the fluid by the mechanisms discussed under the helicity balance, but no new helicity will be created or destroyed. In short, if the viscosity term in the Navier-Stokes is replaced with:

$$\nu(\nabla^2 \mathbf{v} - \frac{(\omega \cdot \nabla^2 \mathbf{v})}{\omega \cdot \omega}\omega)$$

we get an equation which conserves helicity over a periodic volume or a volume which has a boundary without normal gradients of velocity or vorticity (a boundary at which nothing happens). This equation also preserves Clebsch representability.

In the rest of this work, the Navier-Stokes equation with this new term replacing the usual viscosity term will be referred to as "the modified equation" and the term itself will be referred to as "the modified viscosity term".

I emphasize here that the purpose of this modified equation is not to describe some non-Newtonian flow (although possibly it does) nor is the modification made because it makes the integration of the equation easier (it seems to make it harder). The purpose of studying this modified equation is to illuminate the role of topological changes in the vorticity field, especially those involving helical fluctuations in time. The hope is that this equation is in some sense close to the Navier-Stokes, but different in its action on the topology of the vortex field. Further, it is often implied that the essential features of turbulence are from the Eulerian (non-viscous) part of the Navier-Stokes. In this view, helical fluctuations are not important, and the viscous term serves mainly to dissipate energy and prevent discontinuities in the velocity field.

Although there are not many analytical results for this equation, in this respect it is in good company. There is no proof for the Navier-Stokes equation for the existence or uniqueness of a solution. The proofs that do exist for the Navier-Stokes such as dissipation properties and the symmetry of the surface force tensor took many years and minds to develop.

First of all, note that the modified viscosity term can be rewritten with the two terms combined to give:

$$\nu\frac{\omega\times\nabla^2\mathbf{v}\times\omega}{\omega\bullet\omega}$$

or, alternatively, can be written:

$$\nu\mathbf{n}\times\nabla^2\mathbf{v}\times\mathbf{n}$$

where **n** is the unit vector tangent to vorticity.

In this form it is clear that this term will not become infinite due to a zero in the vorticity field, but will lead to discontinuities in the time derivative for certain kinds of singularities in the vorticity field. More specifically, if the limit of $\mathbf{n}\cdot\nabla^2\mathbf{v}$ fails to exist in the neighborhood of a singularity, the time derivative will be discontinuous at that point. This leads to the possibility that the velocity field will become discontinuous, leading to infinities in the vorticity field, even if the original field was completely smooth. The behavior of the enstrophy spectrum observed in the simulations suggests that this might actually occur.

Does this equation dissipate energy, conserve it or create it? I have not been able to show analytically that it does not create energy, but I have also been unable to find a counterexample. Two extremes that do exist have been found, strong Beltrami flows and Couette types of flows.

In the case of Couette type flow, such as laminar flow in a pipe or between two planes, or any shear flow where the direction of shear is orthogonal to the direction of flow, the vorticity is already perpendicular to velocity, and so the modified equation gives exactly the same time derivative as the Navier-Stokes. In this case the dissipation has its full value.

Because of this it can be expected that the modified equation will act normally at fluid boundaries. A problem with Euler's equation is that it cannot in general fit non-slip boundary conditions. It is not realistic near solid boundaries. The modified viscosity term is already in the form that the normal viscosity term assumes at solid boundries for many flows. So the modified equation is perhaps close to the Navier-Stokes in its behavior near solid boundaries.

In a flow with the strong Beltrami property, the vorticity is parallel to the viscosity term, so in this case the time derivative is the same as that give by Euler's equation. This is the minimum dissipation found in any of the flow fields I tried.

This new viscosity term will not necessarily have other of the usual properties of the usual viscous term. I have not been able to show that it can be written as a surface force, that it conserves momentum, either angular or linear. In view of this it is a pleasent surprise in the simulation results that the modified equation seems to act normally in these respects. It has dissipated energy in each case studied for the entire simulation time. The linear momentum is approximately conserved. The one very noticable new effect of the modified viscosity term has been that it transfers energy between different Fourier modes because it is nonlinear. It is, in fact, in some sense more nonlinear than the usual convective term.

An interesting case to consider is one where the initial condition has non-zero helicity. In this case the helicity must be conserved so the motion cannot ever stop. I can think of only three other possibilities. The first is that the energy will increase in some parts of the flow field, even while it decreases in others. This is possible, but seems unlikely in view of the fact that I could not find an example of this and the simulation results do not suggest it.

It is also possible that the volume where velocity is above any given value will become smaller and smaller in time, while enstrophy grows in a manner never observed in the Navier-Stokes. This is possible because the modified viscous term might allows large gradients in the velocity field and possibly even discontinuities.

The final possibility is that the flow will relax to a Beltrami flow, so that dissipation stops, or possibly even a Trkal flow, which is a flow that remains a strong Beltrami flow through time.

Another property of the modified equation that is of great importance, in theory and in the simulation, is the very non-linear nature of the term. First of all, since the term in question is the same one that dissipates energy, the nonlinear transfer of energy between Fourier modes due to this term cannot be reduced by reducing the viscosity. Since it is homogeneous of order one in velocity the nonlinear effects cannot be reduced by reducing the velocities either. Worst of all, the term is in some sense much more nonlinear than the usual nonlinear (convective) term. Consider the modified viscous term in the form:

$$\frac{\omega \times \nabla^2 v \times \omega}{\omega \cdot \omega}$$

The numerator is more nonlinear than the convective term in this sense. If the convective term has no mode with a wavenumber magnitude greater than k, the part of the time derivative calculated for that term will have no Fourier mode with a magnitude no greater than 2k. For the numerator of the modified viscous term, the corresponding time derivative can have modes with wavenumber magnitudes as great as 3k.

But division by a scalar is much worse. The division of a number by a scalar which has modes only between -k and k will, in general, lead to modes from $-\infty$ to $+\infty$. In fact, if there is a zero anywhere in a continuous vorticity field then the size of the Fourier coefficients of the inverse of the magnitude of the vorticity will not decrease rapidly to zero, in fact, the sums of the magnitudes of the Fourier modes will diverge in this case.

This extreme nonlinearity presents great difficulties in the simulation, especially in the attempt to find the long time behavior of the modified equation.

CHAPTER VI

THE METHOD OF THE SIMULATION

As mentioned above, there are two parts to the thesis work: the analytical work, the results of which are described in the last two chapters; and simulation work. The simulation work consists of simulation of the modified equation, and of the Navier-Stokes for comparison. The programs used for the simulations and postprocessing are described in this chapter, as are the procedures used to determine the size of the time steps and the selection of initial conditions for simulation.

Both simulations, those of the modified equation and of the Navier-Stokes will use the same basic method. This is important because there are no clear analytical proofs of the accuracy of the simulation methods, so the use of two very different methods of simulation would introduce many questions about which differences are due to differences in simulation methods and which are due to genuinely different behavior of the two equations.

Both simulations will use spectral methods on a periodic space. This will make comparison with existing successful spectral simulations, such as those by Orzag and Kerr, easy. Also, spectral methods give the best resolution of turbulent flows when the boundaries are simple. The spectral method will be especially convenient because of the periodic boundary conditions. However, problems such as aliasing errors in the normalization step (division by the enstrophy in the modified viscocity term) will make the results of this simulation necessarily preliminary. But it is hoped that they will be suggestive enough to either lead to new suggestions for theoretical results by themselves, or to lead to modifications of the simulation method. Finally, much of the analysis of the results of the simulation is done in Fourier space, which make spectral methods natural to use for the simulation itself.

The term pseudo-spectral is sometimes used to describe the simulation method used for these simulations. The "pseudo" refers to the fact that some modes are truncated each time step. But since this truncation is in fact always done in all spectral simulations I have seen in the literature, I trust that no ambiguity will result in the use of the less cumbersome term "spectral" in this work.

The simulation is done partly in Fourier space, and partly in real space. Because of the linearity of the Fourier transform, each separate term can be calculated in Fourier space or in real space. The terms which are to be calculated in real space will then be transformed to Fourier space, and the time-stepping will be done in Fourier space, because the viscosity term can be implicitly time stepped in a very simple way in Fourier space, and implicit time stepping is more accurate.

All derivatives are calculated in Fourier space, since this involves only a multiplication by the wave vector in Fourier space and would involve complicated interpolations in real space. So for the given velocity computed at the beginning of each time step, the vorticity and Laplacian of velocity are immediately computed in

Fourier space, and then the vorticity, velocity and Laplacian of velocity are transformed to real space.

Two terms are calculated in real space. The convective term is calculated in real space in the form $\mathbf{v}\times\omega$. The calculation is done in real space because all the multiplications in real space become convolutions in Fourier space. To calculate one product in real space requires only one operation per gridpoint. A convolution in Fourier space for two vectors for a grid with N gridpoints in each direction requires on the order of N^6 operations in each direction since it is defined by:

$$(A*B)(\mathbf{k}) = \Sigma\, A(\mathbf{p})B(\mathbf{q}).$$

The sum in this equation is taken over all $\mathbf{p}$ and $\mathbf{q}$ such that $\mathbf{p} = \mathbf{q} + \mathbf{k}$. (In the fast Fourier transform all addition is done modulo N. In the analytical theory, the addition is done normally.) Taking into account that performing the operation in real space requires two three dimensional Fourier transforms (one forward and one reverse), the total number of operations required to compute this term at one grid-point in real space using a fast Fourier transform is on the order of $N^3\log N$.(Orszag 1971)

The other term that will be calculated in real space will be the modification term. Since the calculation of the modification term requires four multiplications it would be expected that this term would be calculated in real space. But far worse than the four multiplications is the inversion of the moduli of the vorticity, for which no easy expression exists in Fourier space. Both of these terms can lead to dealiasing problems, which will be discussed later.

I will now describe a single time step of the simulation. At the beginning of a time step it is necessary to have two velocity fields in memory. I will call the two velocity fields the past velocity field and the current velocity. The field that is being simulated will be called the future velocity field. At the beginning of the time step the past and present velocity fields are both in Fourier space.

First the viscosity term is computed in Fourier space from the present velocity field. That is, each component of the present velocity field is multiplied by the square of the modulus of the wavenumber. The result then transformed to real space. The vorticity field is calculated in Fourier space. This operation consists of forming the sums:

$$F\{\nabla\times v\} = F\{\epsilon_{mnp} v_{p/n}\} = -\iota\epsilon_{mnp} F\{v_p\}\cdot k_n$$

where ι is the square root of a negative one. This vorticity field is then transformed into real space, where the normalized vorticity field is then computed by dividing the vorticity vector at each gridpoint by its modulus. The values of the moduli used to compute the normalized velocity field are saved to avoid recomputing the vorticity field from the Fourier space present velocity.

The magnitude of the modification term at each point is then computed by taking the dot product of the normalized vorticity field and the viscosity term. The result is multiplied by the normalized vorticity vector at each point to give it the right direction. In other words, using **n** for the normalized vorticity vector, the actual modification term is computed using the formula, equivalent to the one given above:

$$\nu(\mathbf{n}\cdot\nabla^2\mathbf{v})\cdot\mathbf{n}.$$

The modification term is transformed back to Fourier space, and the vorticity field is regenerated from the **n** field from the saved moduli of the vorticity field.

If the vorticity at a particular gridpoint is almost zero, an error message is printed, and if this occurs more than twenty times the program stops. However not even for one value of vorticity has this occured except when the initial condition input has zeros in the vorticity field. The reason for avoiding very small values of vorticity is that the numerical noise of the computation can determine the direction of the normalized vorticity field if the value of vorticity is very small at the given gridpoint. If these values are then used, numerical noise then becomes very important near that region, destroying the accuracy of the simulation. To determine whether the value of vorticity at a particular gridpoint in Fourier space is too small, first the absolute values of the smallest (most negative) and largest (most positive) values of the Fourier components for each of the three components of velocity are added together, considering each imaginary component and each real component as a separate component and considering all the modes in Fourier space.

The sum of these six values is then multiplied by ten to the negative ten. If any value of vorticity were to fall below this value, a message would be printed.

An instance of problems arising from the low vorticity points did occur in low Reynolds number runs of the Taylor-Green vorticity field. The initial condition in this case has a symmetry in the x-y plane such that if the x and y axes are switched, the resulting flow field is the same, except that the location of the origin is changed. As a result, the total energy and enstrophy of the x and y directions should be very close throughout the simulation. In early runs, where the whole vorticty field was normalized, not excluding the points of very low vorticity, the x-y symmetries disappeared after the second time step. This is perhaps a worst case scenario since the representation of the vortex used put points of zero vorticity exactly on collocation points. When the program is altered to shift the low values of vorticity away from the gridpoints, this problem did not occur.

In order to compute the convective term, the present velocity field is transformed to real space. Total enstrophy and energy in each direction are written to the output files. The cross product of the velocity and vorticity is computed and transformed back to Fourier space. The present velocity field itself is transformed back to Fourier space.

So far, we have computed Fourier transforms of $\mathbf{v}\times\omega$ and $(\mathbf{n}\cdot\omega)\mathbf{n}$. Before describing the next step, let us look at the way the viscous term is time stepped. As mentioned above, the accurate simulation of the viscosity term involves implicit time stepping. Implicit time stepping would be more accurate for any of the terms, but only for the viscous term is the computation simple enough to make this method useful. To implicitly time step the other terms would involve the use of a predictor-corrector technique, which would involve a much greater amount of computation time. The implicit step uses the average of the past future velocities to compute the present effect of viscosity, making the time stepping a central difference approximation. In Fourier space the equation for this is:

$$\mathbf{v}^{n+1} = \mathbf{v}^{n} + \Delta\mathbf{v} = \mathbf{v}^{n} - \nu\Delta t(k^2\mathbf{v}^{n+1} + k^2\mathbf{v}^{n-1})/2$$

Where Δt is the size of the time step. This can be solved for $\mathbf{v}^{n+1}$ algebraically. In the actual case, there are two terms included in $\Delta\mathbf{v}$, one to be computed explicitly and one to be computed implicitly. The explicit $\Delta\mathbf{v}$ includes the modification term, the pressure term and the convective term. Rewriting the above equation to include the explicitly time stepped term we have:

$$\mathbf{v}^{n+1} = \mathbf{v}^{n} + \Delta\mathbf{v}^{exp} + \Delta\mathbf{v}^{imp} = \mathbf{v}^{n} + \Delta\mathbf{v}^{exp} - \nu\Delta t(k^2\mathbf{v}^{n+1} + k^2\mathbf{v}^{n-1})/2$$

And so the time stepping done in this program will actually be computed as:

$$\mathbf{v}^{n+1} = \frac{\mathbf{v}^{n} + \Delta\mathbf{v}^{exp} - \nu\Delta t k^2/2\mathbf{v}^{n-1}}{1+\nu\Delta t k^2/2}$$

The explicit term can be further subdivided:

$$\Delta v^{exp} = \Delta v^{crs} + \Delta v^{mod} + \Delta v^{prs}$$

Where Δv^{crs} is the cross product of velocity and vorticity in Fourier space, previously computed, Δv^{mod} is the modification term, also previously computed, and Δv^{prs} is the gradient of the pressure plus the square of the magnitude of the velocity.

Note that the second part of the viscosity term (i.e. the modification term) uses the velocity field at a different time than the first part. This can lead to generation of helicity by time stepping errors. Because of this it is necessary to use smaller time steps for the simulation of the modified equation than for the usual Navier-Stokes.

This last term, which includes the pressure, can be calculated from the incompressibility condition. Taking the divergence of the entire modified Navier-Stokes equation, and recalling that the original velocity field is incompressible we obtain Poisson's equation:

$$\nabla^2(p/\rho + v^2/2) = -\nabla\cdot[\mathbf{v}\times\omega - \nu(\mathbf{n}\cdot\nabla^2\mathbf{v})\mathbf{n}]$$

which for periodic boundary conditions has a solution unique up to a physically insignificant constant. Notice that by the incompressibility of the original velocity field, the viscous term does not enter into the equation for the pressure term at all. This is how the time stepping is done in principle. The actual step by step details that follow describe the elegant manner in which this is done with the minimum of memory and computational time. The overall plan is not due to me (except for that part directly relating only to the modified equation), but is due to earlier researchers in the field of spectral simulations, especially Patterson and Orszag.

Recalling that these terms will be time stepped explicitly, we can write explicit formulae for them in terms of the present velocity. Using F for the Fourier transform operator we get:

$$\Delta \mathbf{v}^{crs} = \Delta t \cdot F[\mathbf{v} \times \omega]$$

$$\Delta \mathbf{v}^{mod} = \nu \cdot \alpha \cdot \Delta t \cdot F[(\mathbf{n} \cdot \nabla^2 \mathbf{v})\mathbf{n}]$$

$$\Delta \mathbf{v}^{prs} = \frac{\mathbf{k}}{k^2}\, \mathbf{k} \cdot (F[\mathbf{v} \times \omega] + \nu F[(\mathbf{n} \cdot \nabla^2 \mathbf{v})\mathbf{n}]) \cdot \Delta t$$

Putting all of this together, the next few steps are done in a manner computationally efficient, but not conceptually natural. First an intermediate velocity field is computed that includes part of the viscous term and the cross product term. The subroutine that does this is called "PIVOT2". Calling the result of PIVOT2 $\mathbf{V}^1$ we get:

$$\mathbf{V}^1 = (1 - \nu \Delta t/2) \cdot k^2 \cdot \mathbf{v}^{n-1} + \Delta t \cdot F(\mathbf{v} \times \omega)$$

Then the modification term is taken into account.

$$\mathbf{v}^2 = \mathbf{v}^1 - \nu \cdot \Delta t \cdot F[(\mathbf{n} \cdot \nabla^2 \mathbf{v})\mathbf{n}]$$

Now $\mathbf{v}^2$ includes all of the terms needed to compute the pressure term as well as part of the viscosity term. The viscosity term should have no effect on the computation of the pressure term because of the incompressibility of the present velocity. So the subroutine PRES next calculates this pressure term from $\mathbf{v}^2$ with an expression equivalent to the one given above.

$$\Delta\mathbf{v}^{prs} = \frac{\mathbf{k}}{k^2}\,\mathbf{k}\cdot\mathbf{v}^2$$

Now the subroutine VISC completes the computation of the viscosity time stepping while adding on the pressure term.

$$\mathbf{v} = \frac{\mathbf{v}^2 - \Delta t \cdot \Delta\mathbf{v}^{prs}}{1 + (\nu \cdot \Delta t)/2}$$

This almost completes the reiterative calculation of the velocity. The one operation that remains is the dealiasing step.

Consider the cross product term in the Navier-Stokes equation. In the spectral approximation, we assume that the velocity and vorticity fields can be approximated by a finite number of Fourier modes between -N/2 and N/2. But if the components of velocity field and a vorticity field both fitting this model are multiplied, the result will not be contained in only the modes from -N/2 to N/2, but will in general include modes from -N to N.

The problem now is that these modes will not just be forgotten as we would wish. (One can argue that the higher modes generated are quickly damped out by viscosity or that they continue to exist but have only a minor effect on the lower modes.) An N point fast Fourier transform cannot distinguish between different modes modulo N and will, for instance take the result of the N mode and interpret it as a zero mode. In this way the higher harmonics are not dropped, but reappear under an alias, disguised as lower modes.

A method to correct this problem was developed by Orszag to completely dealias the Navier-Stokes. The first step is to set many of the higher modes to zero by spherical truncation (see Patterson et al. 1971). Then the calculation is carried out on two separate grids and the results averaged. This method is analytically proven to completely dealias the time steps. But it has been discovered over time that if the modes are set to zero in a computationally simpler method, i.e. octodecahedral truncation, the results are, for all practical purposes, the same. It has also been discovered that it is unnecessary to compute on two separate grids, that using only one gives results just as good and saves about half of the computational time. So the current spectral simulation performs only the octodecahedral truncation and nothing more. This is the procedure that will be tried in simulating the modified Navier-Stokes.

There is one difference between the two simulations in terms of the dealiasing procedure. In the simulation of the regular Navier-Stokes equation the (0,0,0) modes are set to zero each time step. This is done because, in spite of the fact that conservation of momentum implies that the (0,0,0) mode, which starts with a value of zero, should remain zero, in actual practice it is found that it drifts away from zero over time. This is due, in part, to aliasing error and in part due to the difference between the digital Fourier transform and the analytical Fourier transform. In the simulation of the modified equation, it was found that this caused a greater drift in helicity than not setting the zero mode equal to zero. So in the simulation of the modified equation the zero mode is not reset to zero. In spite of this, and in spite of the fact that the modified equation has not been shown to conserve linear momentum, the zero mode remains basically zero throughout the simulation. That is to say that it remains smaller than the machine epsilon so that even when an E mask is used to print out the number, the number is printed as zero.

In the modified equation, there is another source of aliasing errors besides the cross product term. That is the modification term. With this term not even the the original procedure that was analytically proven to completely dealias the cross product term will dealias the result. This is because if ω is in the range -N/2 to N/2, the inverse modulus of ω will not just vary from -N to N but will in general include all terms from minus to plus infinity, as described in the previous chapter.

To perform the dealiasing octodecahedral truncation is used. To see if this method of dealiasing is effective, the magnitude of the coefficients of the higher modes are checked. If these are not too large, then it can be expected that the higher modes are dying out rather quickly, and the dealiasing is working acceptably. To allow the reader to judge the accuracy vorticity spectra are included.

The stability of the solution can be further improved by averaging the past and present time step and having the time increment (for instance, every fiftieth step or so will do.) Experience with

Orszag's spectral programs shows that this is sufficient to presume stability.

The question of whether the time step is too large can be resolved by decreasing the size of the time step. If the results with the smaller time step are essentially the same as those with the larger time step, then the larger can be used to save computational time.

The maximum Reynolds number allowable can be checked using the graph of the vorticity versus k^2 in Fourier space. Experience shows that if the Reynolds number is too high, then this graph will show a strong upturn at high k^2. If this does not happen, the Reynolds number is not too high.

Finally, the question of which length scales are being well resolved is addressed by computing the characteristic length scales, such as the Kolmogorov length scale for dissipation. If the characteristic distance is larger than the distance between gridpoints, then it can be assumed that the length scale in question is being well resolved.

Typically for this kind of numerical simulation the question of accuracy of the simulation cannot be answered by an analytical proof of the accuracy of the simulation. Instead, a combination of error estimates, experience with similar simulations and credibility of results is used. For a still greater degree of certainty, the best method is to compare the results of two different methods of simulation, since comparison with experiment is not possible.

I would like to thank Prof. Pelz for his help in constructing the program to simulate the modified equation, in particular for his suggestion that saves three Fourier transforms each step while making the program structure simpler and his suggestions to help conserve helicity more exactly during the course of the run.

CHAPTER VII

POSTPROCESSING: THE QUANTITIES COMPUTED AND THE PROGRAMS THAT DO IT

1. THE QUANTITIES COMPUTED

Since such large amounts of data are generated by a numerical simulation of a flow field, the results cannot be inspected directly. This is one reason for postprocessing programs. A second reason, at least as important as the first, is to check the validity of the results. For validity checking certain quantities are commonly computed: energy in each direction vs time, enstrophy in each direction vs time, Taylor microscale, velocity and vorticity spectra.

The energy should decrease over time for the Navier-Stokes equation monotonically. The energy in each direction should also decrease, but not necessarily monotonically. The decrease in energy should be greatest when the enstrophy is greatest since, in a periodic volume the integral of the enstrophy over the volume is equal to the dissipation in a volume. This result does not hold for the modified equation.

The enstrophy itself always increases at first if the initial condition is a randomly generated velocity field rather than the results of another simulation. The enstrophy then peaks and starts to decline. Statistics near the peak of enstrophy are usually considered the most significant, since at this time the field has had time to develop the enhanced dissipation characteristic of turbulence, yet has not decayed too far. Decay is a problem in turbulence simulation since the initial velocities simulated are limited by the simulation technique. One solution is to inject energy with an external forcing function, but this introduces the complication of the forcing function's statistics influencing the development of the flow field, and this method was not used in this work.

The Taylor microscale is used to characterize the length scale of the convective term and is defined as the square root of the ratio of the average velocity squared in a given direction and the average squared gradient of velocity in the same direction. By using the three directions of the x, y and z axes, we can compute three different Taylor microscales, which give some indication, not only of the length scales involved in the simulation, but also the isotropy of the flow field, differences in the Taylor microscales in different directions indicating anisotropy.

A measure of the length scale on which dissipation occurs is the Kolmogorov length scale. If the Kolmogorov spectrum is assumed to dominate, this can be calculated using only the dissipation rate and the kinematic viscosity. Since in this simulation set the Kolmogorov spectrum did not predominate, I will use a form due to Batchelor (Batchelor 1953). This form assumes homogeneity and isotropy, which do not strictly hold in the simulations, but there is no form of this measure that assumes nothing about the flow field. According to these assumptions, the dissipation length scale, λ, is:

$$\lambda^2 = \frac{10\nu u^2}{du^2/dt}$$

For comparison with these two length scale note that in the simulation the gridpoint separation in real space is $2\pi/32 \approx .2$ These are of course order of magnitude types of estimates, and there is little sense in worrying about more than one digit accuracy.

The velocity (energy) and vorticity (enstrophy) spectra are also important for determining the accuracy of the simulation. The velocity spectrum is deceptive since it looks well behaved even when the vorticity spectrum does not, so the vorticity spectrum is the most useful in this respect. It should not have too strong a turn-up at the high wavenumber end and should not be too high at the high wavenumber end of the spectrum, where truncation of high modes occurs.

All of these measures are discussed in the references given for spectral simulations, particularly in the work cited by Kerr. Other quantities calculated are used mainly for their indications of the development of the structure of the vorticity field lines and the development of helicity. These measure are less well known.

The first of these lesser known measures is the spectrum of H(**k**). H(**k**) is defined as $\mathbf{v}(\mathbf{k})\cdot\omega(-\mathbf{k})$, where $\mathbf{v}(\mathbf{k})$ is the k'th Fourier component of veloctiy and $\omega(\mathbf{k})$ is the Fourier component of vorticity. By the property of complex symmetry, which holds for the Fourier components of the transform of any real quantity, $\omega(-\mathbf{k})$ is the complex conjugate of $\omega(\mathbf{k})$. Note that this quantity is not the Fourier transform of helicity density, which would be given by the convolution of the Fourier velocity and vorticity. The physical meaning of this quantity is that H(k) is the contribution to the total helicity due to the k'th component of velocity. The spectrum of this quantity is also unusual in that, unlike most power spectra, this spectrum can have negative values. In fact, it is typical of this quantity that its spectrum fluctuates strongly. There is some reference to this quantity in the works cited in the literature review by Prof. E. Levich, but since much of this direction of investigation is quite recent, most the the material has not yet been published.

The speculation is that helicity might show a kind of inverse cascade similar to that described for enstrophy in two dimensions (Levich '83a). Since the cascade is inverse in the sense of going to larger scales, it could be a mechanism for the formation or evolution of large scale structures. If the mechanism is shown to be responsible for the splitting or death of large scale structures, this is similarly significant to showing it to be responsible for the birth of large scale structures. It is also felt that the strong fluctuations already observed in other simulations of H(k) show some general, of as yet not well understood, mechanism for the organization of turbulent flow.

Besides the H(k) spectra, the distribution of cosine theta is also computed. This quantity has been discussed in the literature review.

Two very new quantities were also computed, referred to here as alpha and beta. Alpha is merely the integral over all of k space, of $H(\mathbf{k})\bullet H(-\mathbf{k})$. This quantity is a measure of the total amount of fluctuation of H(k). According to the speculation, this quantity should grow in the initial stage of turbulence if the Reynolds number is high enough. For smaller Reynolds number, the viscous decay will predominate, and alpha will decrease.

Beta is the sum over some of k space of $H^2(\mathbf{k})$ divided by the maximum possible $H^2(\mathbf{k})$, which is $[\mathbf{v}(\mathbf{k})\cdot\mathbf{v}(\mathbf{k})]^2\cdot[\mathbf{k}\cdot\mathbf{k}]$. After the sum is computed, it is divided by the total number of points included, giving a normalized value that is between zero and one. The sum should not necessarily be taken over all of k space since, as defined, each point is weighted equally, and the quantity will include modes that are mainly noise for simulations in the periodic case.

The choice made for the condition for sampling k space to calculate beta was perhaps not the best. It was very convenient to use the size of $H^2(\mathbf{k})$ as a criterion, computing different betas for different values of the cutoff point. If $H^2(\mathbf{k})$ is less than the cutoff point that point is not used in calculating the respective beta. The problem with this is that this condition for sampling includes the effect of alignment of the real and imaginary parts of the velocity and the k, which is part of what determines the ratio of $H^2(\mathbf{k})$ to its maximum value. In fact the ratio of $H^2(\mathbf{k})$ to its maximum possible value is exactly the square of the volume element described by the unit vector in the same directions as the real part of $\mathbf{v}(\mathbf{k})$ the imaginary part of $\mathbf{v}(\mathbf{k})$ and $\mathbf{k}$. The closer this set of three vectors is to an orthogonal triad, the larger $H(\mathbf{k})$ will be, and the more likely that point will be to be included in the ensemble for the given cutoff point. The overall effect of this can be expected to be that the higher the cutoff point, the higher the corresponding value of Beta will be.

To get some idea of what the beta values mean, we can compute the expected value of a single term of beta, which, except for the conditional sampling problem, will the be the expected value of the normalized beta. Of course there is in turbulence no complete description of the correlations between the vectors involved, so I will make the naive assumption that the real part of velocity, the imaginary part of the velocity, and the **k** to which these Fourier components correspond are all independent. The assumption of independence give the joint probability distribution of the angles involved. Defining the angle between the real and imaginary part of to be theta and the angle between the cross product of the real and imaginary part of the velocity and the **k** vector to be phi, we use the well known (and easily derivable) result when space is isotropic that the probability density of the angle between two vectors is proportional to the since of the angle between the two vectors. This leads to a joint probability distribution for theta and phi:

$$P(\theta,\phi) = 1/4 \sin(\theta)\sin(\phi)$$

Recalling that the value of the term in the sum for beta is the volume element of the three vectors, using t for the term we get:

$$\langle t\rangle = \int P(\theta,\phi)\sin(\theta)\cos(\phi) = \pi^2/32 \approx .309$$

The results will show that the actual value computed is never this low even for the initial condition, a result I expect is due to the conditional sampling. Because of these objections to the conditional sampling used for beta, the full results that were computed for this quantity are not reported here.

THE METHOD OF THE POST PROCESSING

Since the output of the simulation is the velocity field in Fourier space (unlike BIGBOX, which uses a mixed, Fourier - real space representation) the calculation of the spectra consists only of adding up all the components of the quantities for the wavenumbers in a given range of magnitudes. This is done by taking each component in k space, computing its value, computing the magnitude of the wavenumber and adding it to the results already accumulated in the spot in memory reserved for that range of wavenumbers. Alpha and beta are computed in a single do loop, computing first $H^2(k)$, adding it to the partial sum for alpha, and then using that alpha to determine what partial sum of betas will have a term added to them for the given k.

The Taylor microscale is also computed in Fourier space, simply dividing, for instance, the total energy in the x direction by the total $(dv/dx)^2$ (where v is the x component of velocity). It is not necessary to go to real space to find the sum of these squares, because Parseval's theorem says that the sum of the square of the real space quantities over the whole space is equal to the sum of the squares of the Fourier components over all of Fourier space. The Kolmogorov length scale is computed by hand using the values of energy put out by the simulation itself.

So, we almost escape the need to use the Fourier transform in the post processing, but not quite. In order to find the distribution of cosine theta it is necessary to go to real space since there is no neat expression for this quantity in Fourier space. The velocity and vorticity are transformed to real space, and terms of the sum are computed there directly, and added up.

CHAPTER VIII

THE RESULTS OF THE SIMULATIONS

The main results of the simulations are two pairs of runs. Each pair consists of one run using the Navier-Stokes equation, and one run using the modified equation. The first pair of runs starts with an initial condition which is generated using Clebsch variables, and so starts with zero initial helicity. The second pair of runs has an initial condition generated using the usual velocity variables, and so has non zero initial helicity.

The first pair of runs is referred to here using the term "Clebsch initial condition runs". The second pair of runs is referred to with the phrase "random initial condition". This is, of course, a casual use of the word random, which properly applies only to ensembles with some probability density function. Both initial conditions were generated using a standard pseudo-random number generator (RANF), so both are equally random. The chosen terms of reference are not exact, but more descriptive than using terms like "run A" and "run B".

To generate the random initial condition, we used a subprogram already written for INCORE. This routine generates independently the Fourier components of the three Cartesian components of velocity. The complex phase angle, the arctangent of the ratio of the real component of the velocity to its imaginary component, is uniformly distributed between zero and two pi. The magnitude of the Fourier component of velocity has a distribution in which the magnitude of the wavenumber occurs as a parameter. The probability density dependence on the magnitude of the wavenumber is:

$$C^1 k^s \exp(-C^2 k^2)$$

where k is the magnitude of the wavenumber, and C^1, C^2 and s are parameters which can be chosen to give the desired total energy, location of the maximum of the energy spectrum and steepness of decent of the energy spectrum from its maximum value to the small values at high wavenumbers. The above quantity is then multiplied by a variable distributed between zero and infinity. More precisely, it is multiplied by:

$$\sqrt{-2 \cdot \mathrm{Alog}(R1)}$$

where R1 is the variable given by the random number generator RANF which gives a uniform distribution between zero and one, and the square root extends over the entire expression.

Since the velocity field generated in this way will not in general be incompressible, it is made incompressible using the same procedure (and the same subroutines) used to enforce incompressibility in the time stepping, and is described in an earlier chapter. Finally the field is dealiased, again in the same way as in the time stepping part of the program.

When generating fields to use as initial conditions, we looked at a large number of fields generated in this way. We checked the distribution of cosine theta, and found that it never had the horns that were observed after turbulent evolution of the field. This confirmed the supposition that the horns of cosine theta are not due solely to some slight spreading of the spectrum as the simulation progressed, which might otherwise be supposed to be the case. In the most extreme case, the energy contained in the modes with magnitudes between fifteen and sixteen were one fifteenth of the energy contained in the modes with magnitudes between three and four, which was the location of the maximum of the energy spectrum in this case.

A slight skewness is seen in the distribution of cosine theta for fields generated in this way. This is very much to be expected since cosine theta is a kind of normalized helicity density. So if the helicity density tends to be more of one sign than the other, so might the normalized version of it.

To formulate the Clebsch variable initial condition, one variable was generated as described above for the components of velocity. But then each component was assigned to either λ or μ, again using RANF to assign the values equally to each. Whenever one of these two variables was given a non-zero value at a particular wavenumber, the value of the Fourier component of the other was left zero, so that for each wavenumber in Fourier space, only one of λ or μ was given a non-zero value. This was done to avoid giving the resulting field a large (0,0,0) mode velocity. Otherwise the (0,0,0) mode tends to have the largest value. (Recall that the expression for the velocity, before the imposition of incompressibility in Fourier space, is the convolution of λ and $k\mu$, and for the (0,0,0) mode this is the sum over k of $\lambda \cdot k\mu$). The (0,0,0) mode becomes zero after incompressibility and dealiasing, but this process involves the difference of large numbers if the (0,0,0) mode is very large, which is a classical source of numerical error. The resulting field has much smaller helicity if the (0,0,0) mode of the velocity field is initially zero before the imposition of incompressibility and dealising, so the above described method was used. The helicity of field generated in this way is typically smaller than ten to the minus tenth, compared with a typical helicity of ten to the third for a random initial condition for which other statistics are similar. This makes the generation of the zero helicity field far and away the most accurate result of the entire project except, one hopes, for the analytical results.

The distribution of cosine theta of fields generated in this way is not skewed. This is expected since the distribution of helicity density is not skewed. However the distribution of cosine theta is not flat but shows a distinctly convex shape. This was also obseved in the Clebsch initial condition field reported in Pelz et al. 1986. That article does not report the method of generating the field so the two methods of generation cannot be compared here. The appearance of this convexity is not yet explained. Note that the symmetric convex shape puts the maximum of cosine theta at zero, which corresponds to zero helicity density, and this fact could be part of the explanation.

For both pairs of simulations, we chose a relatively low wavenumber magnitude for the maximum of the energy spectrum, between two and three. This was done to make the most of the resolution available, the greatest wavenumber magnitude which included all its possible modes was only fifteen. It was done also in anticipation of spectral truncation problems, especially for the modified equation, which indeed were important. For the Clebsch initial condition, the maximum of the energy spectrum was at two. For the random initial condition it was at two and one half.

The total amount of energy was chosen to be of order one in Fourier space for both runs. Rescaling velocity in the Navier-Stokes or in the modified equation is equivalent to rescaling time and viscosity, so the questions of choice of magnitude of initial velocities is equivalent to the choice of viscosity, since the size of the time steps is determined later, by experimenting with different sizes. We chose the viscosity to be the maximum that we felt we could resolve well enough, even pushing the limit of the simulation, to assure that the result would be of interest in the theory of turbulence. If one choses an initial condition too conservatively, then the initial increase in enstrophy characteristic of turbulence does not occur, or does so only slightly.

The last parameter that determines the steepness of decent of the energy spectrum was chosen to give an initial spectrum that was very low at the wavenumber magnitude where truncation begins (the fifteenth), yet so that the dropoff after the maximum was not extremely sudden. This was done mainly by looking at the energy and enstrophy spectra. These spectra can be found in the appendix. A quick look will assure the reader that they are natural enough, fitting well into the available range of wavenumbers and having the sort of shape one expects for power spectra of a fluid flow.

The size of the time step was chosen by guessing an initial value, running the simulation for a short time, choosing a smaller value and running that simulation for an equal amount of simulation time and comparing the results. When the results are noticeably different, then a still smaller step must be tested. When they are not, the larger step is taken. For the Navier-Stokes equation this procedure resulted in a time step of .005 in the units of the simulation. For the modified equation, a step size of .005 looked good enough when the usual quantities are considered, but led to a greater drift in the value of total helicity than was considered acceptable. A time step four times smaller than that for the Navier-Stokes was used, .00125, and this led to noticeably better conservation of helicity.

The viscosity of the modified equation was chosen to be larger than that of the Navier-Stokes equation for the same initial condition. If this is not done and the lower viscosity of the Navier-Stokes run is used (1/100 for both initial conditions) then the enstrophy spectrum quickly shows significant truncation errors and the total enstrophy "goes through the roof". For the Clebsch initial condition runs of the modified equation, the viscosity was set at 1/70 and for the random initial condition run it was set at 1/65.

Following is a description of the results of these runs. Some comments on the errors expected are given here, but a more detailed analysis is given in an appendix. The graphs referred to are in a separate appendix.

For a quick overview of the runs, refer to the first set of graphs Energy vs time, enstrophy vs time and helicity versus time.

The term "Reynolds number" when used in the graphs means the inverse of the viscosity and is a set parameter of the simulation, rather than a quantity computed from the results of the simulation.

The helicity vs time graphs give a good idea of how well helicity was conserved by the simulations of the modified equation. The results seem to be as good as can be expected, especially for the random initial conditions. Note that in both cases the helicity drifts in the modified equation in the same direction as it moves in the Navier-Stokes. This is probably due to the fact that the modification term lags in time behind the usual viscosity term, since explicit time stepping uses the present time only, but implicit time stepping uses an average of the present and future time. The drift in helicity is about the same in absolute magnitude for either case. A difference of scales of the graphs is responsible for the larger visual difference between the two cases.

Energy vs time is the good news. The modified equation seems to dissipate energy throughout the course of both simulations, as it did in all other runs not discussed fully in this work. There is a difference in the shapes of the curves however. If the curves were to be approximated with a power law in time, the modified equation would have an exponent with a smaller absolute value. An analytical result for homogeneous, isotropic turbulence in the final stage of decay gives an exponent of -5/2 for the Navier-Stokes case, but there is not enough information to derive a similar exponent for the modified equation since the long time behavior of the modified equation is unreliable, for reasons described below. A look at the energy spectra shows no particular truncation errors, but for this the enstrophy spectra are more reliable.

Enstrophy vs time shows the initial increase typical of turbulence. This shows that the parameters chosen are sufficient to give genuine turbulence. Since turbulence is the point of this study, this increase is the most important characteristic to be considered in the choice of parameters. The times chosen for presenting the spectra graphically are the initial condition, an intermediate time, and the spectra for the end of the simulation run. The intermediate time chosen is the time at which the Navier-Stokes equation reaches its peak of enstrophy. This time is the one at which the field is considered the most turbulent, and so is the most appropriate for describing the mechanisms of turbulence. The enstrophy spectra for the initial condition are definitely alright, they show no truncation. The spectra for the times of the maxima of enstrophy, 1.11 for the Clebsch initial condition and 1.36 for the random initial condition, suggest that the simulation parameters are being pushed as far as they will go and are, not surprisingly, worse for the modified equation than for the Navier-Stokes. For the Navier-Stokes equation, the vorticity spectra from this point on look fairly similar. Skipping ahead to the end of the simulation for the Navier-Stokes for either initial condition, one sees a spectrum which looks similar. The truncation at the end of the spectrum looks a little worse, but this is due to a change of scale, since dissipation has by this time brought the maximum of the spectra down.

Looking again at enstrophy vs time, one sees that in the modified equation the enstrophy peaks at a later time than in the Navier-Stokes. Graphs of the vorticity spectra for the times when the rate of increase in enstrophy are beginning to drop noticeably are included for the modified equation. One can see that the enstrophy in both cases tends to drop only after truncation errors become significant. This suggests that the dissipation of enstrophy might be due only to truncation errors. In any case, the data for the times after the peak in enstrophy for the modified equation must be viewed with a large measure of suspicion. The enstrophy spectra for the modified case get only worse, as a glance at these spectra for the ends of the runs show.

In an effort to get around these difficulties, we attempted a run of the modified equation using a velocity field generated by a long Navier-Stokes run at large (1/40) viscosity. This attempt did not succeed well. There is a simple reason why all of these attepmts to simulate the modified equation failed. In a run of the regular Navier-Stokes equation, if the vorticity spectra seem bad, one can always increase the viscosity and so increase the dissipation, especially at the high wavenumbers. The cascade of energy and vorticity from the low wavenumbers will not be increased by this, so a sort of quasi-equilibrium is established, at a level that can be manipulated. Alternatively, one can decrease the initial velocities, and since the convective term is homogeneous of order two in velocity and the viscous term is homogeneous of one, this will increase the viscous decay relative to the cascade.

In the case of the modified term, however, the nonlinear transfer of energy to high wavenumbers from low ones is also due to the same term which dissipates the energy. So increasing viscosity also increases the cascade of energy and will not sufficiently slow the growth of vorticity at high wavenumbers. Again, since this second nonlinear transfer of energy is homogeneous of order one, decreasing velocities will not reduce it compared to the dissipation either.

Now let us look at the more novel quantities measured in this simulation. The best known is the distribution of cosine theta. Graphs comparing the distribution of cosine theta at the same time for the two equations are given in the appendix. It has been proposed that the growth of the horns of cosine theta is due somehow to fluctuations in time of helicity. This idea is not supported by the results of the simulation. In fact, the modified equation formed horns noticeably faster than the regular Navier-Stokes event though it has almost constant helicity, even with the computational errors. The greater speed of growth of the horns is probably due to the more rapid growth of enstrophy for the modified equation.

It is surprising that at the ends of the simulations the horns of cosine theta have grown remarkably for the modified equation, even though by this time the results of the simulation are doubtful. The reason for this could be that the simulation of the modified equation is still mainly valid, even with truncation and aliasing errors (an optimisitic thought). Another explanation could be that aliasing errors cause growth of horns of cosine theta.

The low wavenumber parts of some spectra for H(k) are also given in the appendix for a few different times. The theory of the inverse cascade would suggest that the lower modes of these spectra should grow in time. This effect should occur for modes of lower magnitude than the maximum of energy (Levich et al. 1987) Since in this simulation the maximum of energy was at two or two and a half, H(k) would be expected to grow only for the modes with magnitudes between two and one. This was observed in all runs for both the usual Navier-Stokes and for the modified equation starting sometime after the peak of enstrophy and last until nearly the end of the simulation. For the larger modes there is no growth in time, but rather a decay.

This result is significant because, at the times discussed, the velocity and vorticity are both decreasing, in general, and in the bottom part of the spectrum. One would expect as a result that the the quantity H(k) would also decrease. The reason that it is expected not to decrease is the inverse cascade, which is discussed briefly in the literature review and more fully in references given therein. Another reference, not yet in publication, but accepted for publication, will be discussed briefly here.

The publication is "Helicity Fluctuations and Coherence in Developed Turbulence" by E. Levich and L. Shtilman, accepted for publication in the book "Scaling Fractals and non-Linear Variability Geophysics" to be published by Reidel. There it is pointed out that it is expected that H(k) will grow for low magnitudes of k. The quantity alpha, the sum of the squares of H(k), should perhaps grow for these low wavenumbers, but not necessarily for the high ones. It would be expected that the sum over k of $H^2(k)/k^2$ will not decay, even if alpha does. In the results of the simulations we see that in all cases alpha decays with time. However the magnitude of the H(k) spectrum for the modes between one and two grows for the time after the peak of enstrophy until the end of the simulations in all cases.

Thus the theory of inverse cascade is not contradicted by the results of the simulations. This same result has been reached in the results of a simulation with greater resolution, 128^3, which is also reported in the above mentioned reference, and one graph from that simulation is also presented in the appendix.

In summary then, the simulations show no remarkable difference between the two equations in terms of helicity related quantities. This implies that the topological constraints introduced by the use of Clebsch variables and the conservation of helicity are not very important in the aspects of the flow measured in these simulations. Of course many qualifications must be added about the lowness of the Reynolds number, the possibility of aliasing errors and truncation errors. The inverse cascade conclusions were not really the subject this work, but are cited to show that whatever may be occurring seems not to be due to the source term in the helicity balance equation.

CHAPTER IX

CONCLUSIONS

The comparison of the simulation results for the two different equations suggests that some properties of the viscosity term are important to the development of turbulence, and that some are much less so. Reviewing the properties of the viscosity term discussed in this work the results are:

1)Evolution in time of total helicity - not crucial for the development of turbulence, even with respect to helicity related quantities such as H(k) and probability of cosine theta.

2)Preservation of Clebsch representability - also not crucial to the development of turbulence, even with respect to helicity related quantities.

3)Linearity of the viscous term - important for the development of the turbulent flow field, especially in the case where the alternate term is very nonlinear in the sense that it causes a strong cascade of energy between wavenumbers.

Of course no one can say what the complete significance of these conclusions are, especially since there is at present no successful theory of turbulence, but a number of implications in terms of the present directions of research can be drawn.

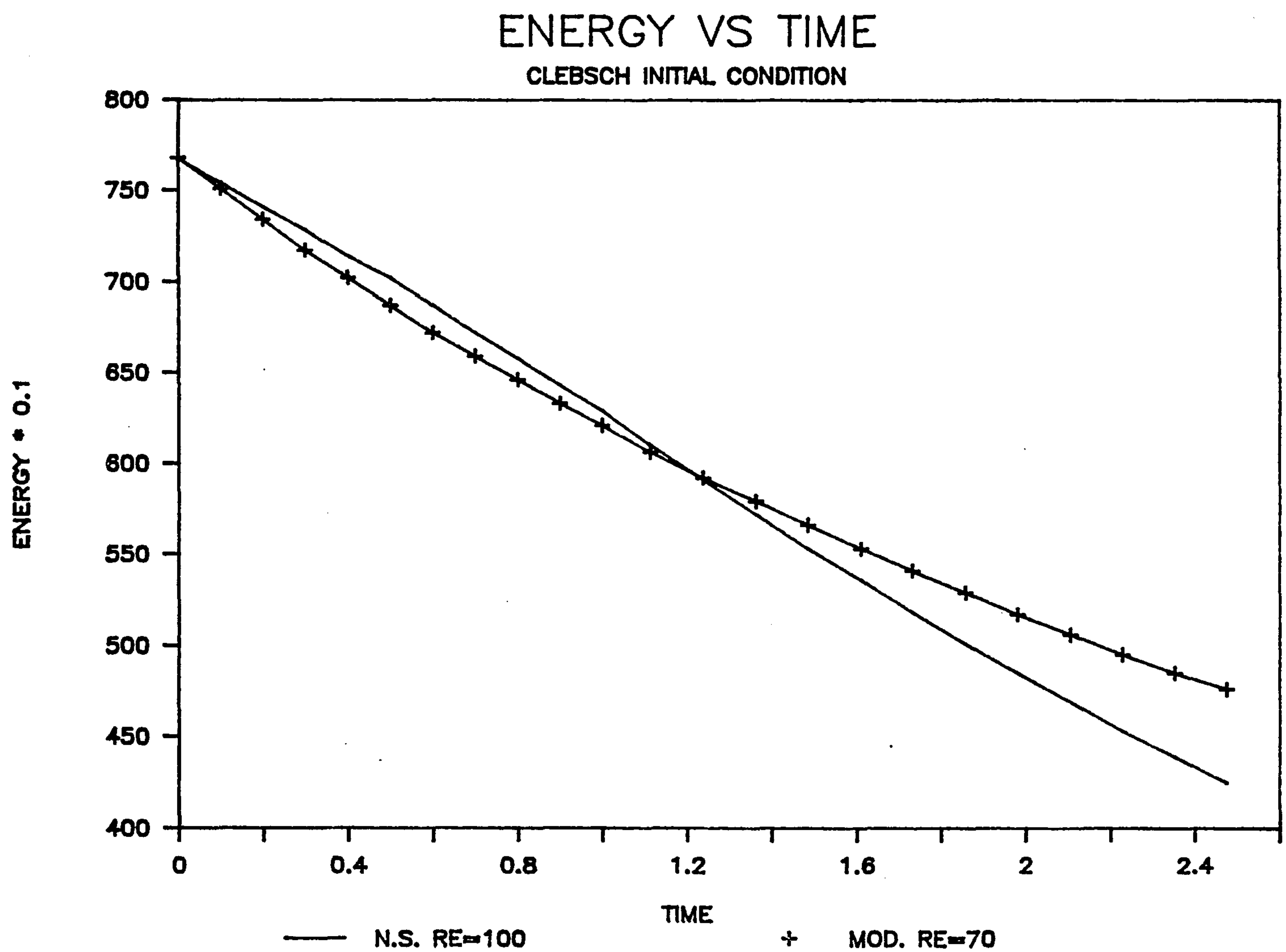
1)In analytical work - the significance of the total helicity of the entire flow field should not be accounted of great importance for the development of small scale turbulence, instead other helicity related quantities could be considered. Among these are: the helicity of subvolumes of particular interest, H(**k**), distribution of cosine theta.

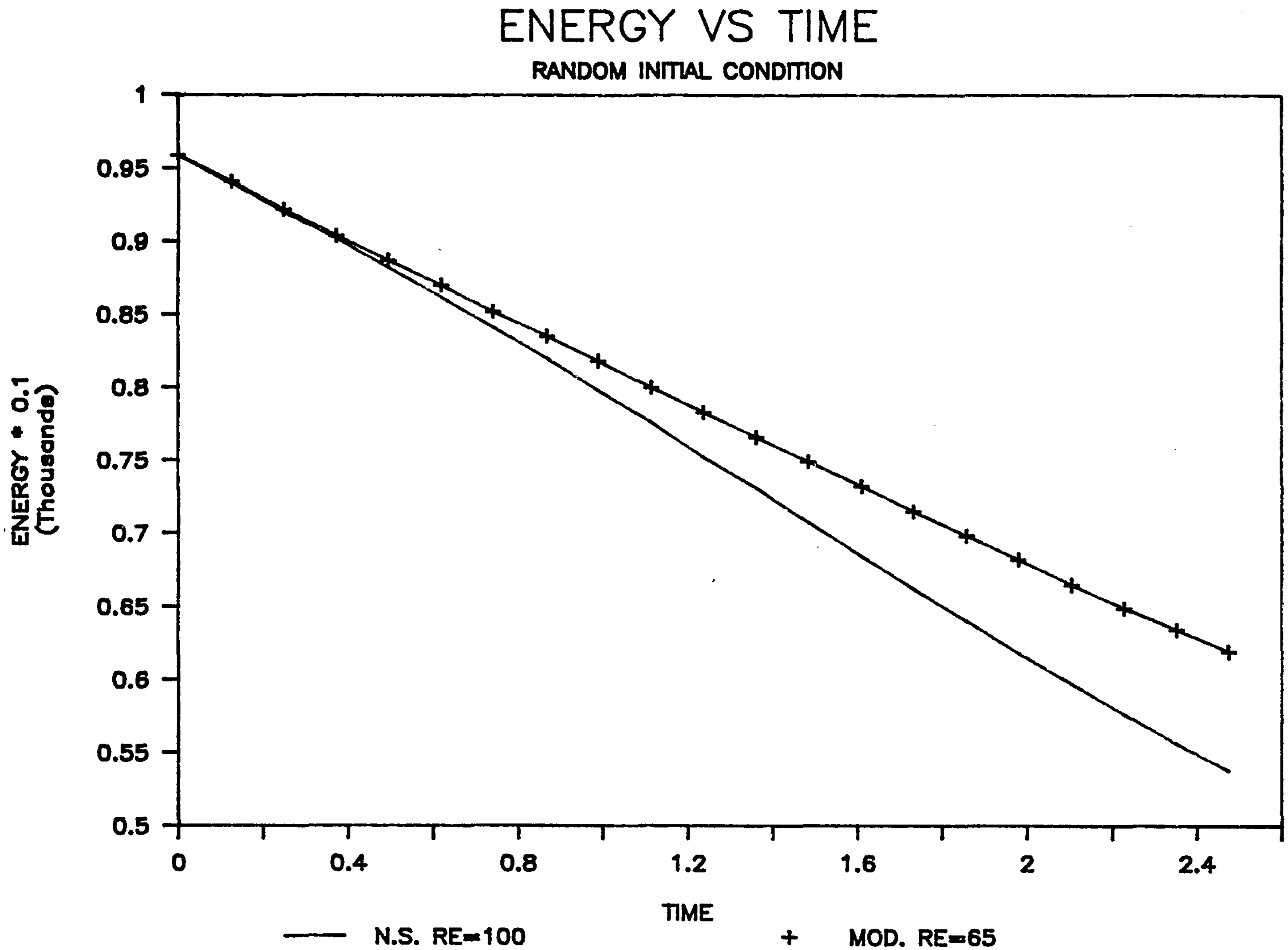
2)In computational work - substitution of the viscosity term with others which are easier to calculate is encouraged by the simulation results, especially if the substituted term is linear or nearly so. This has already been done in some cases. For instance in large eddy simulation, instead of the usual viscosity term with constant viscosity, a term with the same differential form is substituted, but with a non-constant, position dependent viscosity. In cited works by Grossmann simulation results are reported from simulations with an (unintentionally) modified viscosity term which are more accurate than other simulations using comparable computer resources but with the usual (and more difficult to simulate) viscosity term.

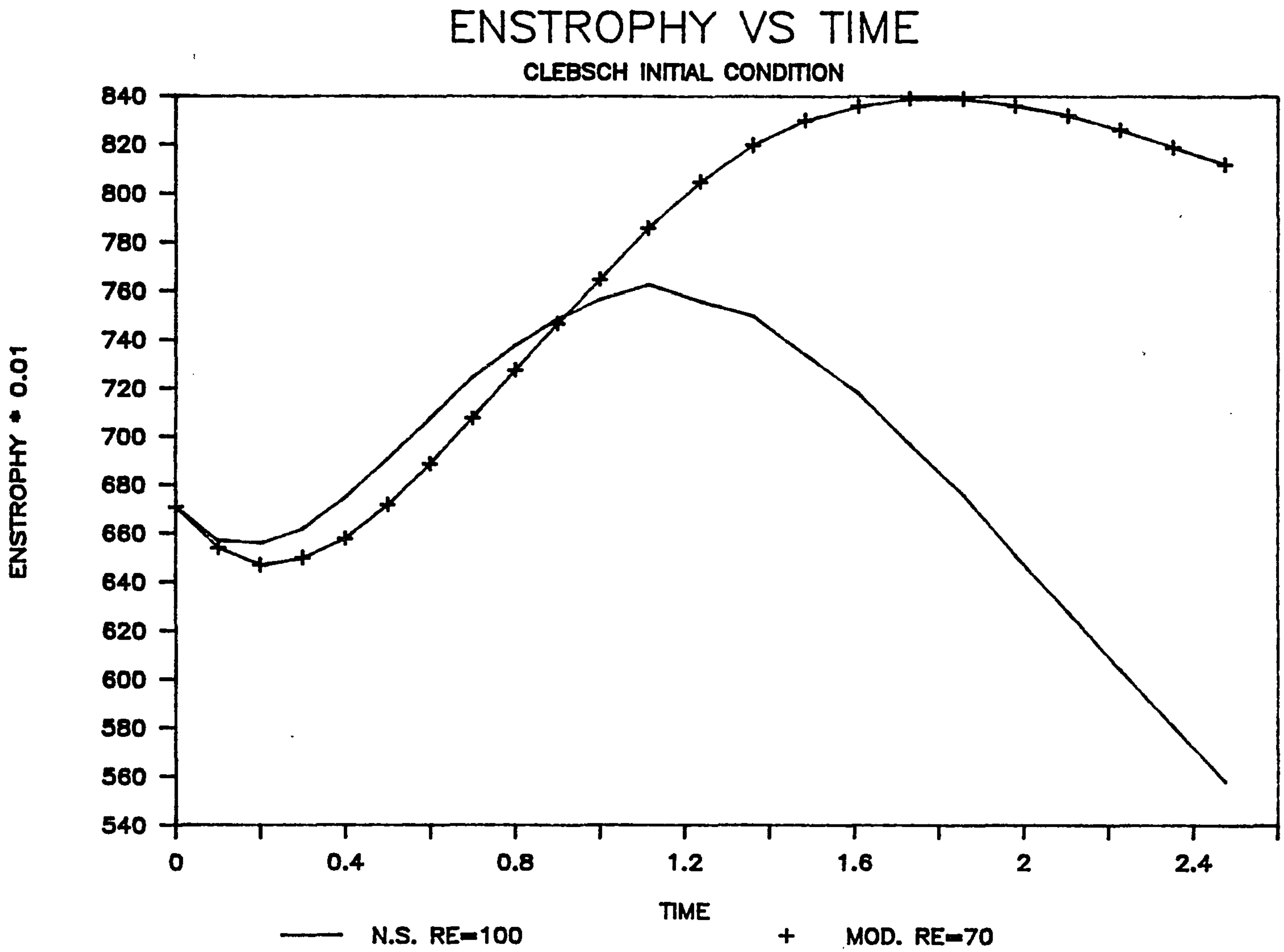
3)Experimental - turbulence in non-Newtonian flows may be more similar to turbulence in Newtonian flows than might have been expected. Groups of Non-newtonian flows should be studied to see what non-Newtonian properties change the character of turbulence.

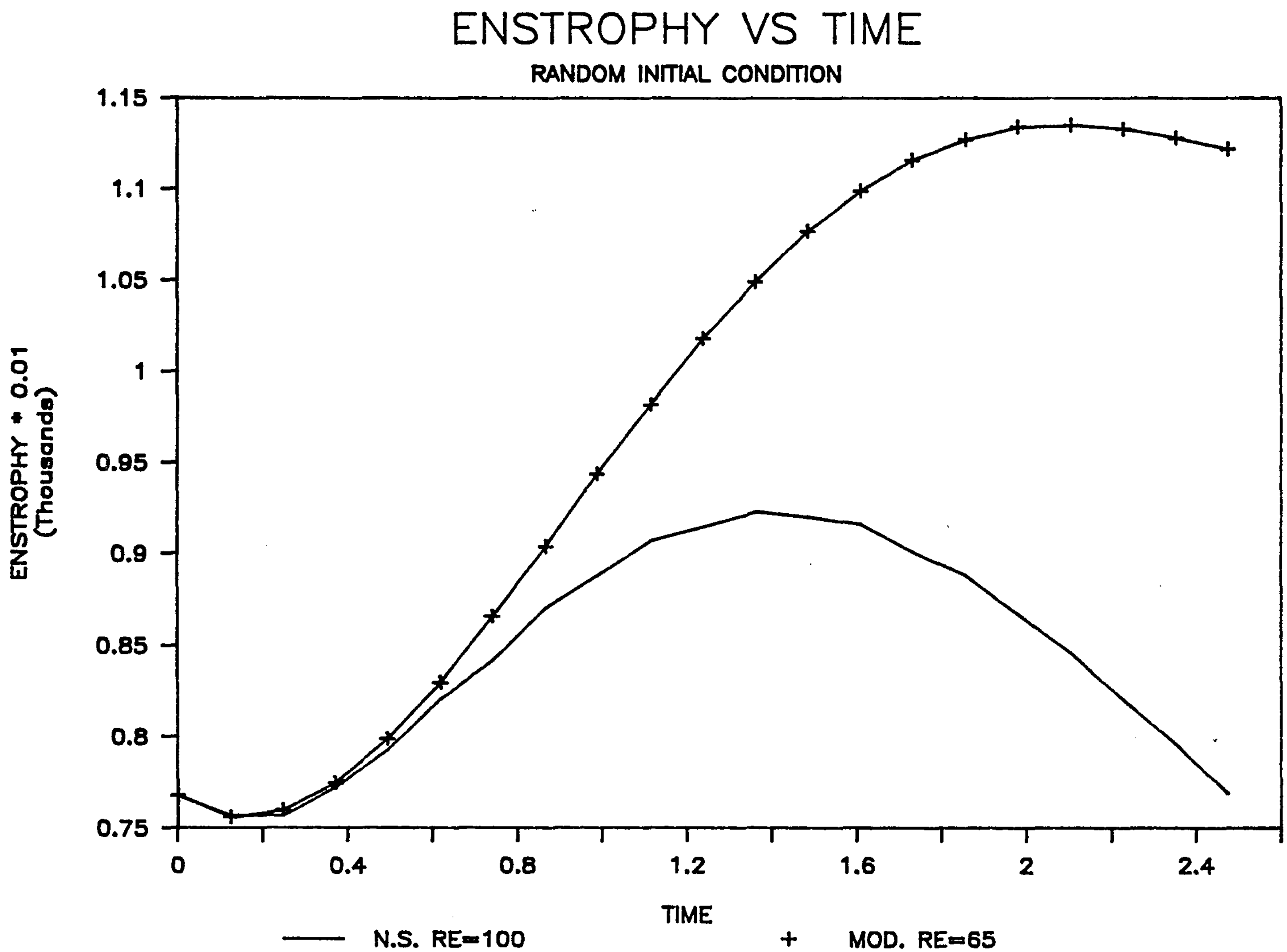
4)Computer aided modelling of turbulent non-Newtonian flows - Existing programs that model turbulent Newtonian flows could be tried with no modifications. If the results of this are unsatisfactory, easy modifications can be tried such as position dependent viscosity or frequency dependent viscosity.

GRAPHS


ENERGY VS TIME
CLEBSCH INITIAL CONDITION
ENERGY * 0.1
800
750
700
650
600
550
500
450
400
0
0.4
0.8
1.2
1.6
2
2.4
TIME
N.S. RE=100
MOD. RE=70

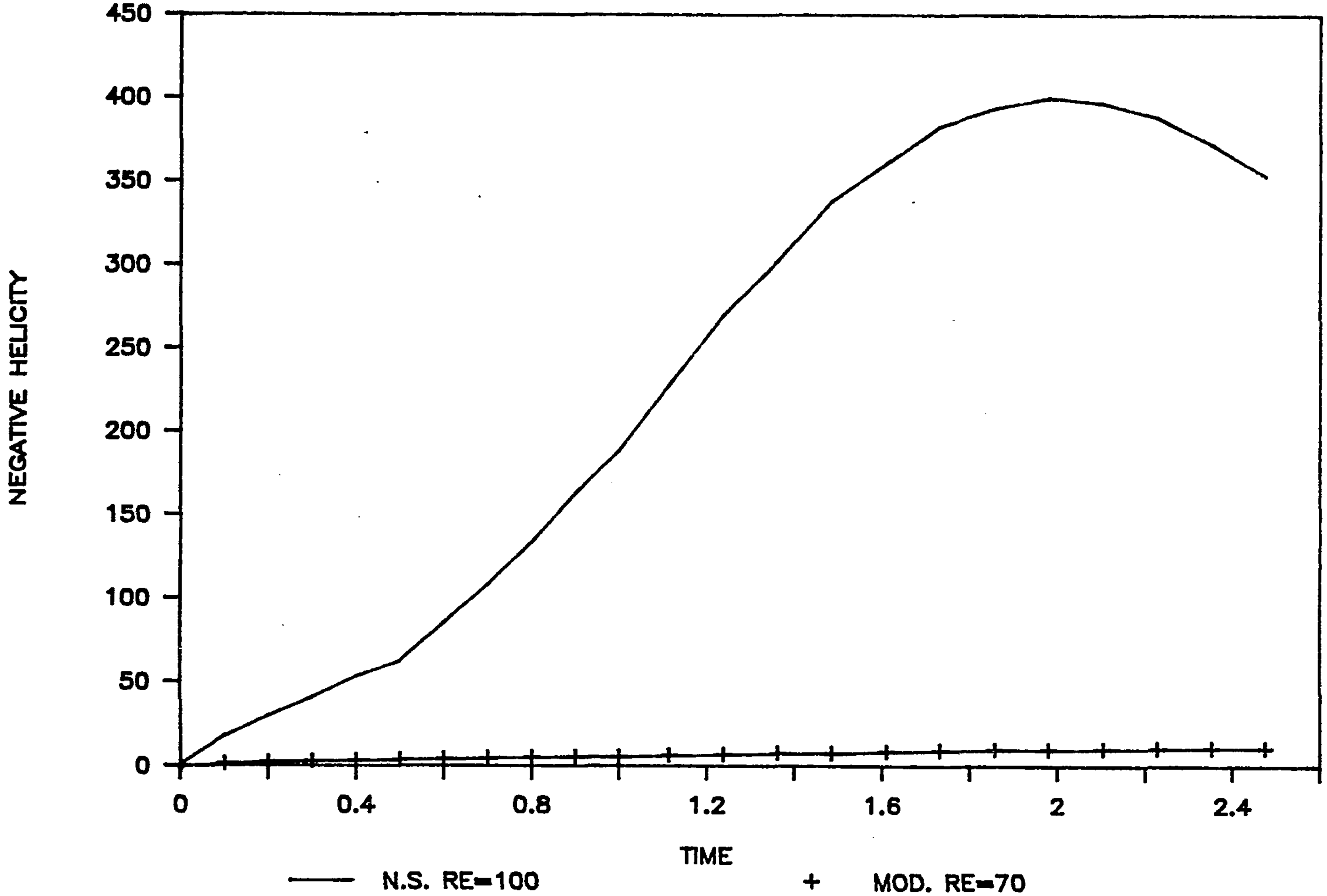

ENERGY VS TIME
RANDOM INITIAL CONDITION
ENERGY * 0.1
(Thousands)
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0
0.4
0.8
1.2
1.6
2
2.4
TIME
N.S. RE=100
+ MOD. RE=65

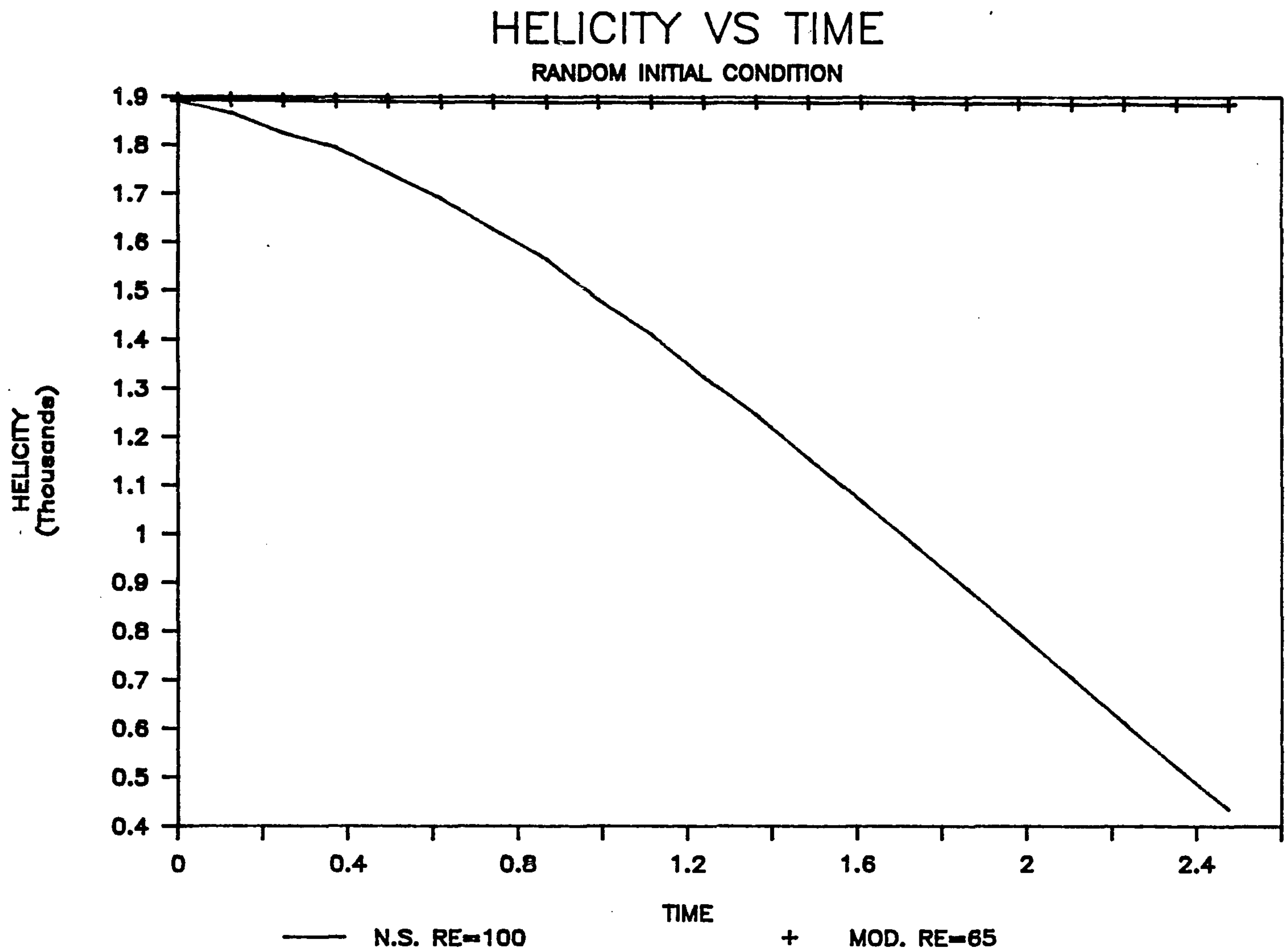

ENSTROPHY VS TIME
CLEBSCH INITIAL CONDITION
ENSTROPHY * 0.01
840
820
800
780
760
740
720
700
680
660
640
620
600
580
560
540
0
0.4
0.8
1.2
1.6
2
2.4
TIME
N.S. RE=100
MOD. RE=70


ENSTROPHY VS TIME
RANDOM INITIAL CONDITION
ENSTROPHY * 0.01
(Thousands)
1.15
1.1
1.05
1
0.95
0.9
0.85
0.8
0.75
0
0.4
0.8
1.2
1.6
2
2.4
TIME
N.S. RE=100
MOD. RE=65

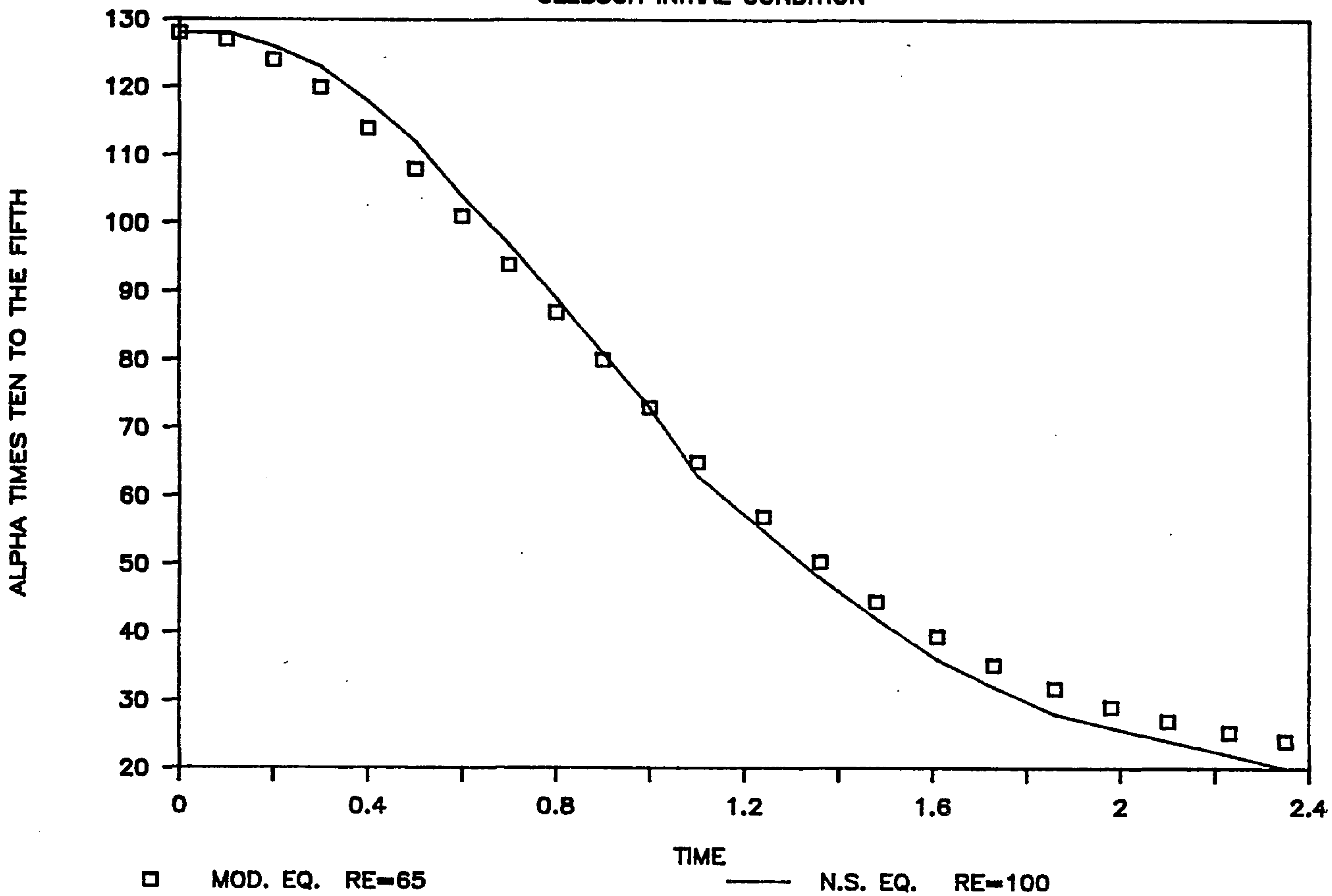
HELICITY VS TIME

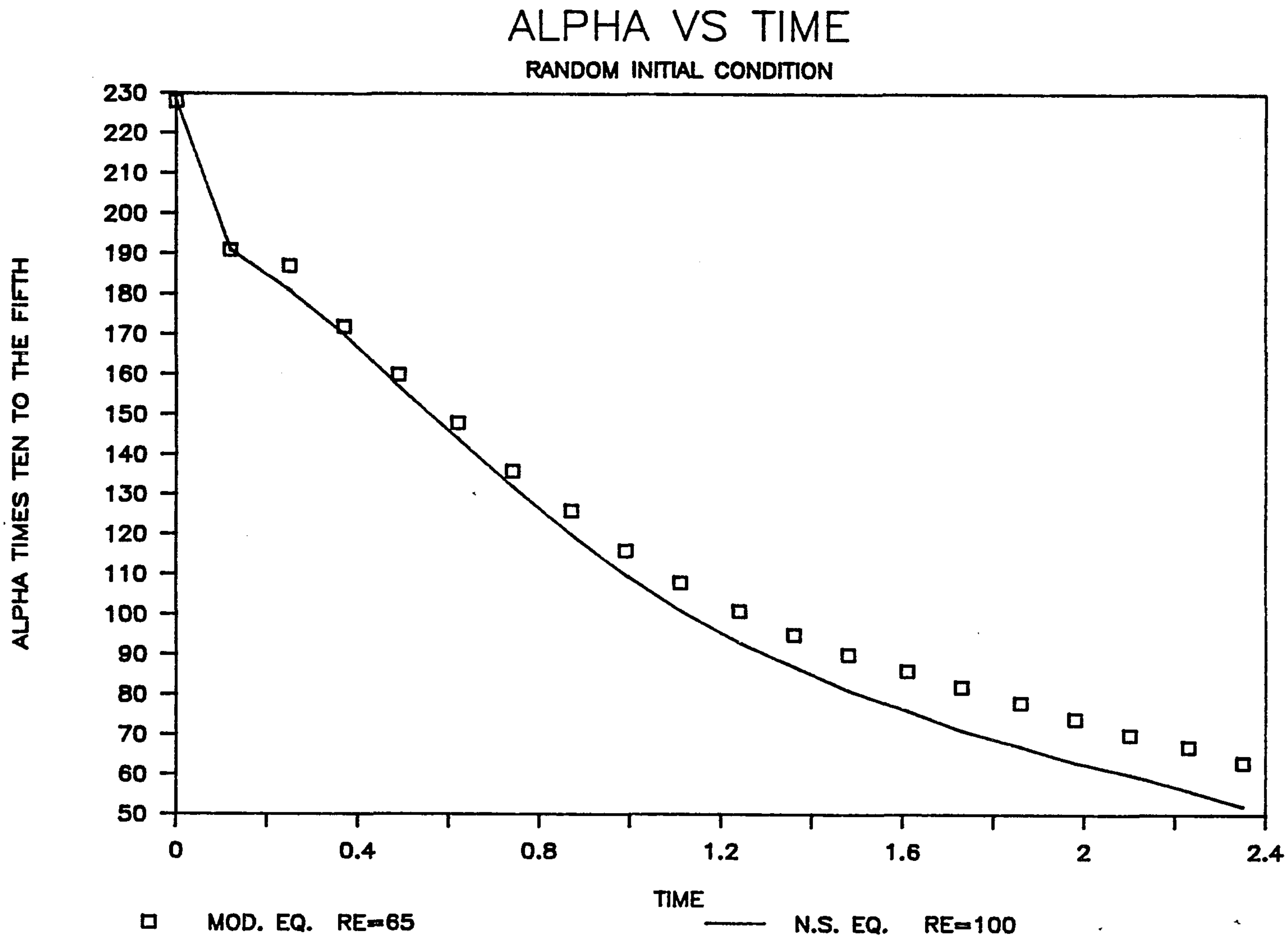
CLEBSCH INITIAL CONDITION




HELICITY VS TIME
RANDOM INITIAL CONDITION
HELICITY
(Thousands)
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0
0.4
0.8
1.2
1.6
2
2.4
TIME
N.S. RE=100
MOD. RE=65

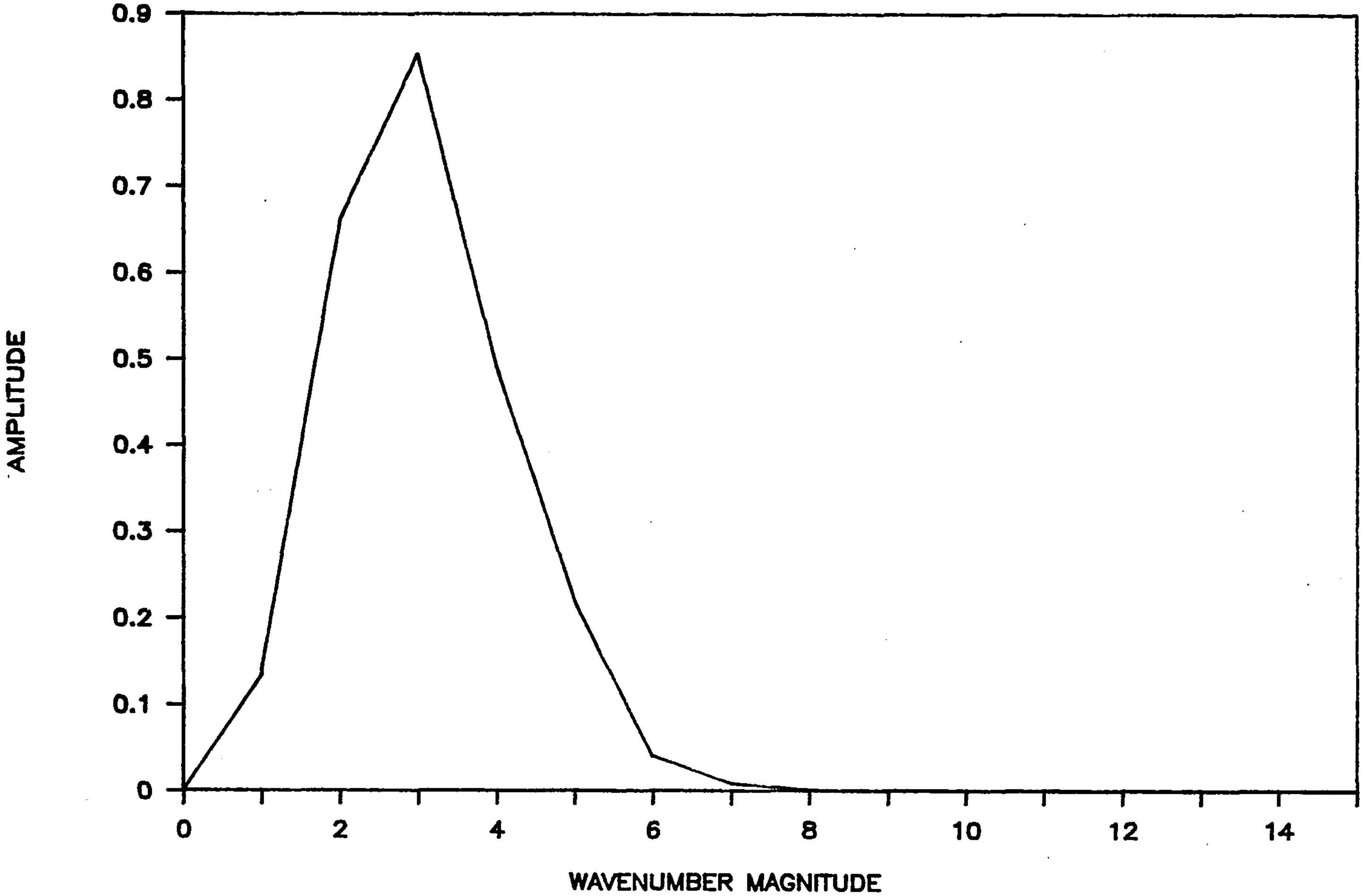
ALPHA VS TIME




ALPHA VS TIME
RANDOM INITIAL CONDITION
ALPHA TIMES TEN TO THE FIFTH
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
0
0.4
0.8
1.2
1.6
2
2.4
TIME
MOD. EQ. RE=65
N.S. EQ. RE=100

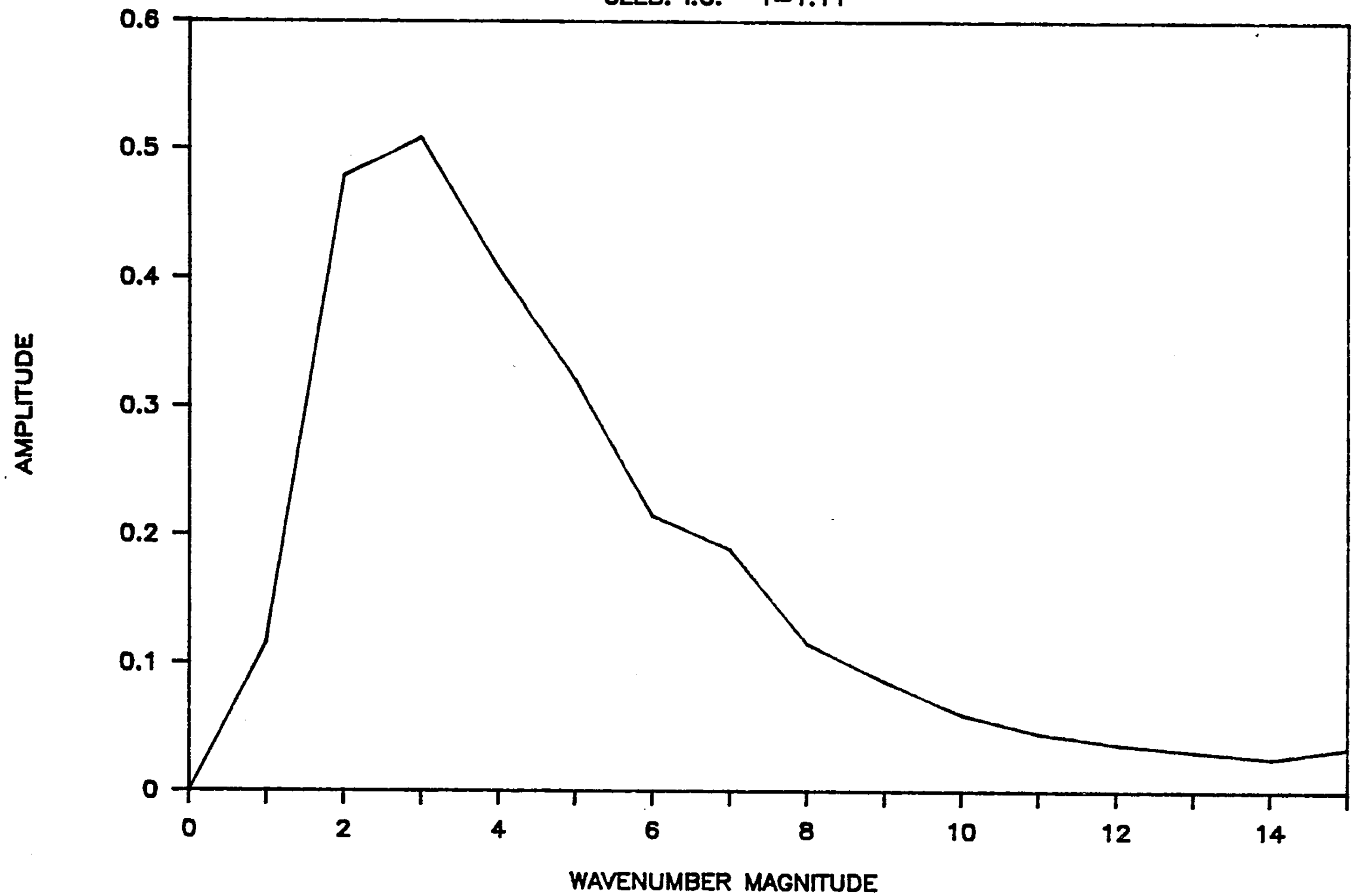
ENSTROPHY SPECTRUM

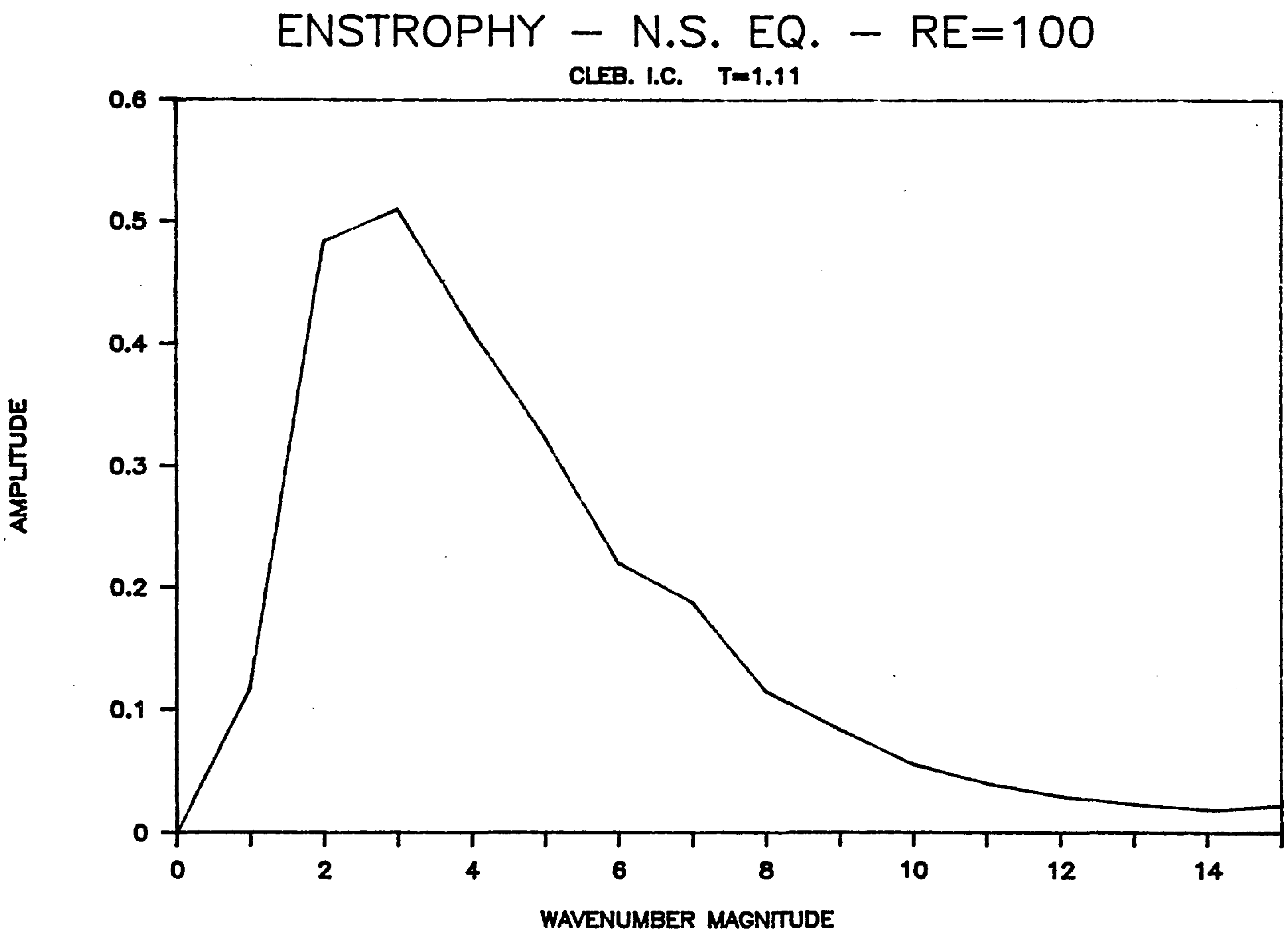
CLEBSCH I.C.

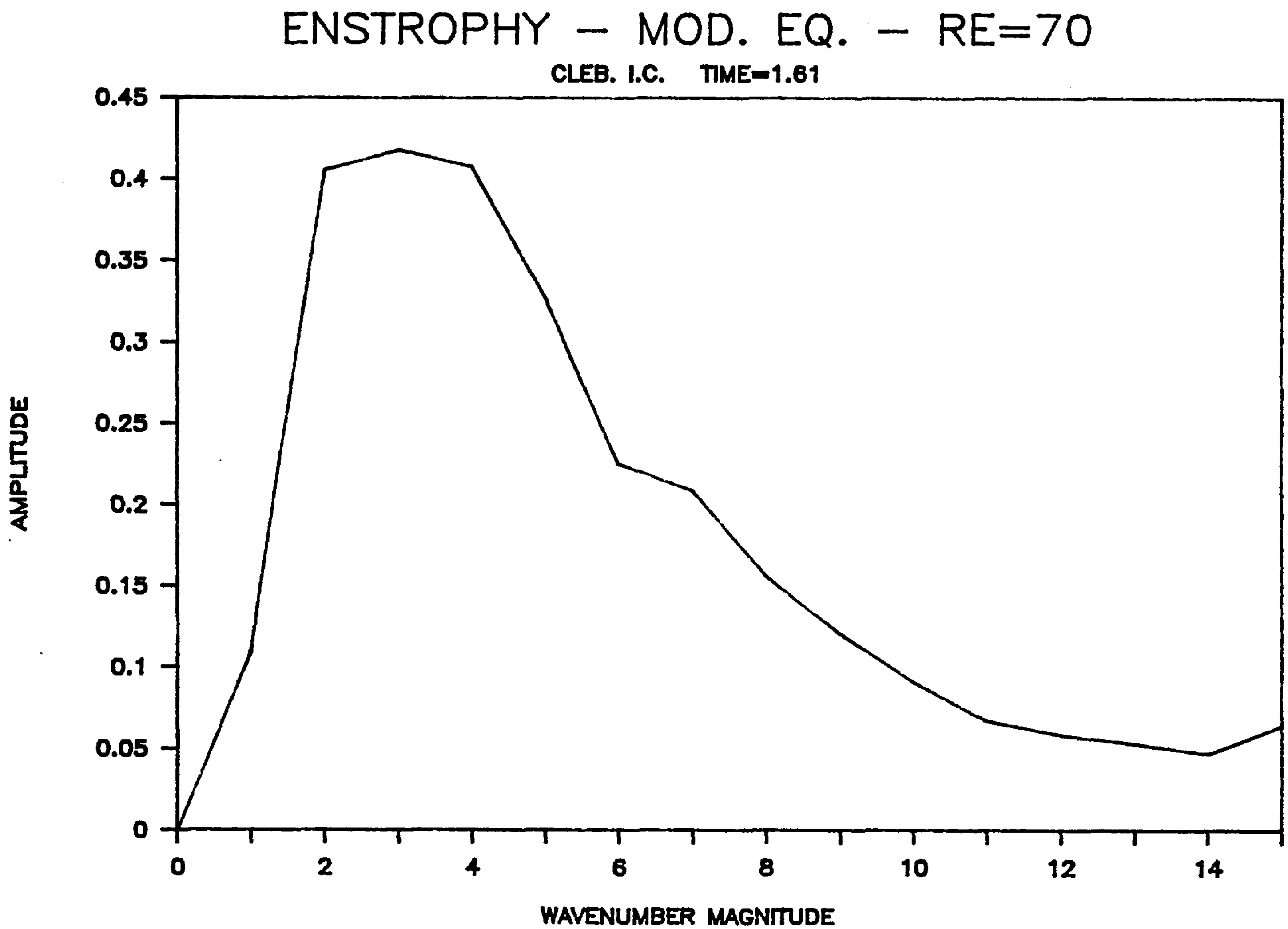


ENSTROPHY – MOD. EQ. – RE=70

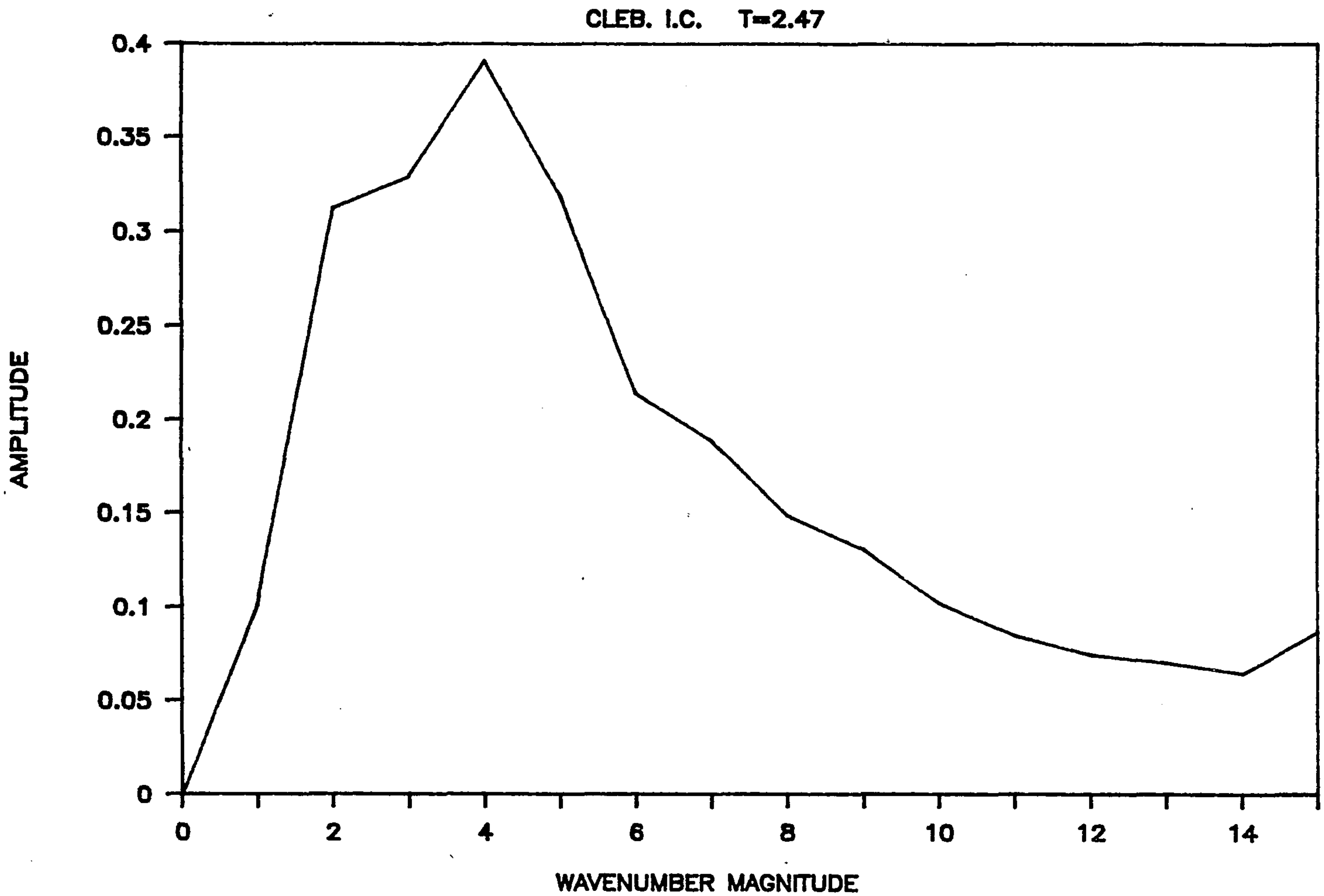
CLEB. I.C. T=1.11




ENSTROPHY – N.S. EQ. – RE=100
CLEB. I.C. T=1.11
AMPLITUDE
0
0.1
0.2
0.3
0.4
0.5
0.6
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

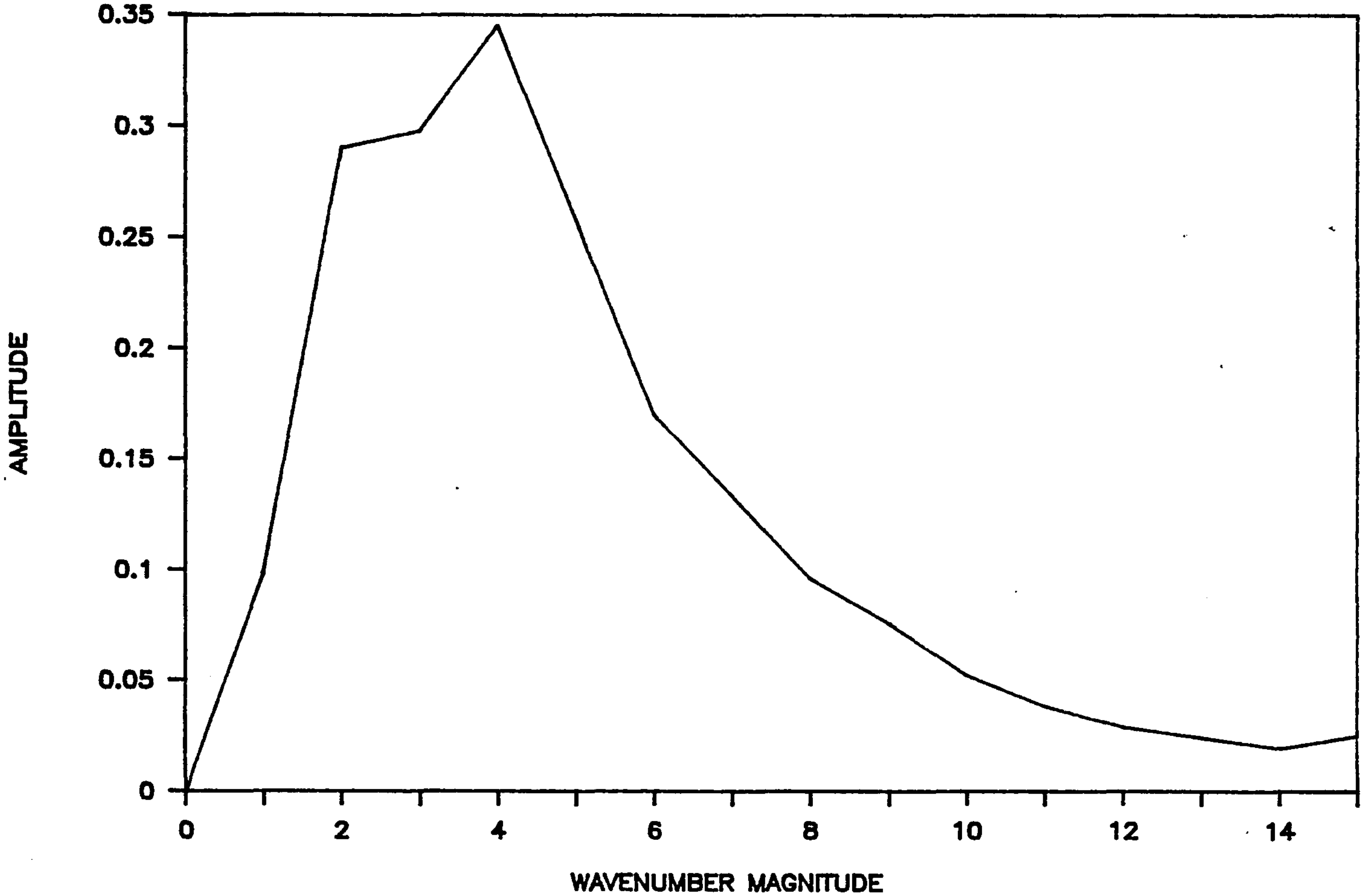

ENSTROPHY - MOD. EQ. - RE=70
CLEB. I.C. TIME=1.61
AMPLITUDE
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

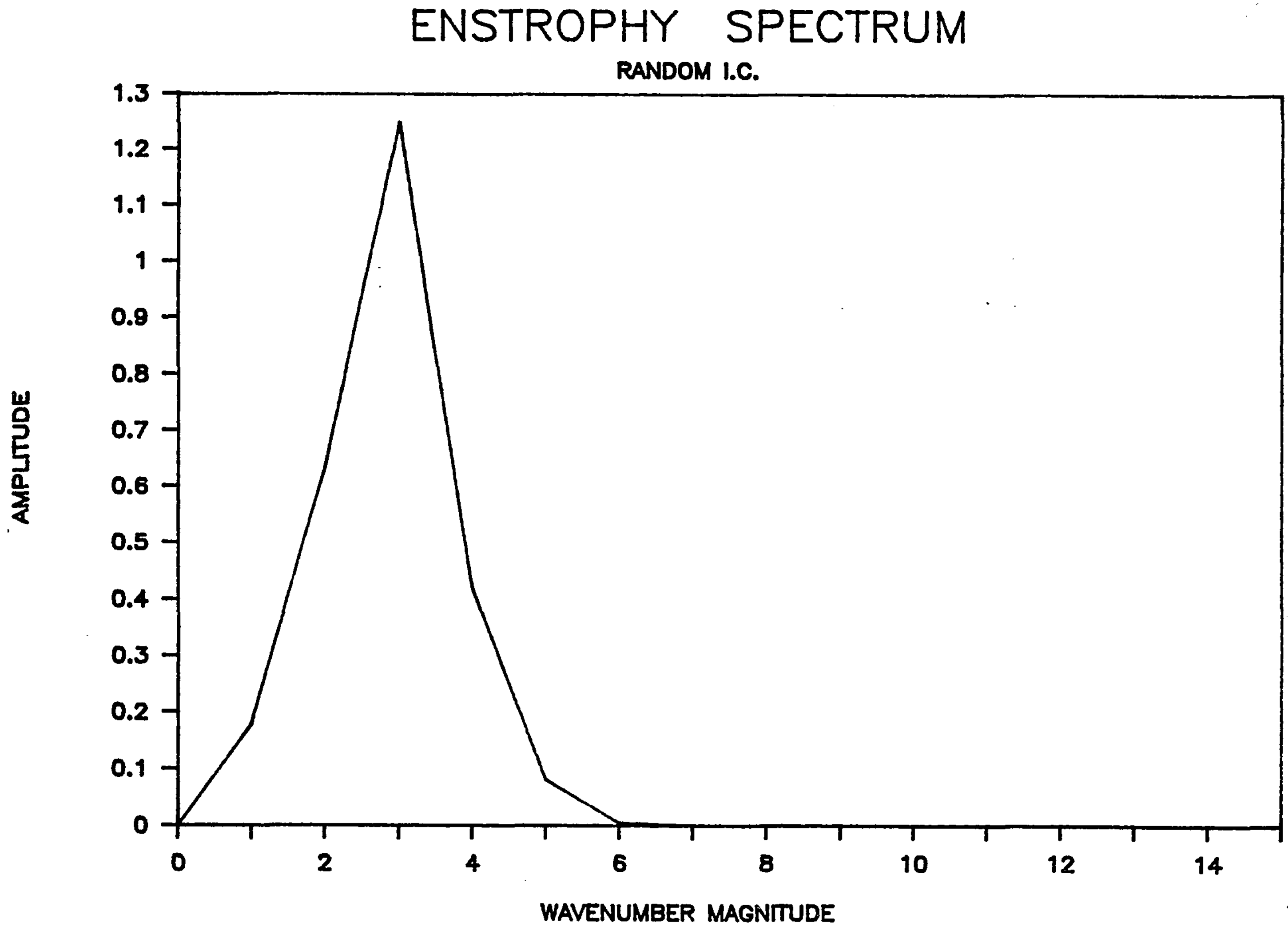
ENSTROPHY – MOD. EQ. – RE=70

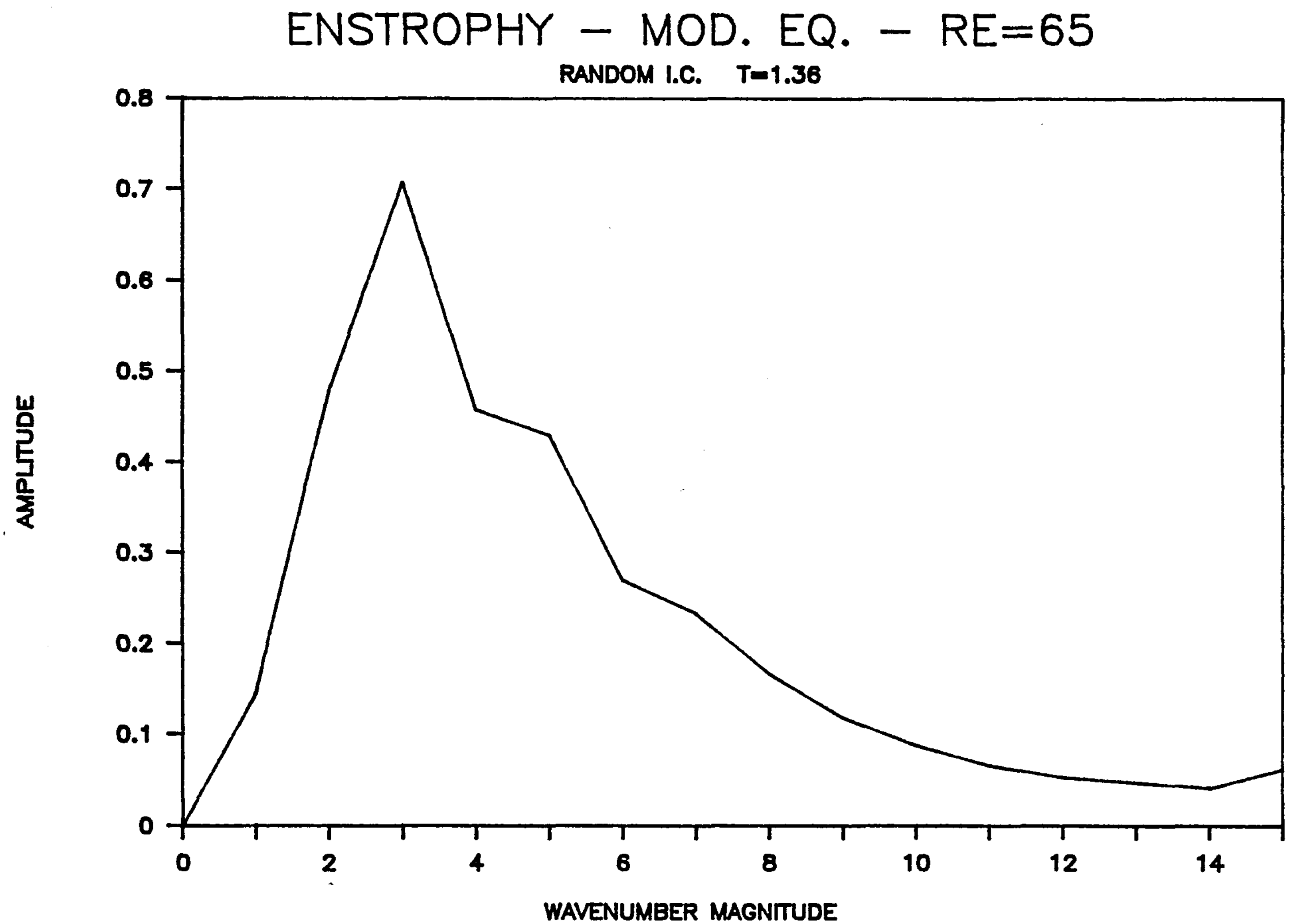


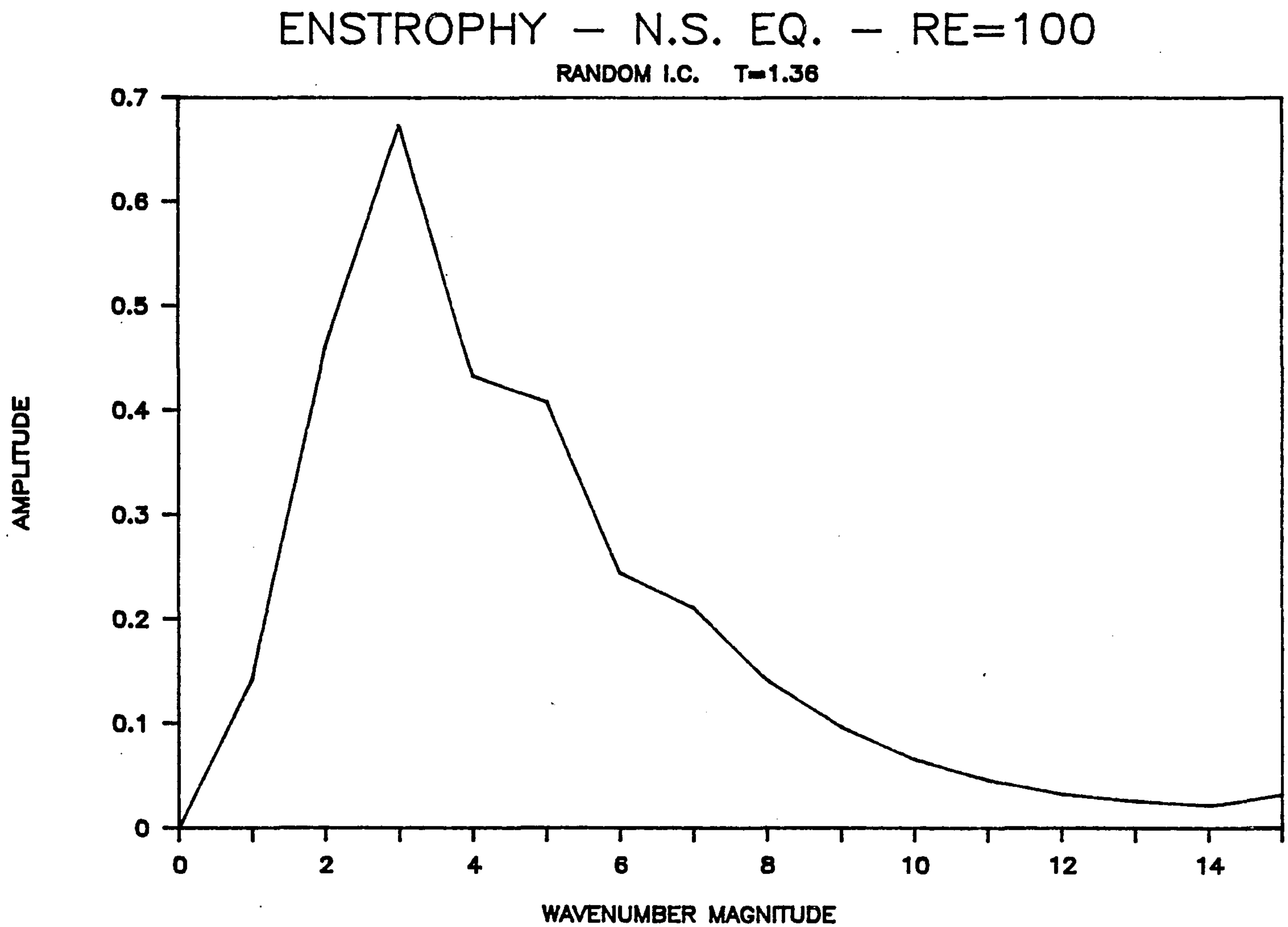
ENSTROPHY – N.S. EQ. – RE=100

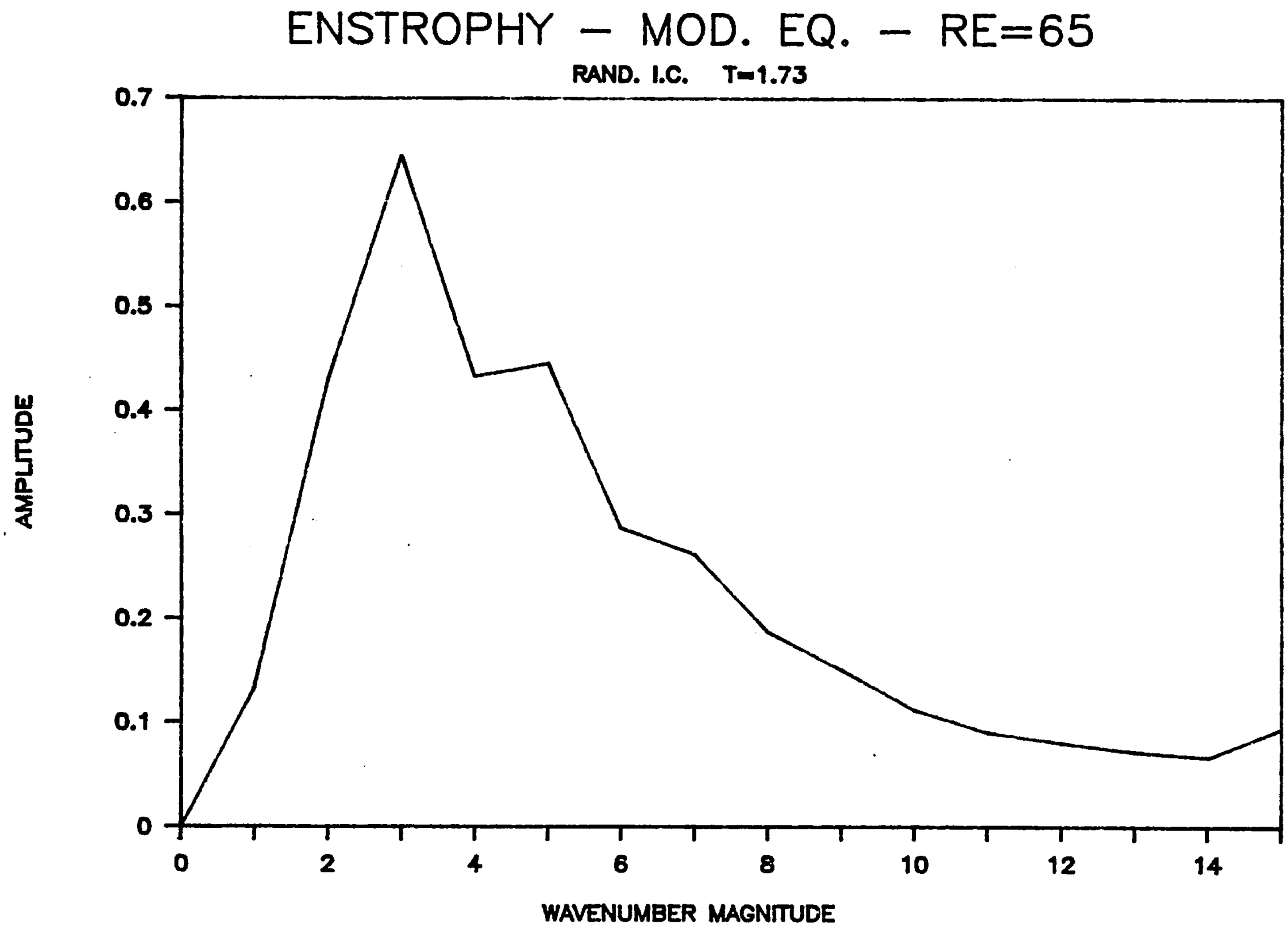
CLEB. I.C. T=2.47



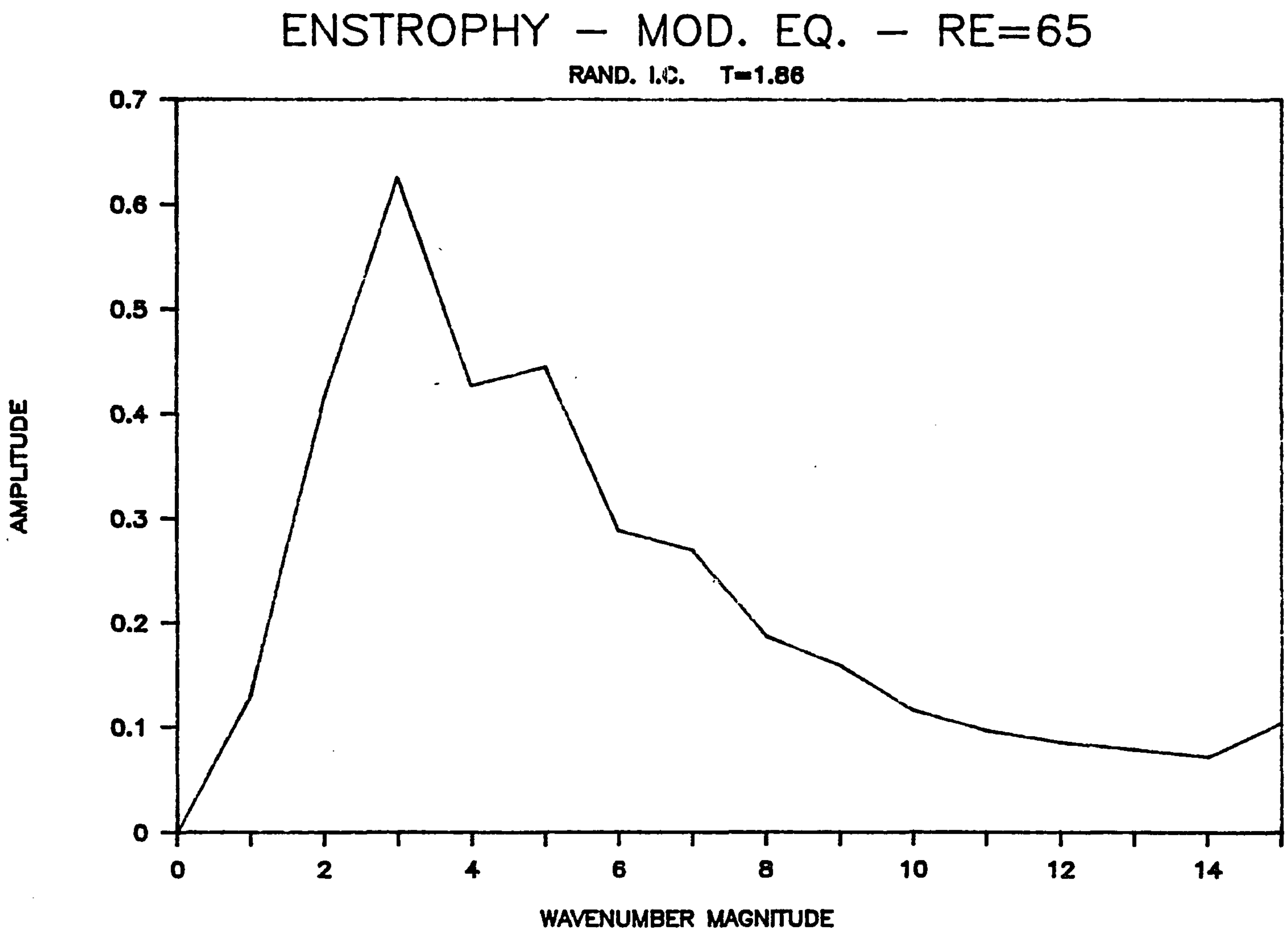

ENSTROPHY SPECTRUM
RANDOM I.C.
AMPLITUDE
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

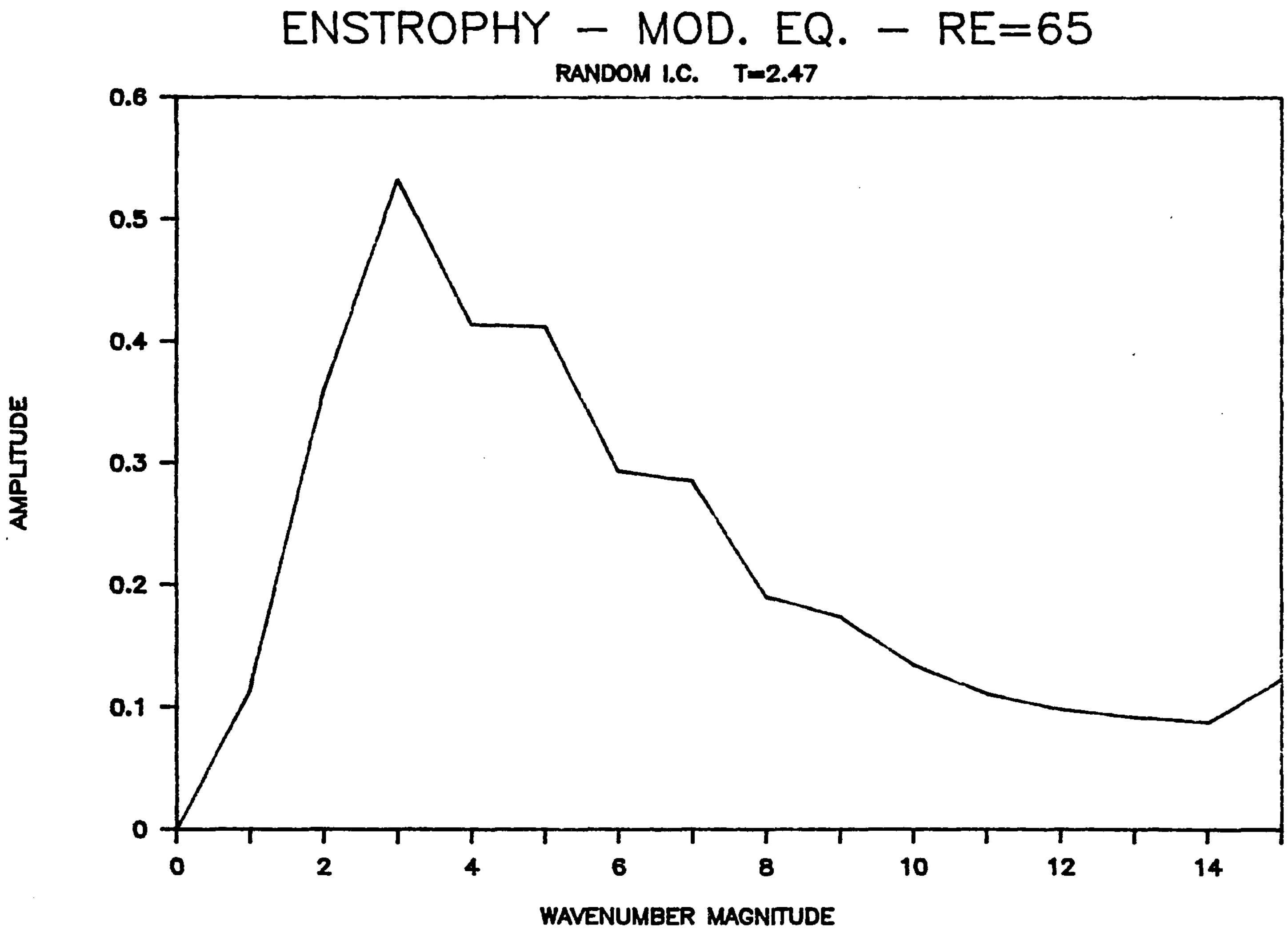

ENSTROPHY - MOD. EQ. - RE=65
RANDOM I.C. T=1.36
AMPLITUDE
WAVENUMBER MAGNITUDE
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
2
4
6
8
10
12
14

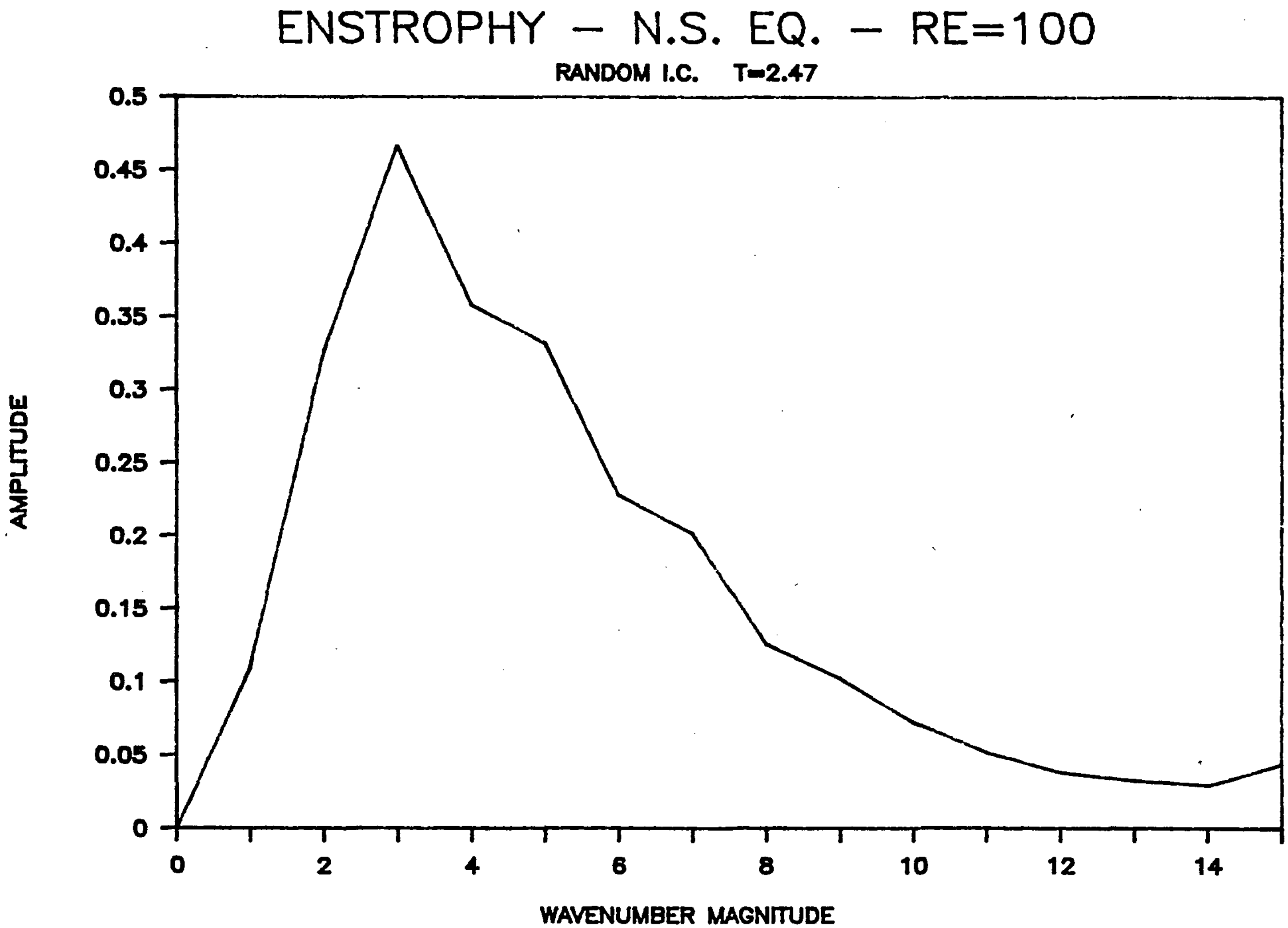

ENSTROPHY – N.S. EQ. – RE=100
RANDOM I.C. T=1.36
AMPLITUDE
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

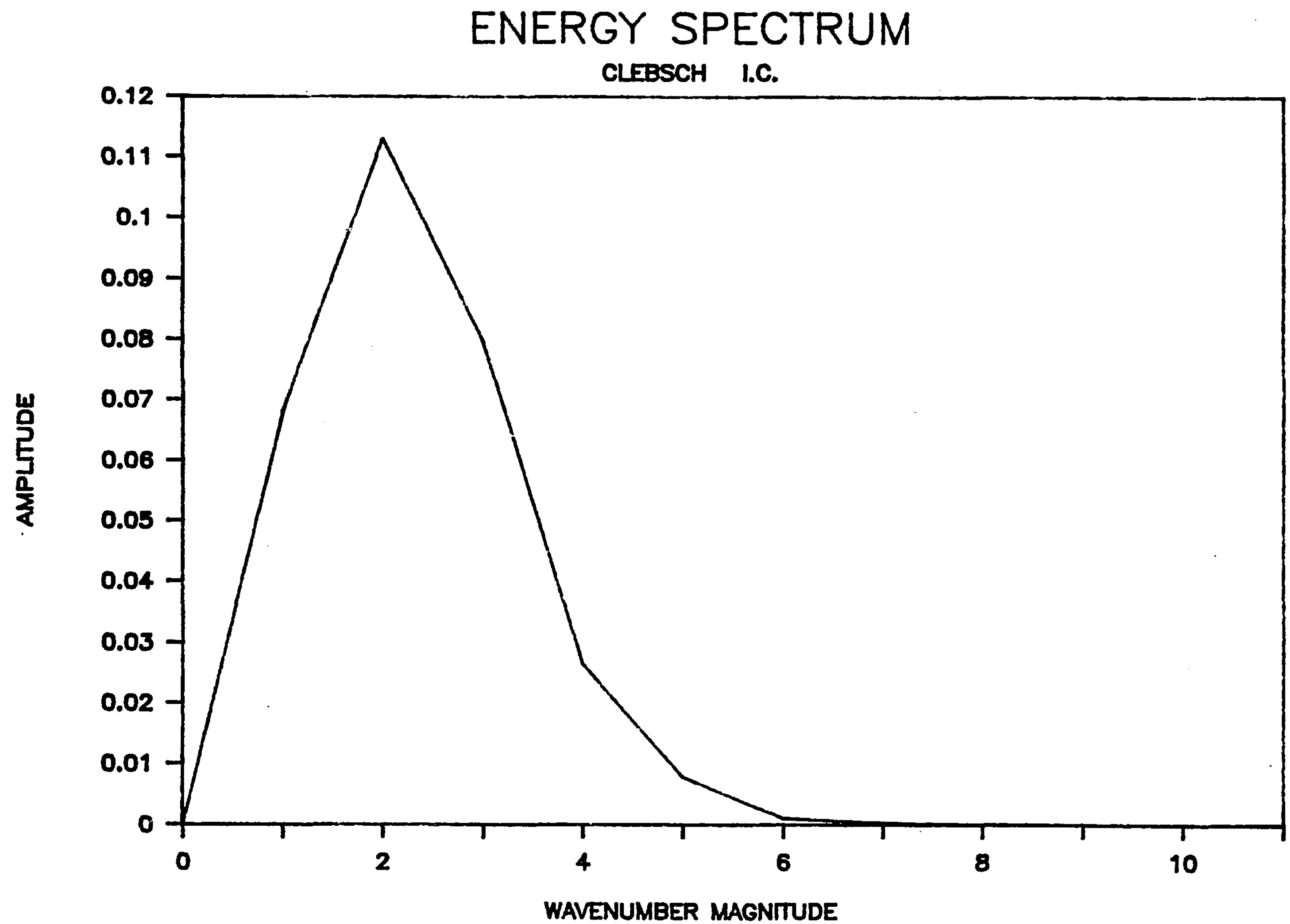


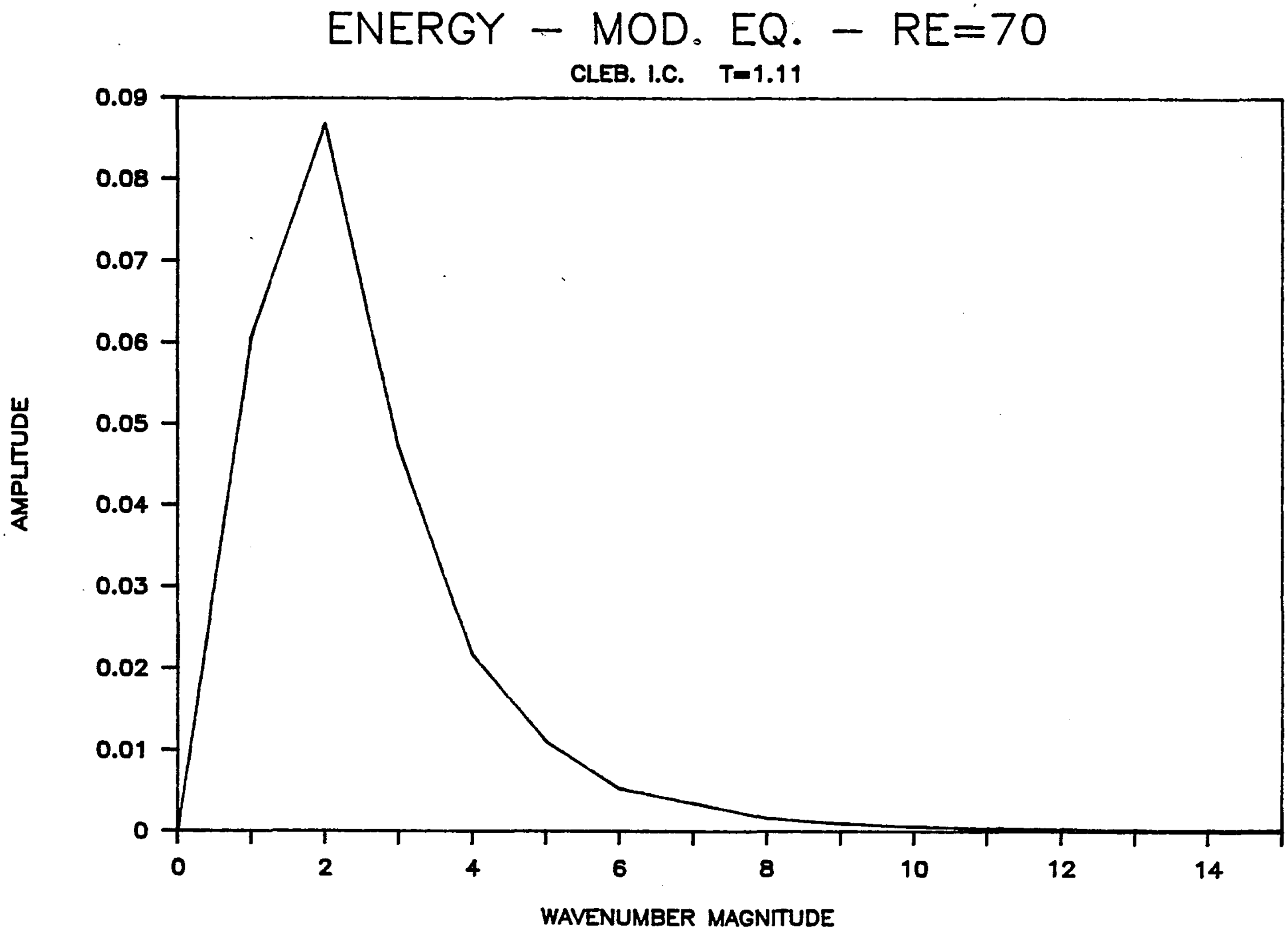
ENSTROPHY - MOD. EQ. - RE=65
RAND. I.C. T=1.73
AMPLITUDE
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

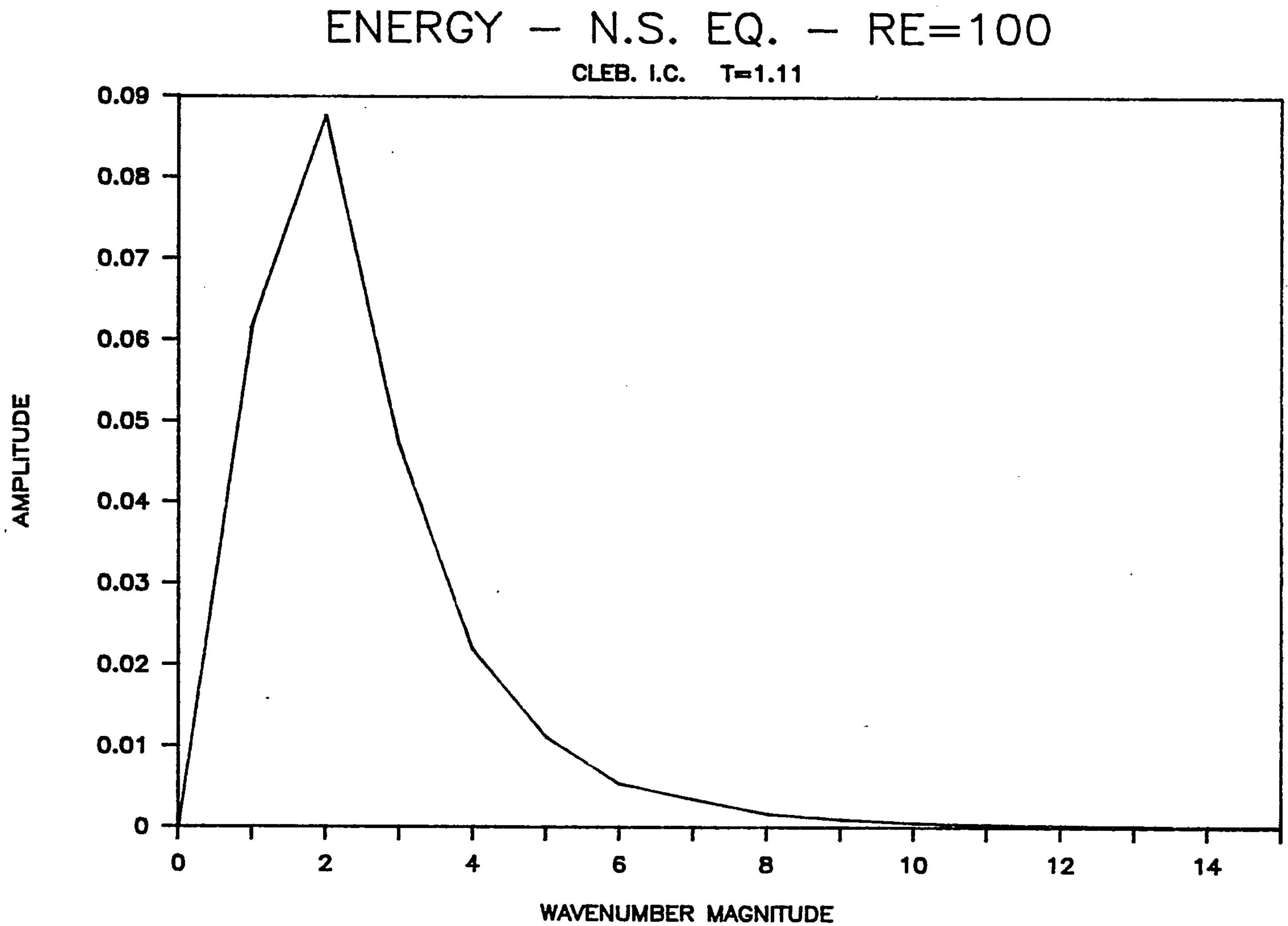

ENSTROPHY - MOD. EQ. - RE=65
RAND. I.C. T=1.86
AMPLITUDE
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

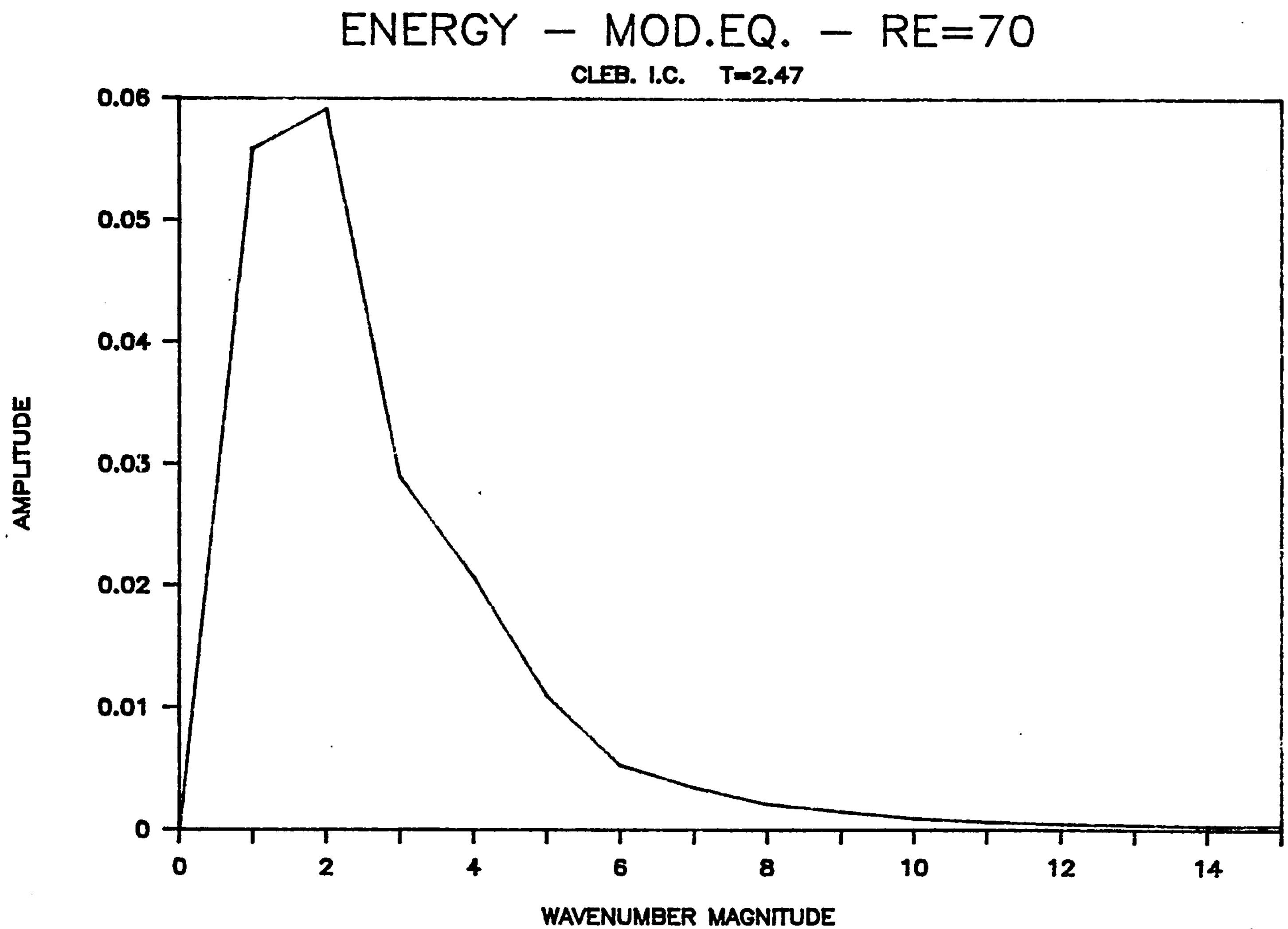

ENSTROPHY - MOD. EQ. - RE=65
RANDOM I.C. T=2.47
0.6
0.5
0.4
0.3
0.2
0.1
0
AMPLITUDE
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

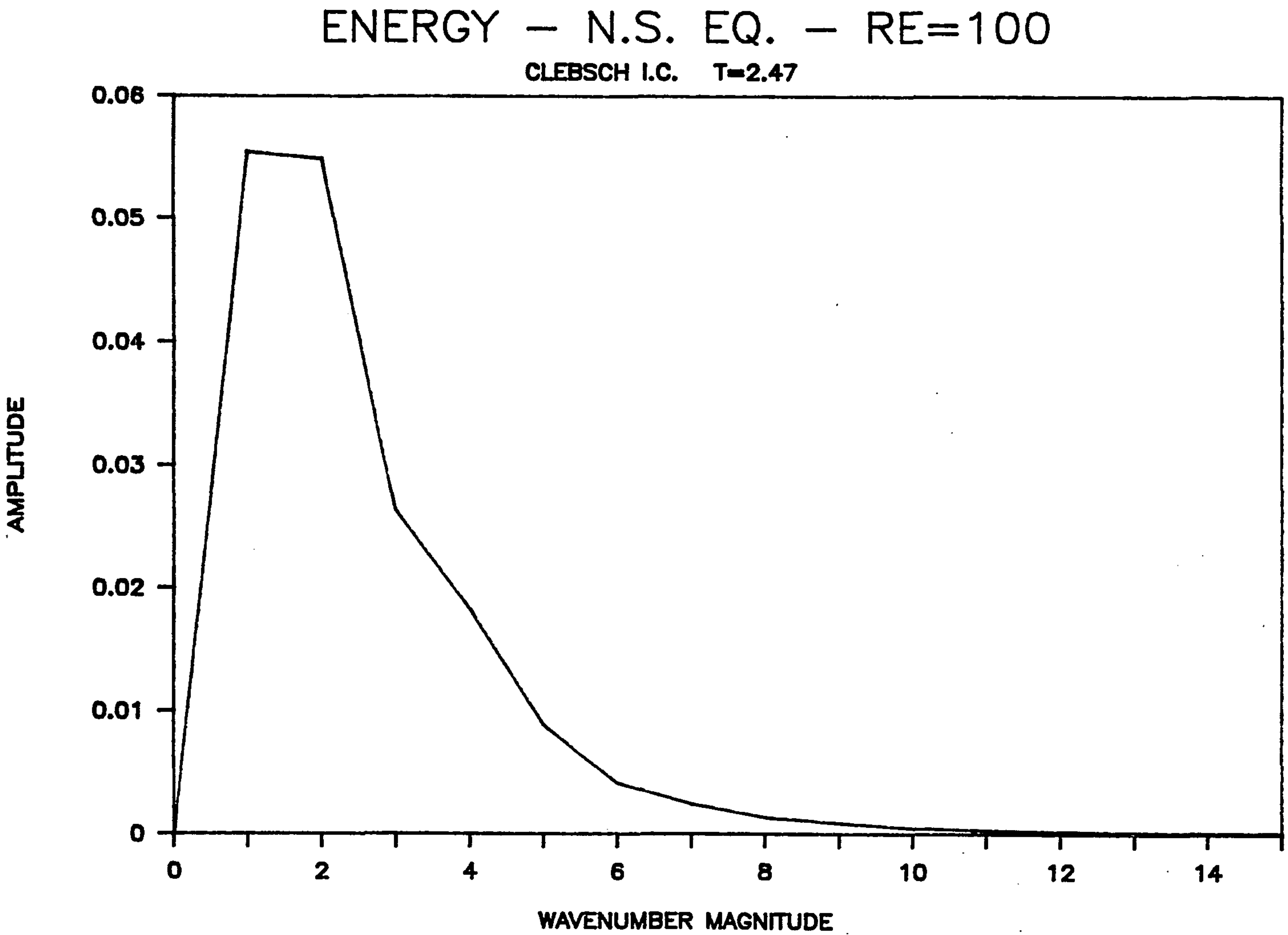

ENSTROPHY - N.S. EQ. - RE=100
RANDOM I.C. T=2.47
AMPLITUDE
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

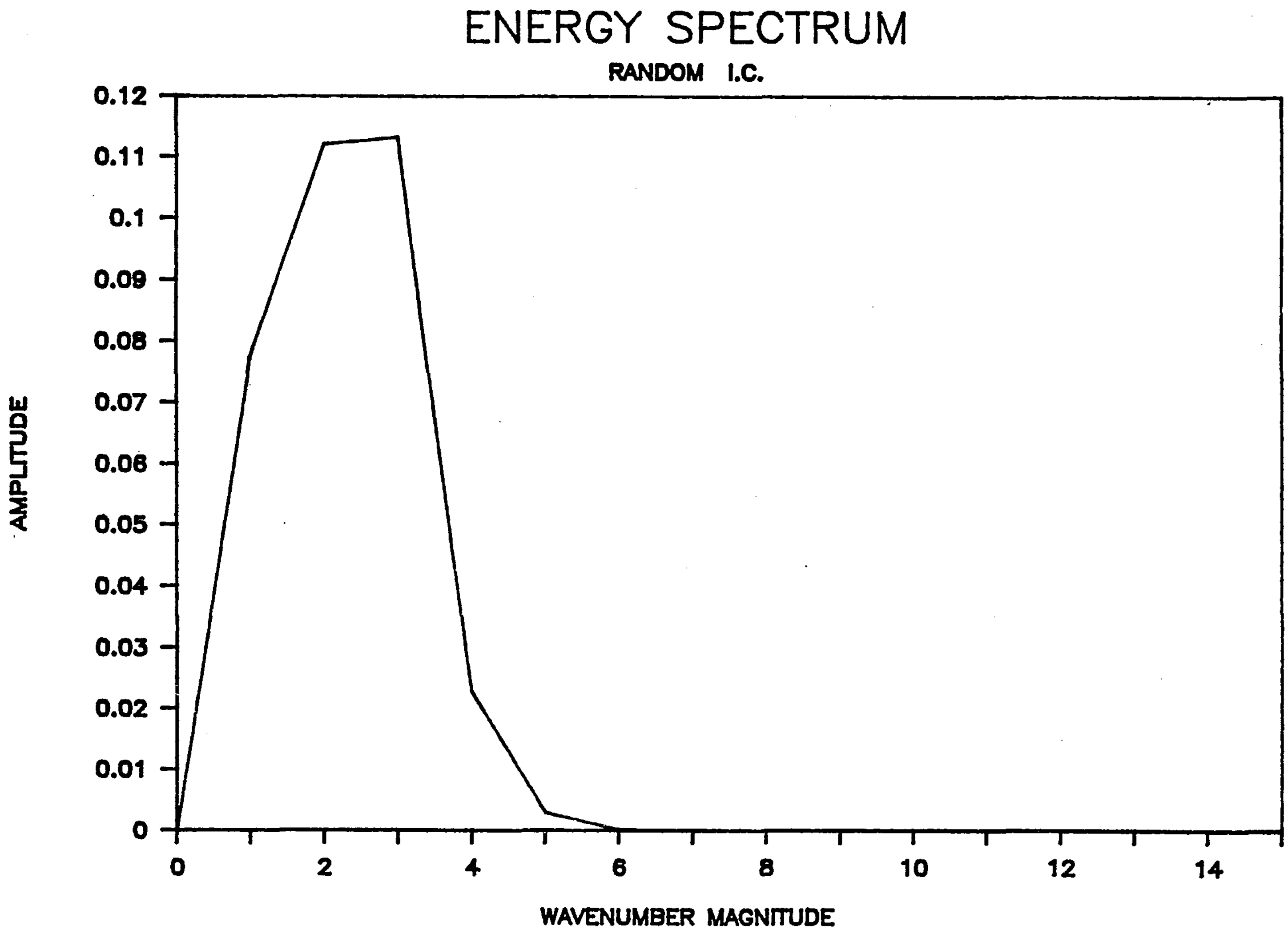

ENERGY SPECTRUM
CLEBSCH I.C.
AMPLITUDE
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
2
4
6
8
10
WAVENUMBER MAGNITUDE

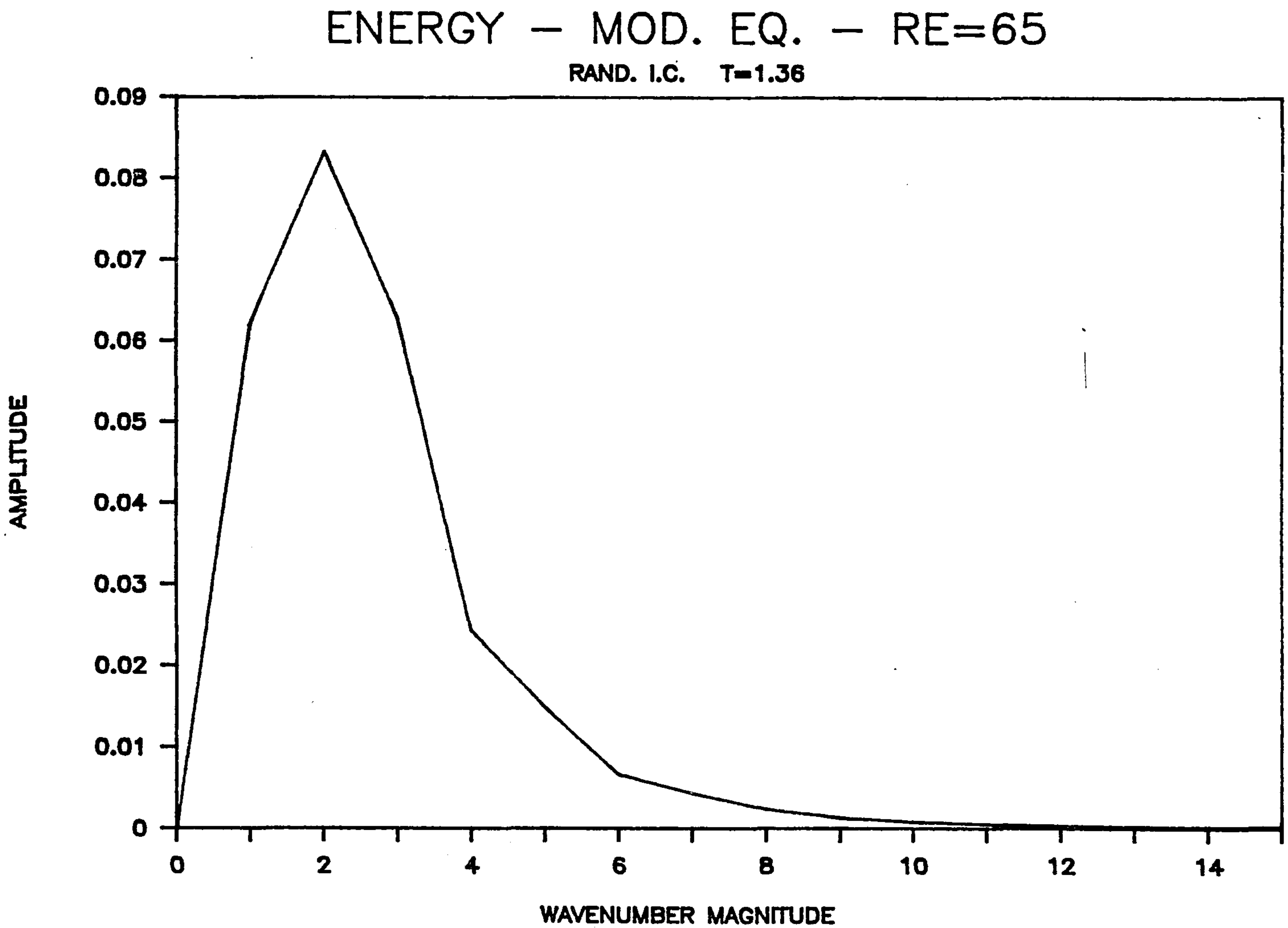

ENERGY - MOD. EQ. - RE=70
CLEB. I.C. T=1.11
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
AMPLITUDE
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

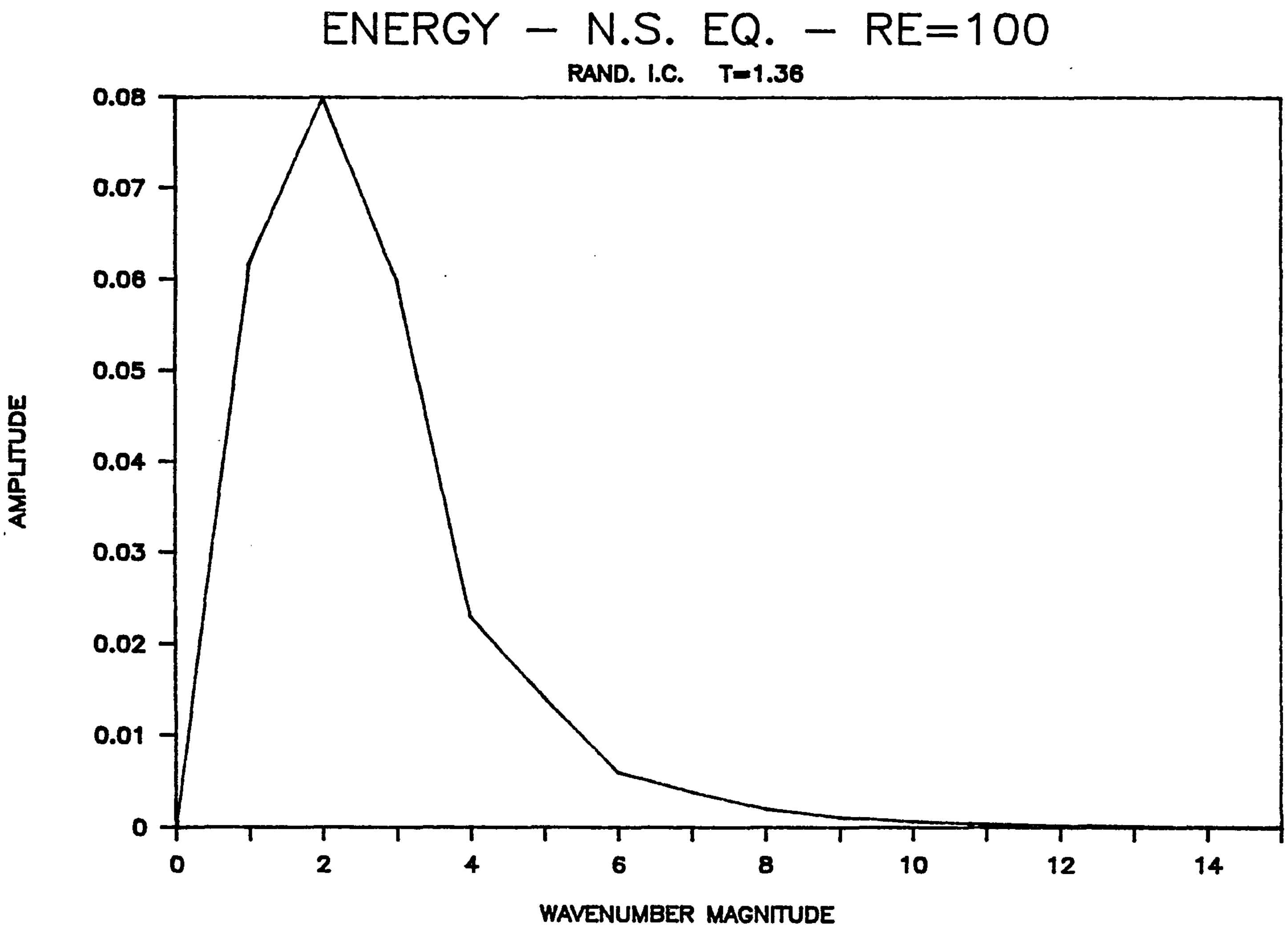

ENERGY - N.S. EQ. - RE=100
CLEB. I.C. T=1.11
AMPLITUDE
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

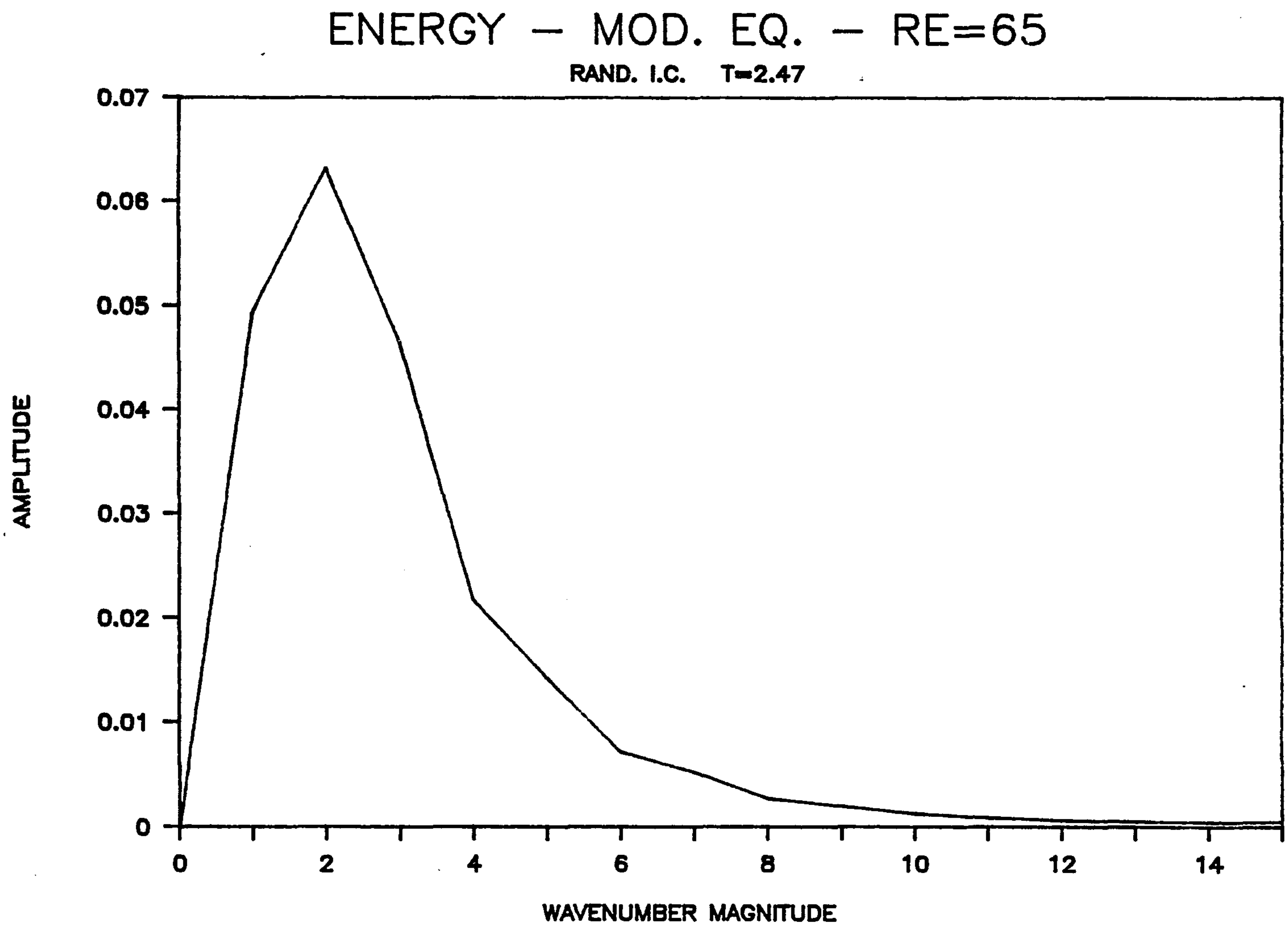

ENERGY — MOD.EQ. — RE=70
CLEB. I.C. T=2.47
AMPLITUDE
0.06
0.05
0.04
0.03
0.02
0.01
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

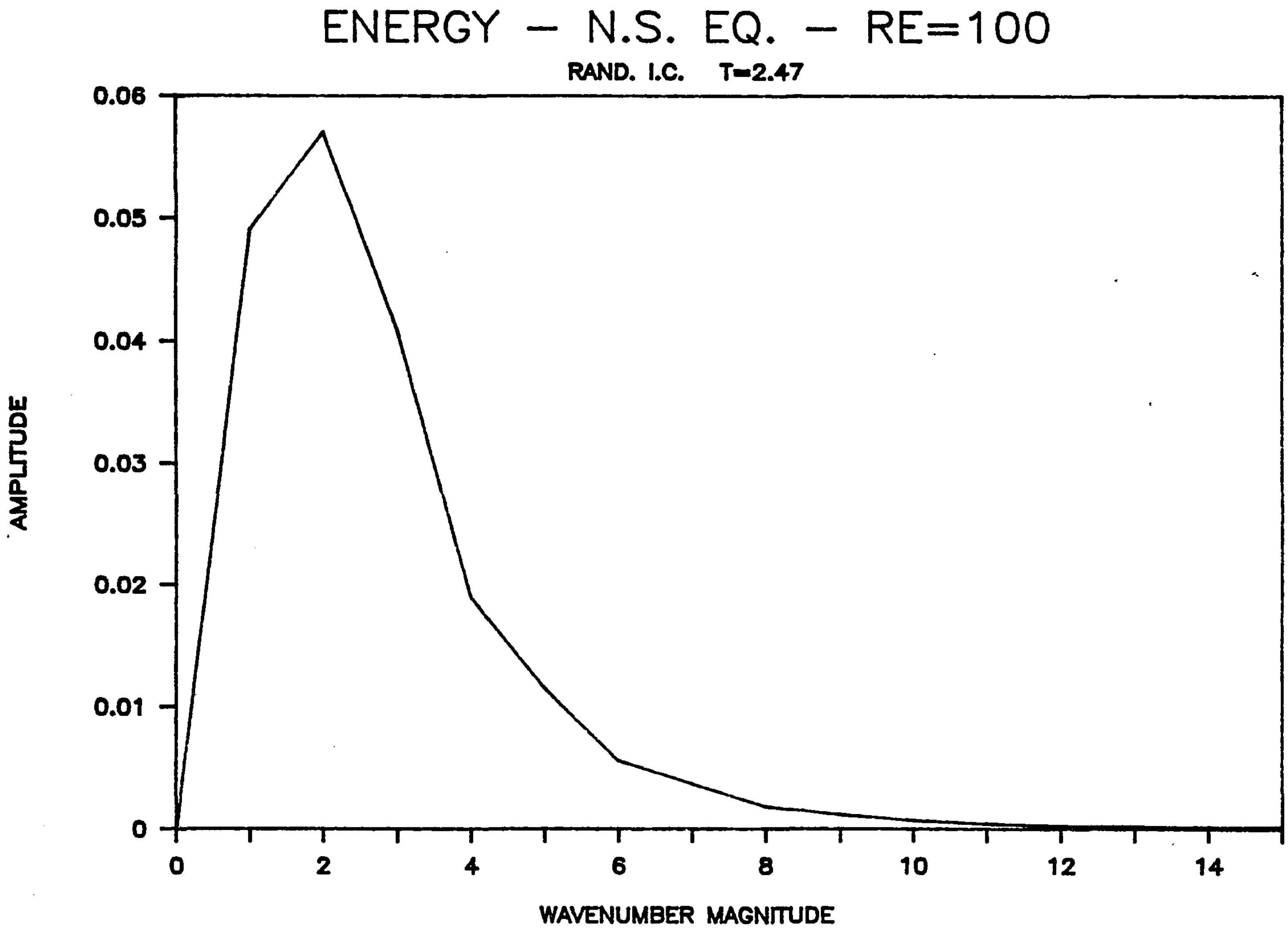

ENERGY - N.S. EQ. - RE=100
CLEBSCH I.C. T=2.47
AMPLITUDE
0.06
0.05
0.04
0.03
0.02
0.01
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

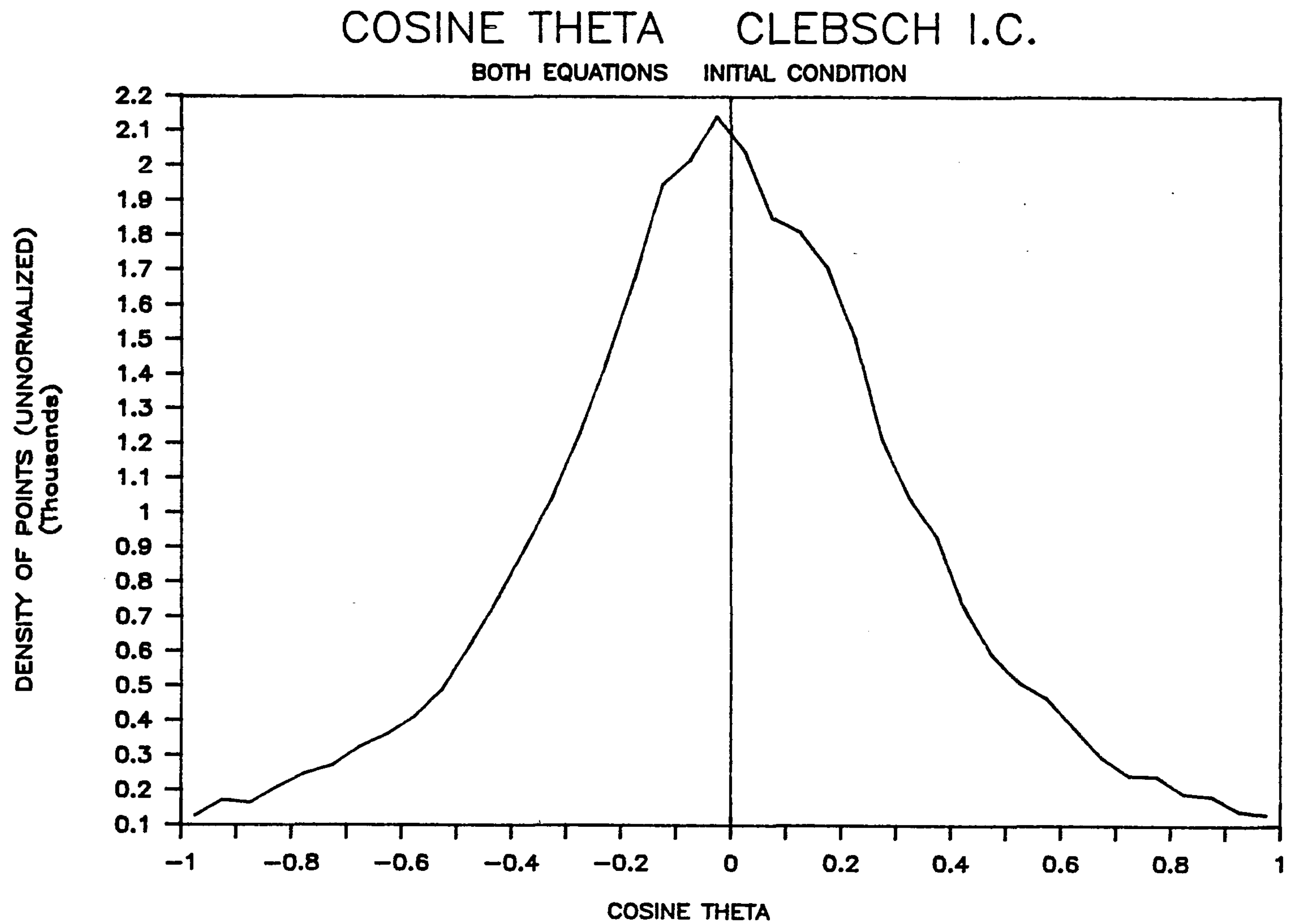

ENERGY SPECTRUM
RANDOM I.C.
AMPLITUDE
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

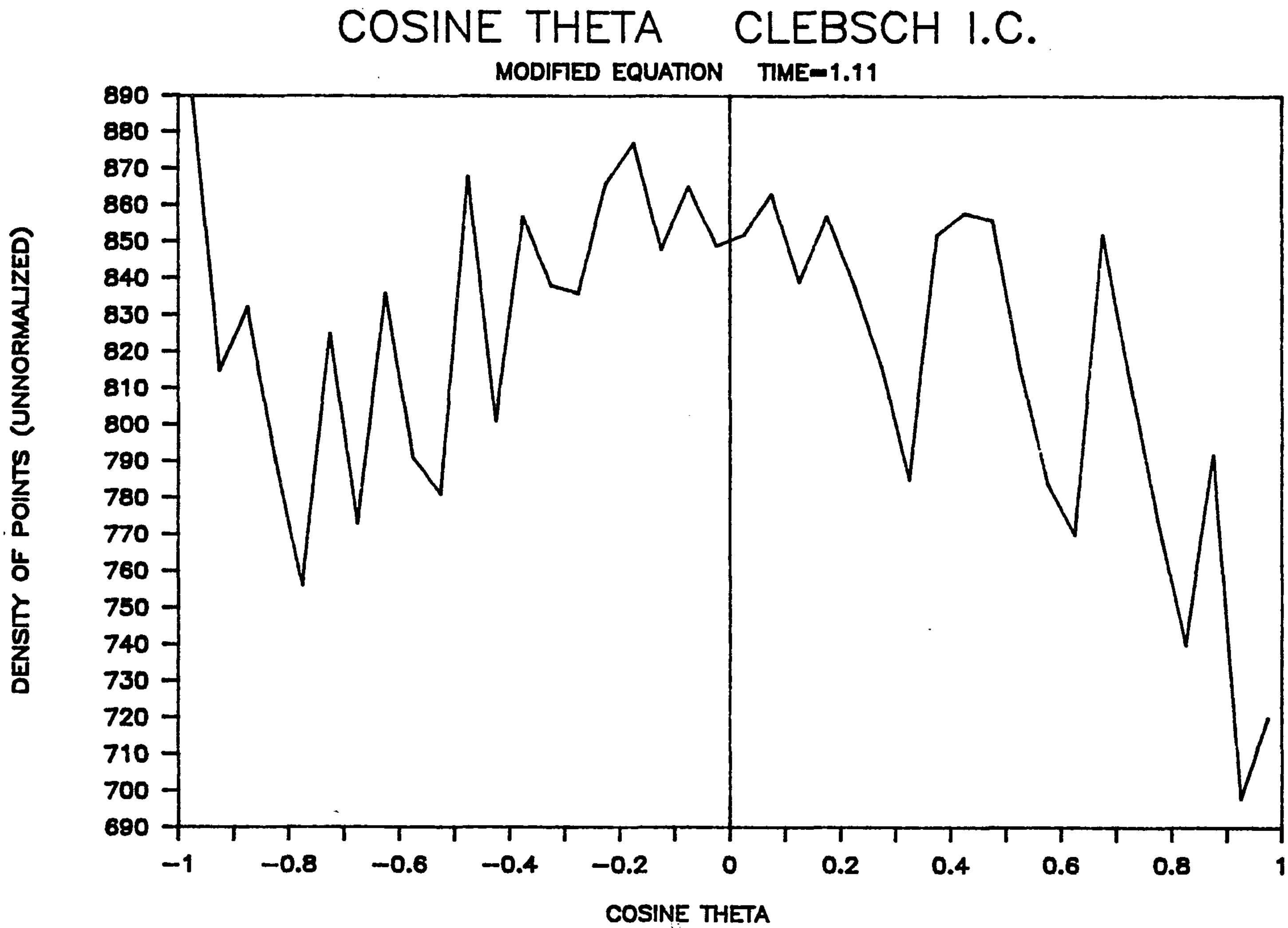

ENERGY - MOD. EQ. - RE=65
RAND. I.C. T=1.36
AMPLITUDE
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE


ENERGY – N.S. EQ. – RE=100
RAND. I.C. T=1.36
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
AMPLITUDE
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE


ENERGY – MOD. EQ. – RE=65
RAND. I.C. T=2.47
AMPLITUDE
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE


ENERGY - N.S. EQ. - RE=100
RAND. I.C. T=2.47
0.06
0.05
0.04
0.03
0.02
0.01
0
AMPLITUDE
0
2
4
6
8
10
12
14
WAVENUMBER MAGNITUDE

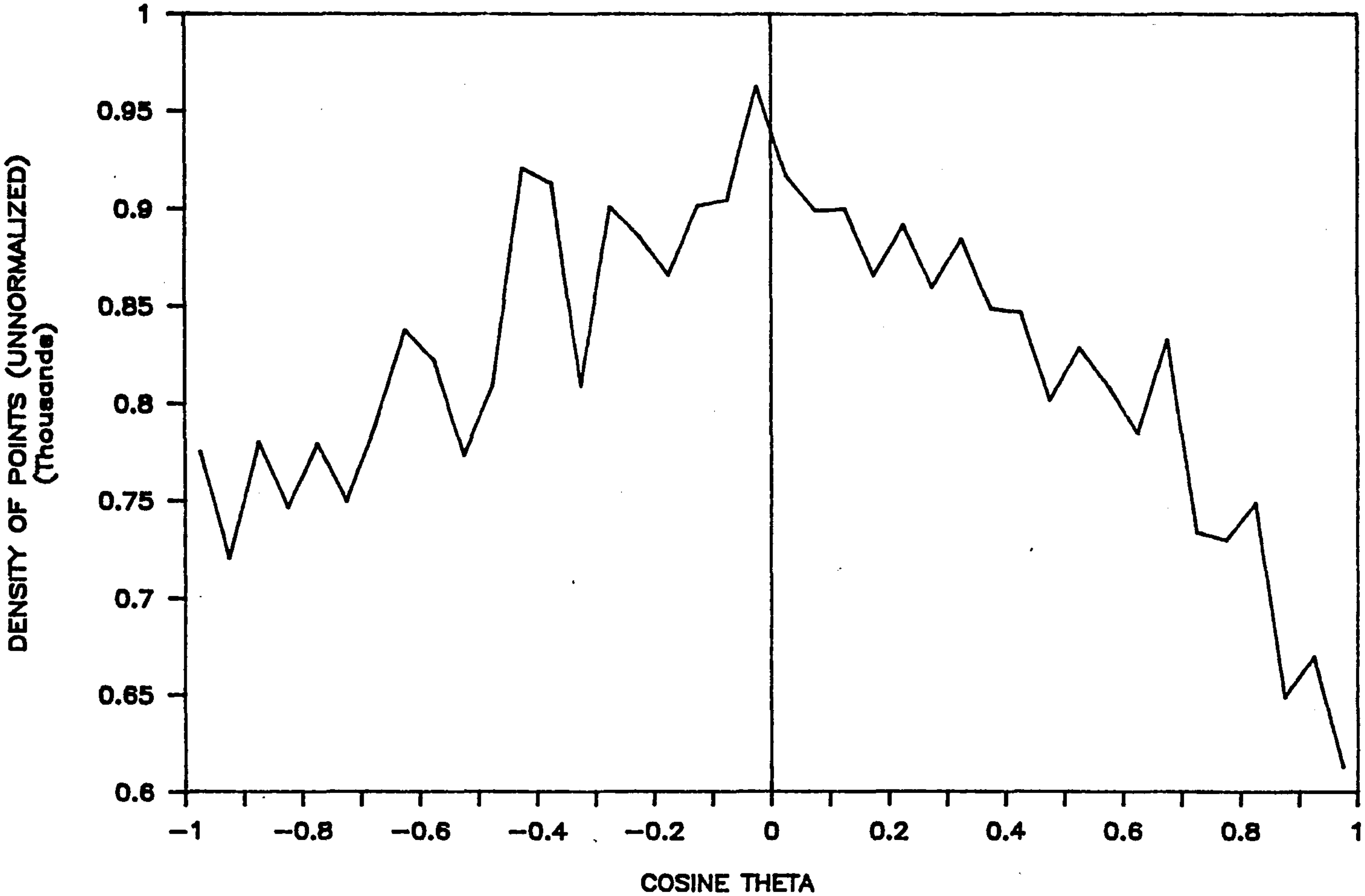

COSINE THETA CLEBSCH I.C.
BOTH EQUATIONS INITIAL CONDITION
DENSITY OF POINTS (UNNORMALIZED)
(Thousands)
2.2
2.1
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1
COSINE THETA

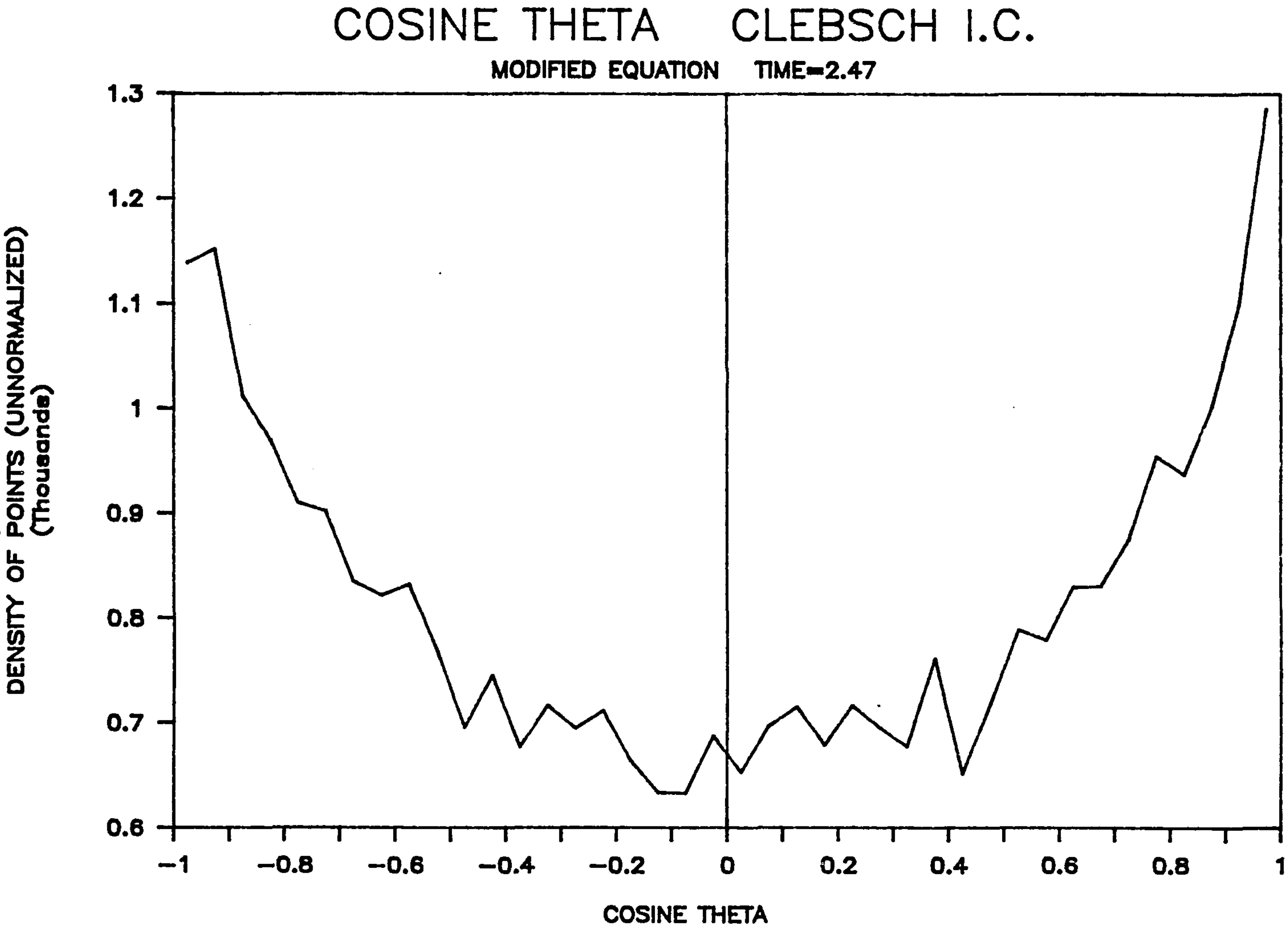


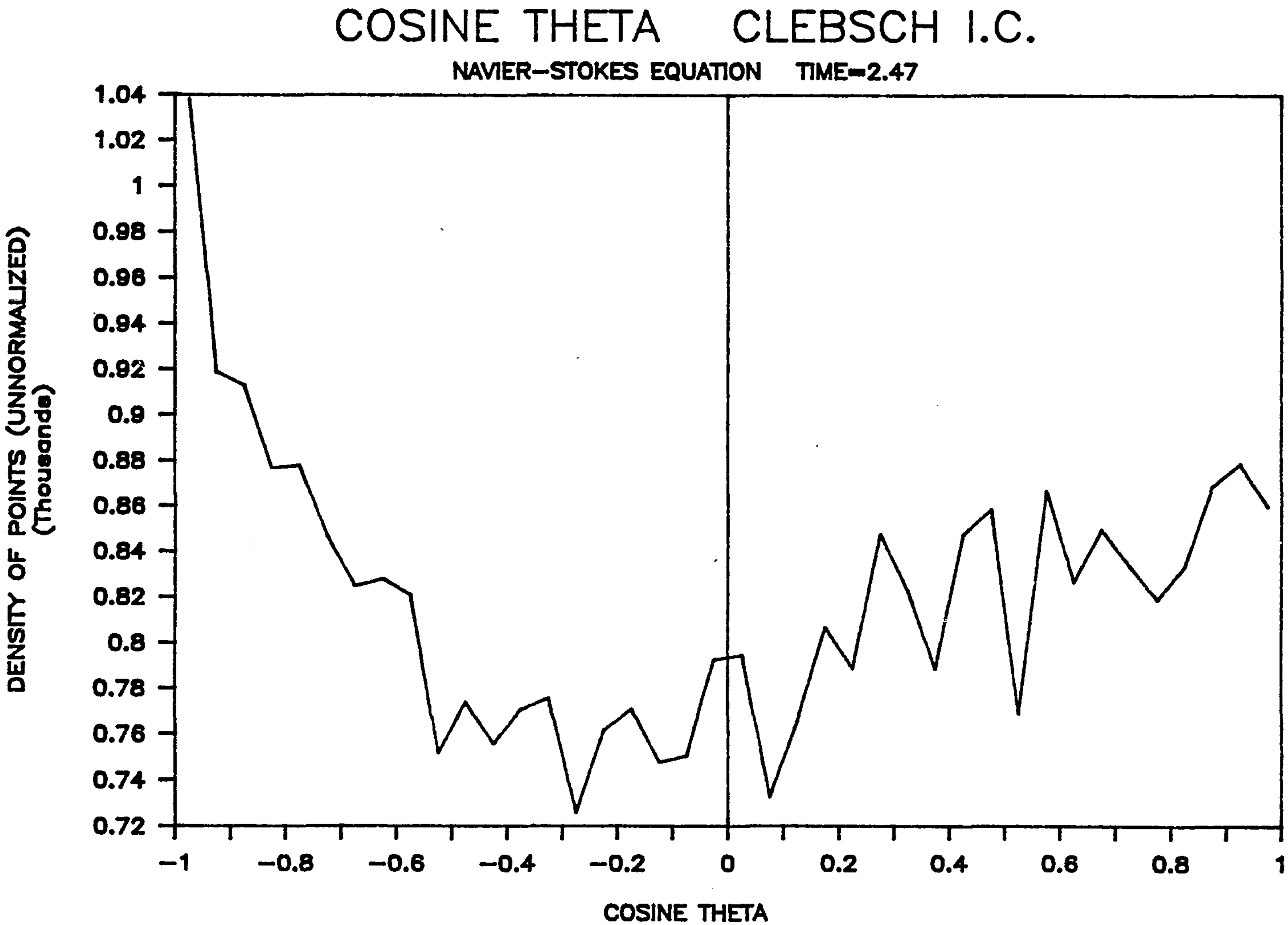
COSINE THETA CLEBSCH I.C.
MODIFIED EQUATION TIME=1.11
DENSITY OF POINTS (UNNORMALIZED)
890
880
870
860
850
840
830
820
810
800
790
780
770
760
750
740
730
720
710
700
690
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1
COSINE THETA

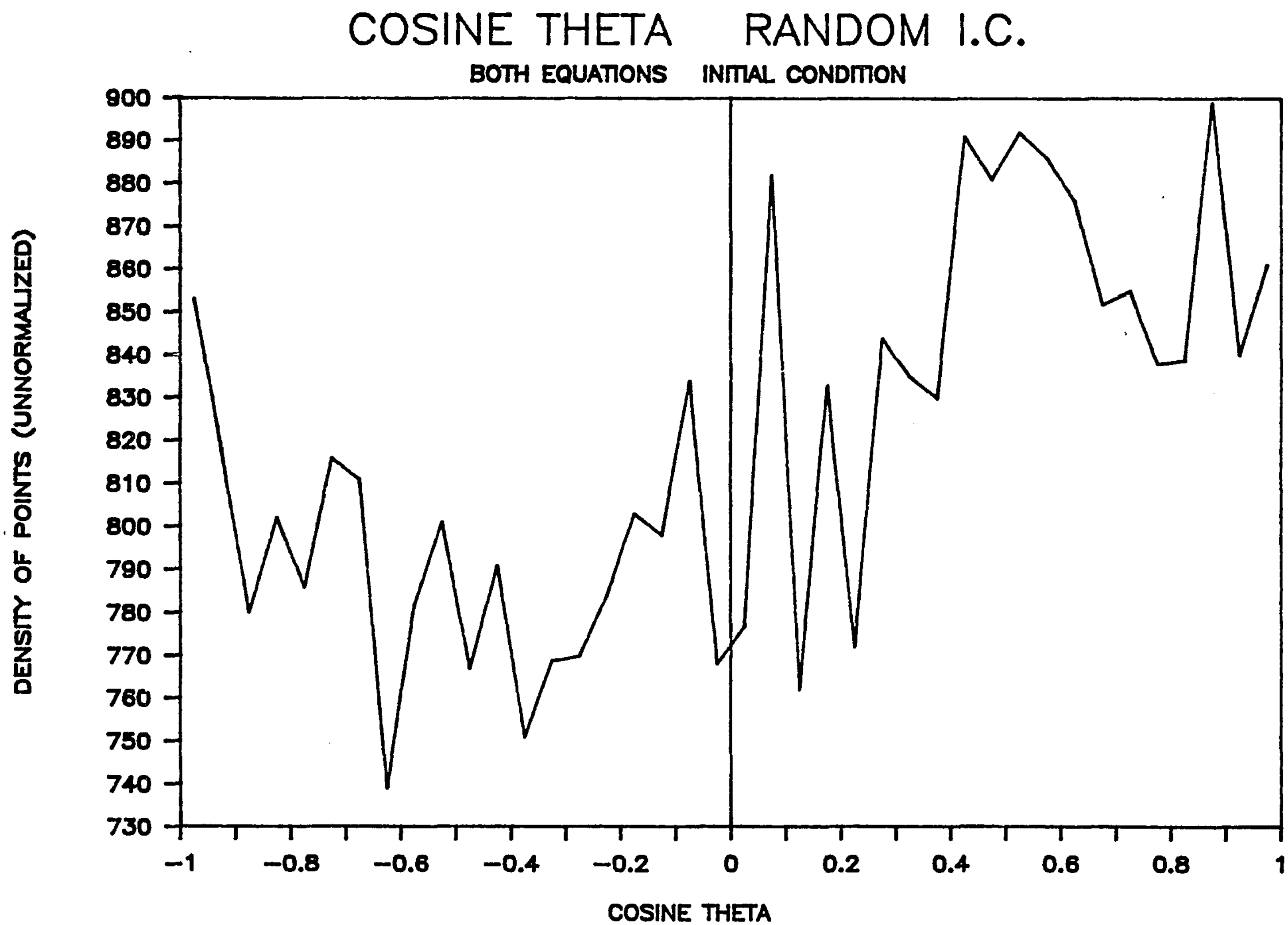
COSINE THETA CLEBSCH I.C.

NAVIER–STOKES EQUATION TIME=1.11



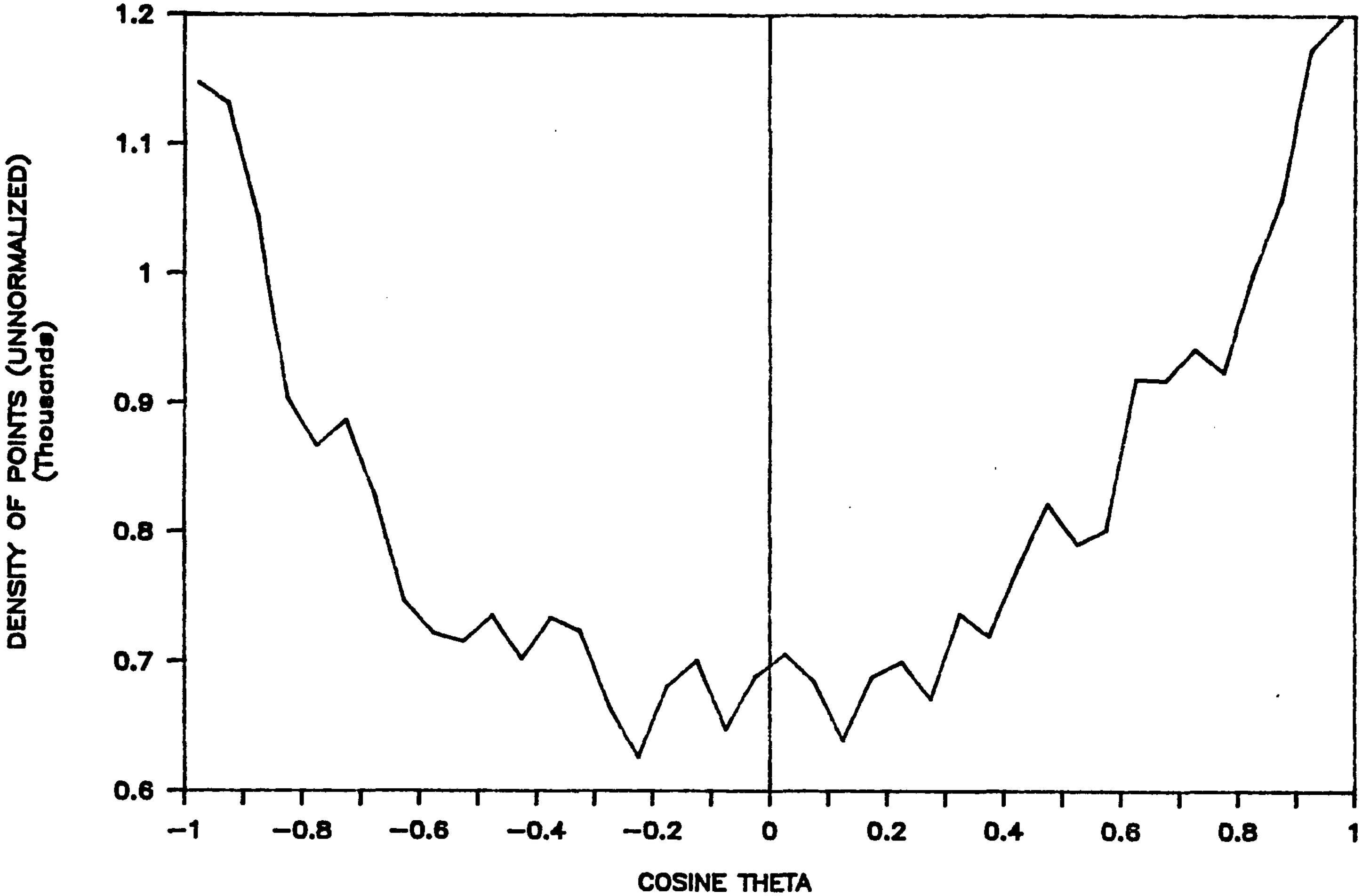

COSINE THETA CLEBSCH I.C.
MODIFIED EQUATION TIME=2.47
DENSITY OF POINTS (UNNORMALIZED)
(Thousands)
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1
COSINE THETA

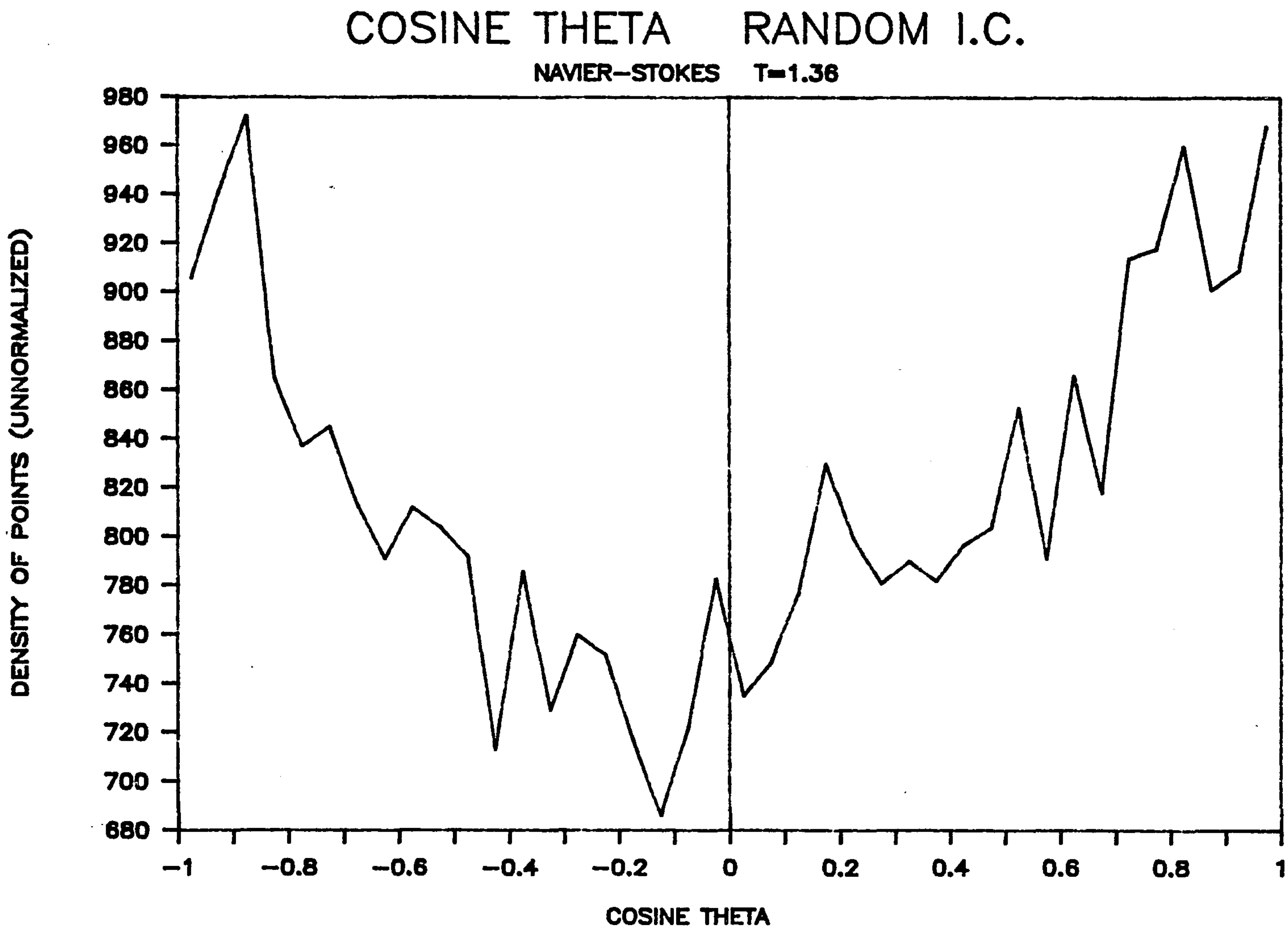

COSINE THETA CLEBSCH I.C.
NAVIER–STOKES EQUATION TIME=2.47
DENSITY OF POINTS (UNNORMALIZED)
(Thousands)
1.04
1.02
1
0.98
0.96
0.94
0.92
0.9
0.88
0.86
0.84
0.82
0.8
0.78
0.76
0.74
0.72
–1
–0.8
–0.6
–0.4
–0.2
0
0.2
0.4
0.6
0.8
1
COSINE THETA

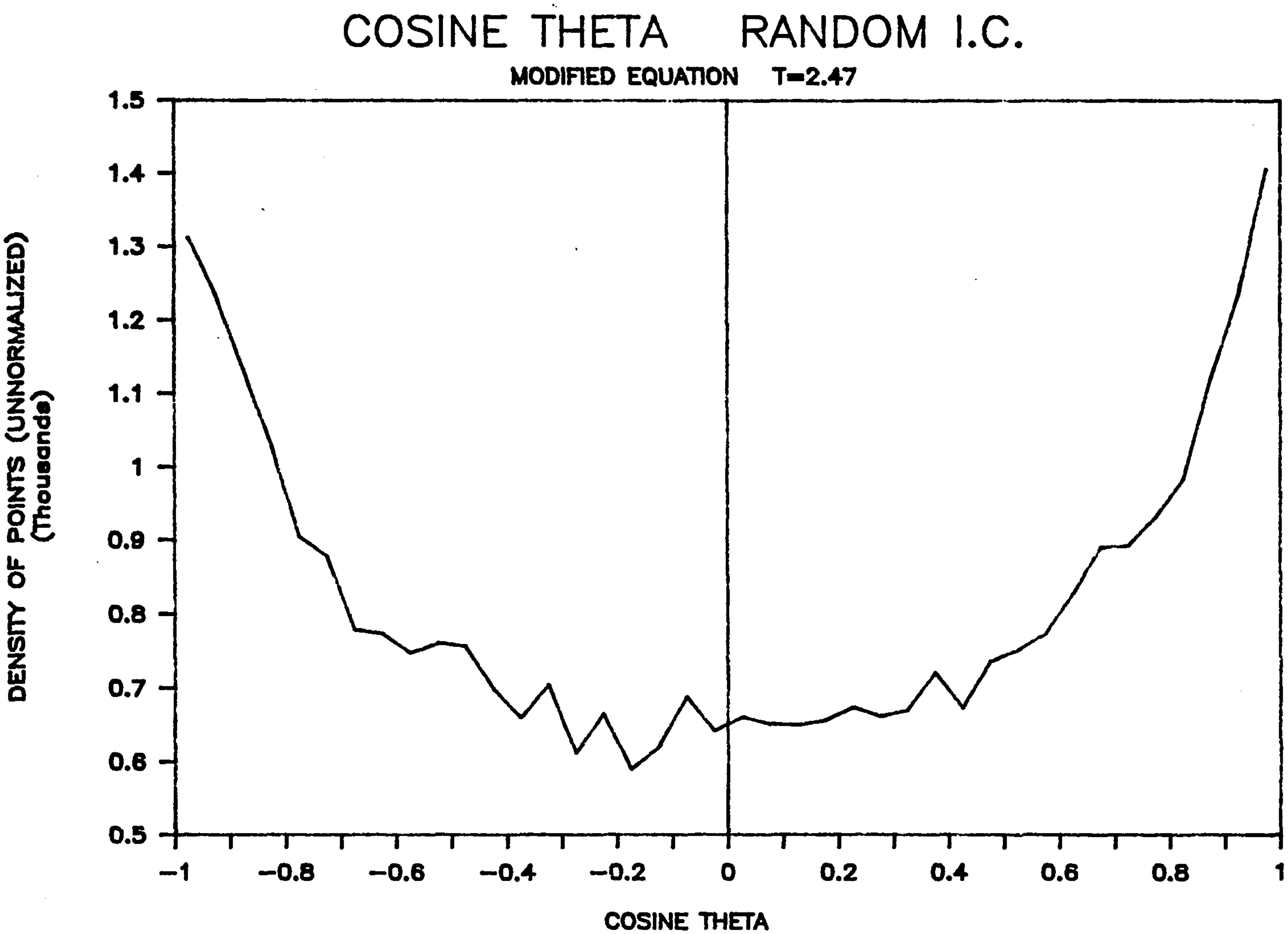

COSINE THETA RANDOM I.C.
BOTH EQUATIONS INITIAL CONDITION
DENSITY OF POINTS (UNNORMALIZED)
900
890
880
870
860
850
840
830
820
810
800
790
780
770
760
750
740
730
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1
COSINE THETA

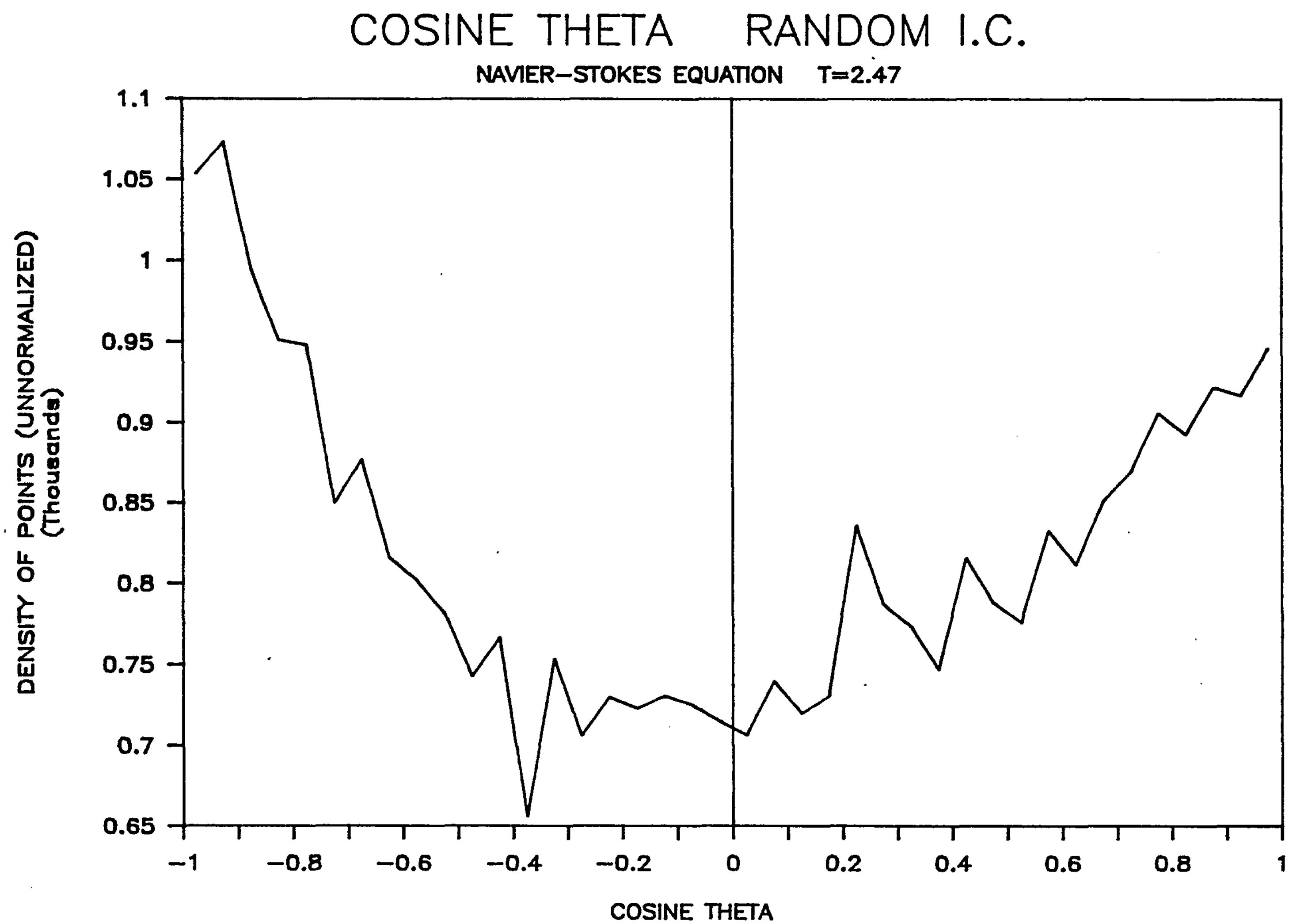
COSINE THETA RANDOM I.C.

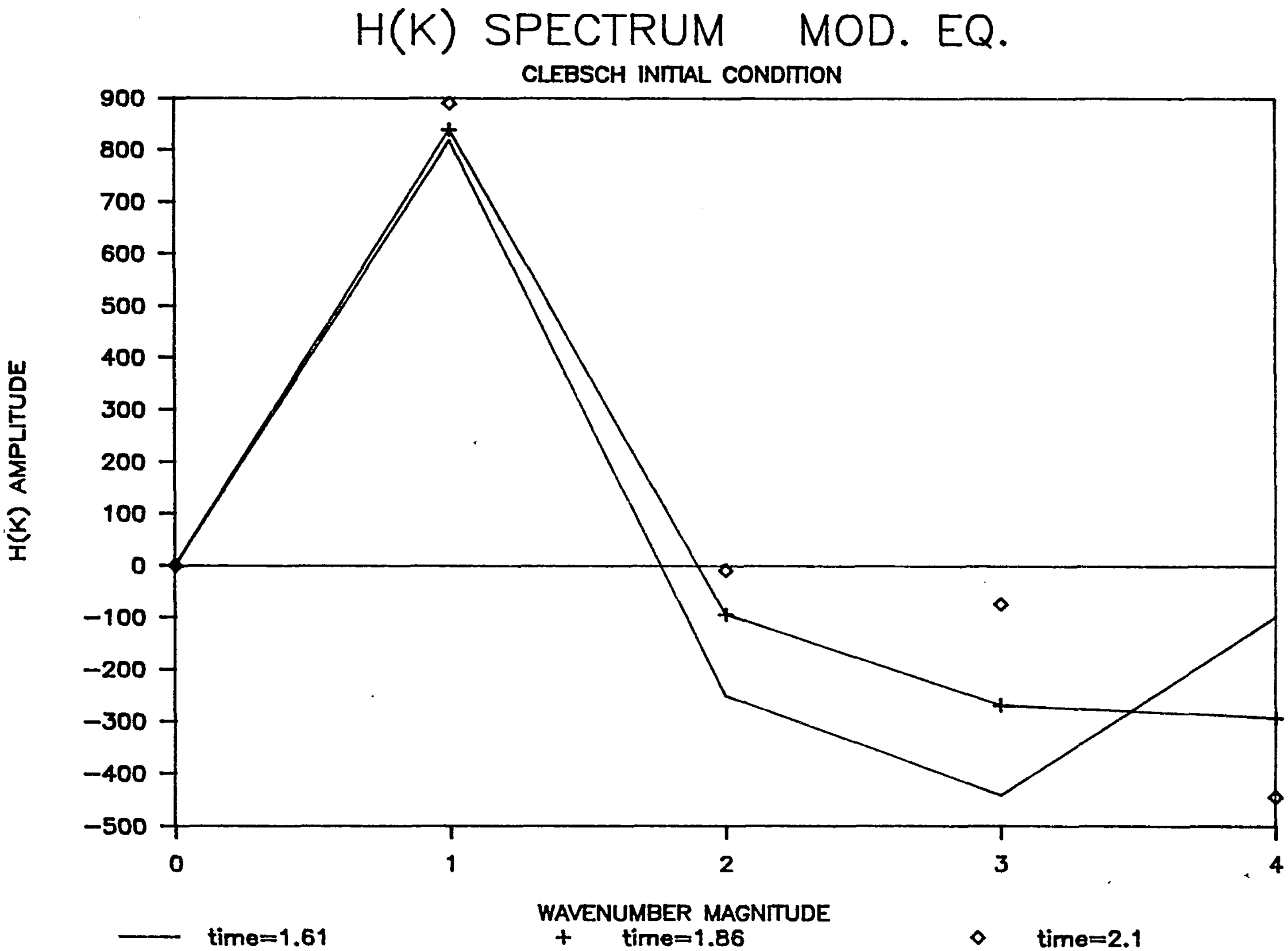
MODIFIED EQUATION T=1.36

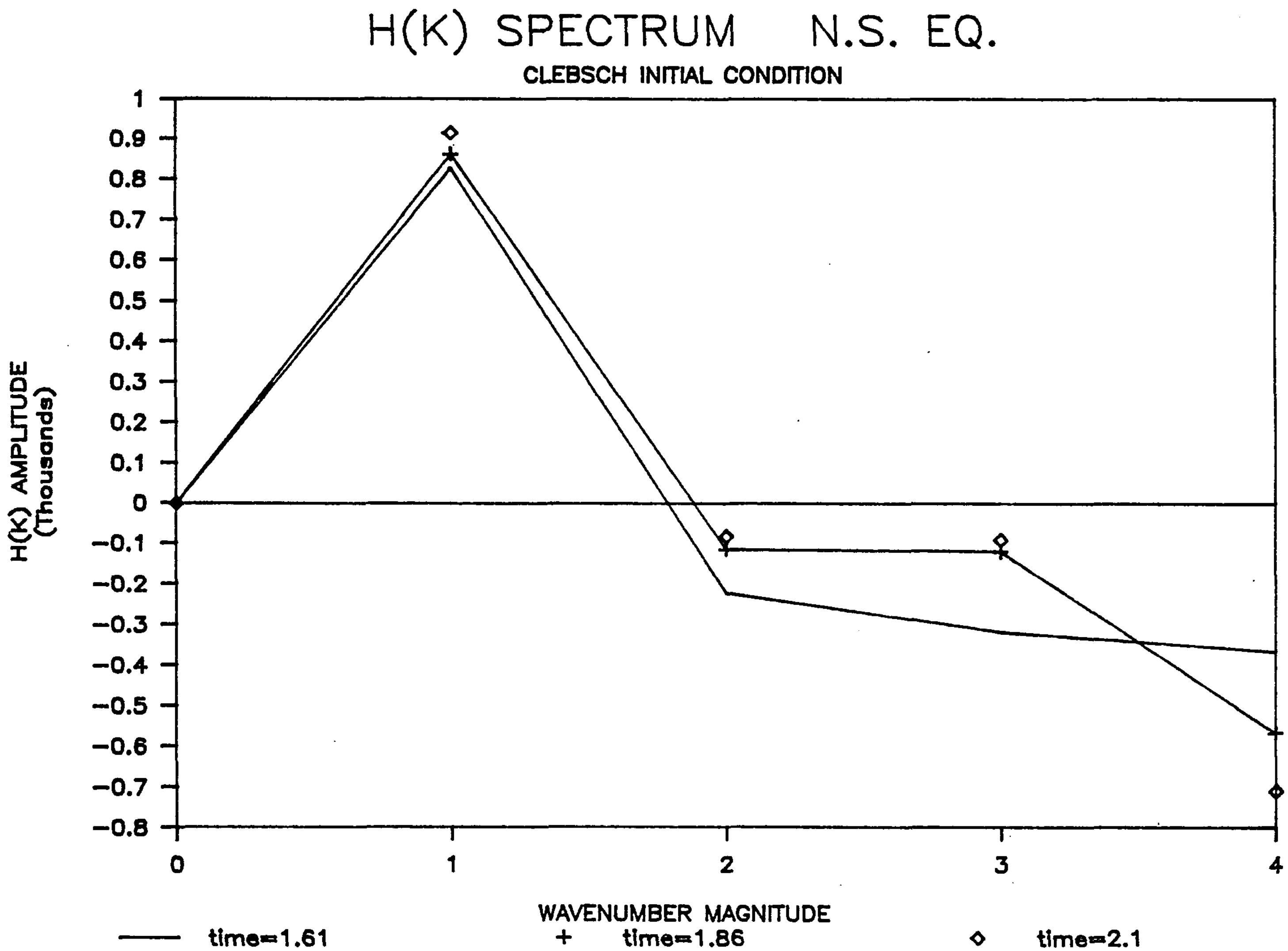


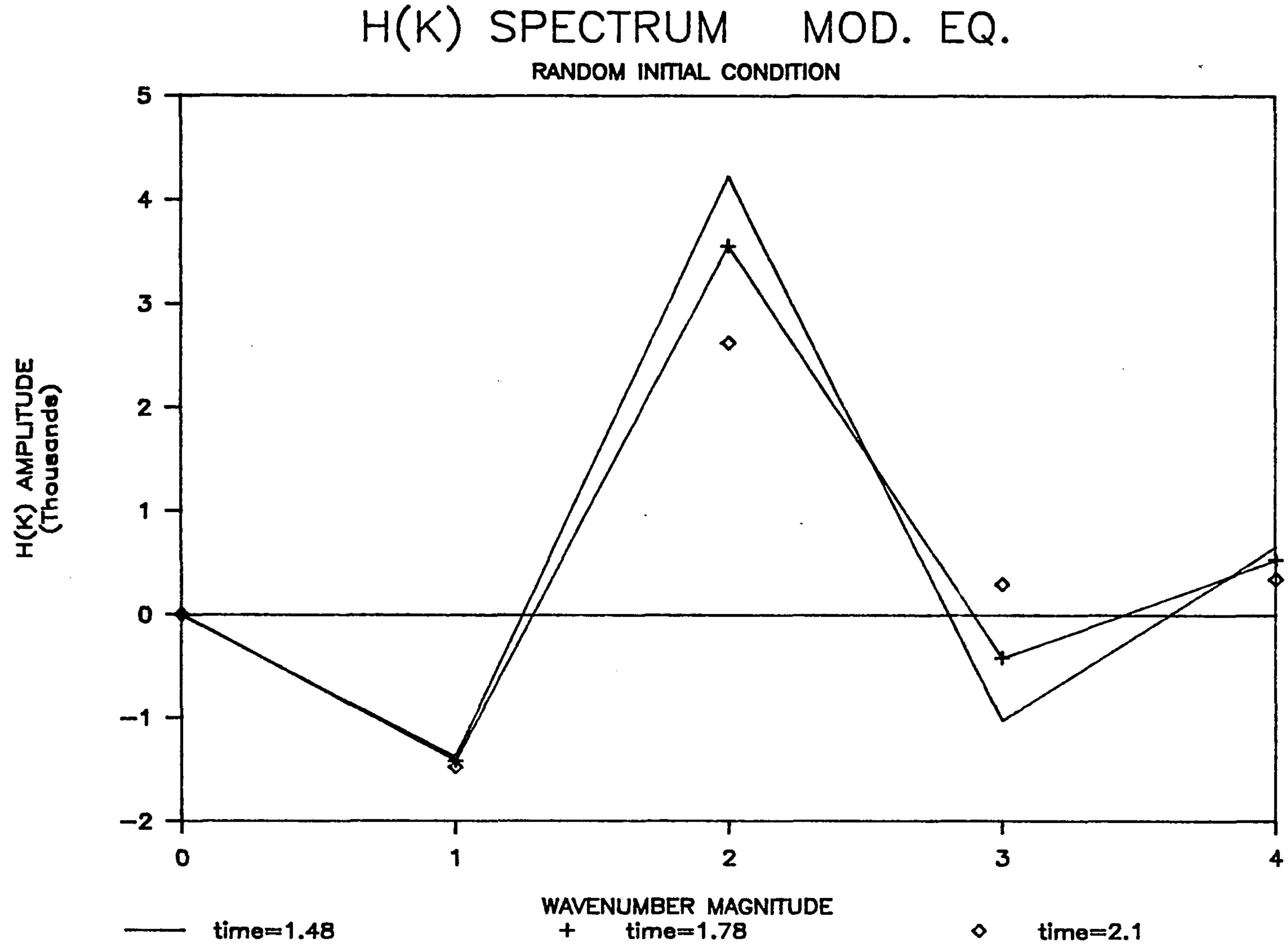

COSINE THETA RANDOM I.C.
NAVIER–STOKES T=1.36
DENSITY OF POINTS (UNNORMALIZED)
980
960
940
920
900
880
860
840
820
800
780
760
740
720
700
680
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1
COSINE THETA

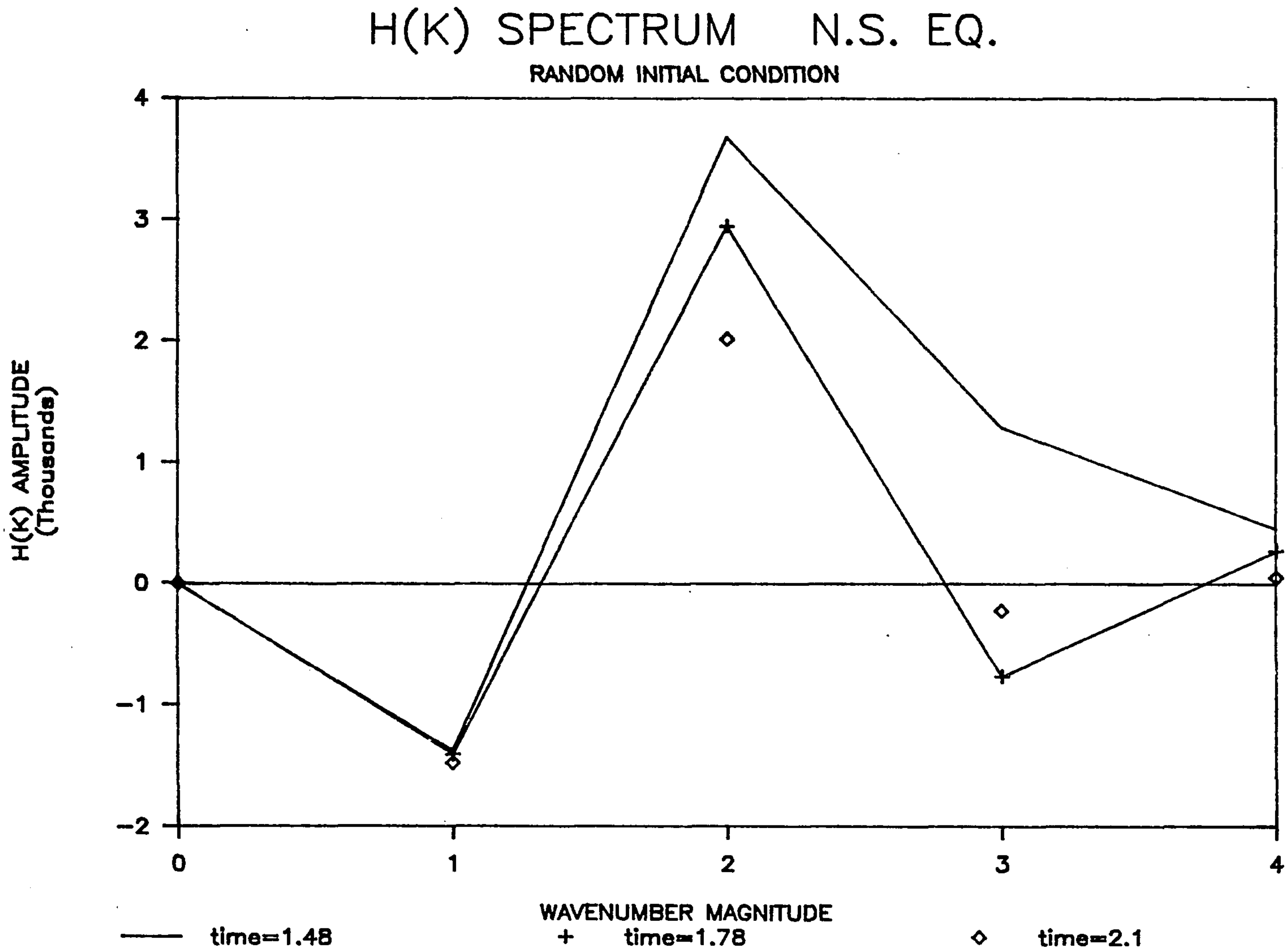

COSINE THETA RANDOM I.C.
MODIFIED EQUATION T=2.47
DENSITY OF POINTS (UNNORMALIZED)
(Thousands)
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1
COSINE THETA

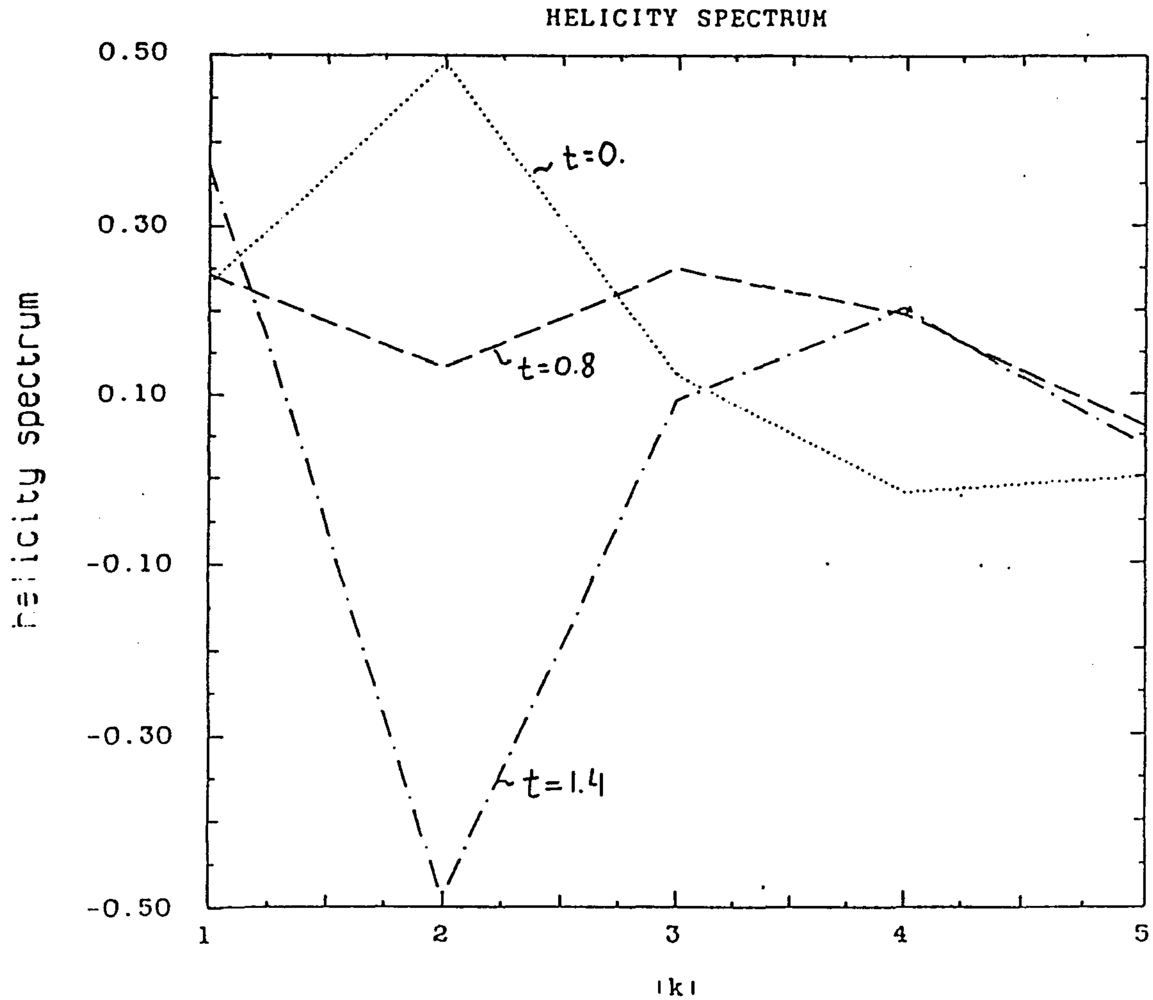

COSINE THETA RANDOM I.C.
NAVIER–STOKES EQUATION T=2.47
DENSITY OF POINTS (UNNORMALIZED)
(Thousands)
1.1
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
–1
–0.8
–0.6
–0.4
–0.2
0
0.2
0.4
0.6
0.8
1
COSINE THETA


H(K) SPECTRUM MOD. EQ.
CLEBSCH INITIAL CONDITION
H(K) AMPLITUDE
900
800
700
600
500
400
300
200
100
0
−100
−200
−300
−400
−500
0
1
2
3
4
WAVENUMBER MAGNITUDE
time=1.61
time=1.86
time=2.1


H(K) SPECTRUM N.S. EQ.
CLEBSCH INITIAL CONDITION
H(K) AMPLITUDE (Thousands)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
−0.8
0
1
2
3
4
WAVENUMBER MAGNITUDE
time=1.61
+ time=1.86
◇ time=2.1


H(K) SPECTRUM MOD. EQ.
RANDOM INITIAL CONDITION
H(K) AMPLITUDE
(Thousands)
5
4
3
2
1
0
-1
-2
0
1
2
3
4
WAVENUMBER MAGNITUDE
time=1.48
time=1.78
time=2.1

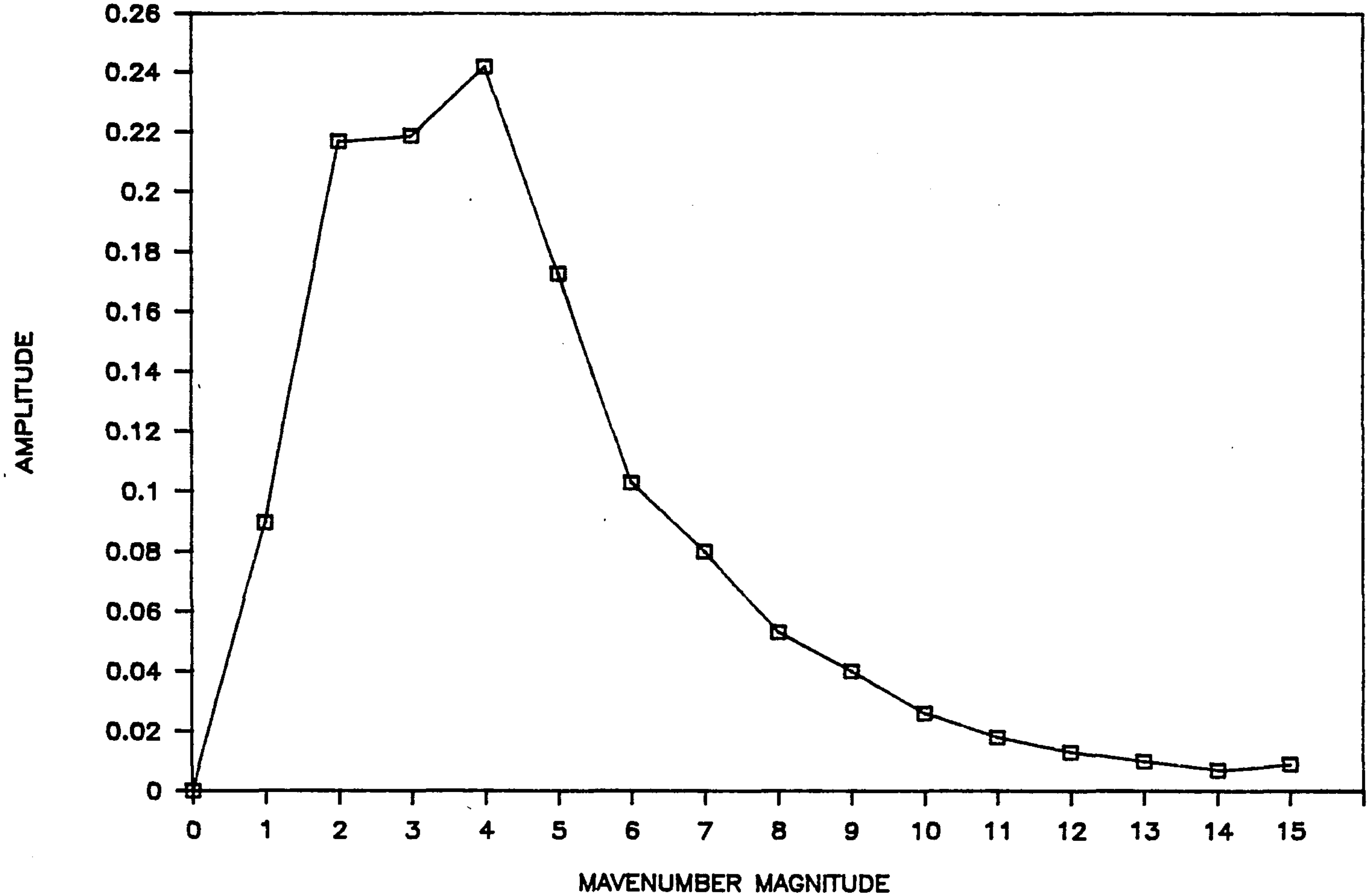

H(K) SPECTRUM N.S. EQ.
RANDOM INITIAL CONDITION
H(K) AMPLITUDE
(Thousands)
4
3
2
1
0
−1
−2
0
1
2
3
4
WAVENUMBER MAGNITUDE
time=1.48
+ time=1.78
◇ time=2.1



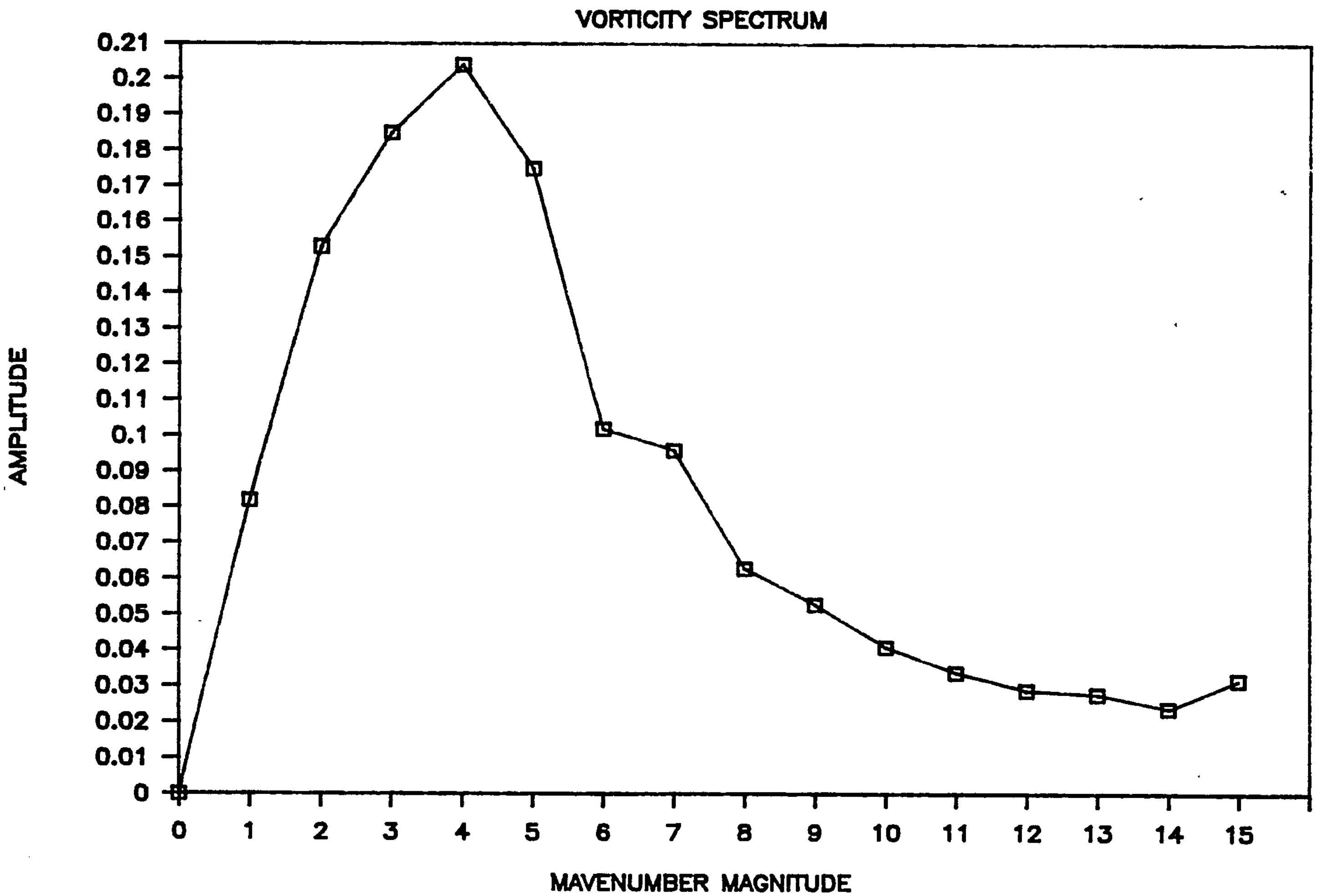
simulation 128**3 of a BIGBOX

APPENDIX RUN INITIAL CONDITION

VORTICITY SPECTRUM



APPENDIX RUN FINAL CONDITION



APPENDIX

APPENDIX

ERROR ANALYSIS

For the Navier-Stokes equation the argument that truncation errors are unimportant if the vorticity spectrum is low enough where the high wavenumber truncation begins makes sense. That the high wavenumbers are damped very strongly is an analytical result. For the modified equation there is no such result. For the Navier-Stokes we were also able to control the parameters so that the viscous decay balances the the cascade, and the high wavnumbers do not grow too strongly. For the modified equation this was not the case. For this reason the results of the simulation of the Navier-Stokes equation are necessarily more trustworthy than the result of the modified equation. Let us first quickly review the evidence for the validity of the Navier-Stokes simulations.

The vorticity spectra are the first evidence, and these should be reviewed by eye. There is only a small upturn at the high wavenumber end and the height of the line is moderate. Recalling that many modes past this point are still represented (though not all) it would seem that these results look acceptable. The Taylor and Kolmogorov length scales are given in the table below for the times: the beginning of the run, the maximum of enstrophy, the end of the run. The Taylor microscale is given for each of the three orthogonal directions. The calculation of the Kolmogorov microscale uses a formula from Batchelor which assumes isotropy, so only one can be given. (The formulae can be found in the text)

Random initial condition

time	K. length	Taylor x direction	Taylor y direction	Taylor z direction
0	0.7	0.6	0.7	0.6
1.36	0.7	0.4	0.4	0.3
2.47	0.5	0.4	0.4	0.3

Clebsch initial condition

time	K. length	Taylor x direction	Taylor y direction	Taylor z direction
0	0.8	1.	0.6	0.6
1.11	0.7	0.8	0.4	0.4
2.47	0.6	0.8	0.3	0.4

For the modified equation, the results are necessarily tentative. We have already discussed the spectra. The Kolmogorov length scale makes no sense in this case because the dissipation is different and the viscosity is two dimensional. The Taylor length scales are:

Random initial conditions

time	Taylor x direction	Taylor y direction	Taylor z direction
0	0.6	0.7	0.6
1.36	0.4	0.4	0.3
2.47	0.3	0.3	0.2

Clebsch initial condition

time	Taylor x direction	Taylor y direction	Taylor z direction
0	0.6	0.7	0.6
1.11	0.5	0.5	0.4
2.47	0.4	0.4	0.3

The time stepping error for helicity generation seems to be second order in time. The following figures are for the Clebsch initial condition run, so any non-zero helicity is an error.

size of time step	value of helicity at t=.4
.005	.78
.0025	.51
.00125	.33

It would seem that there is some residual error not due to time stepping apparently of a size between .1 and .2.

Finally, we present the result of an attempt to assure that the modified equation was simulated accurately by using an initial condition that was already far decayed. The results were negative.

Other attempts were made as well, but this is presented as one example. Following are the vorticity graphs for the initial condition and a later time. I claim only that the simulation was as accurate as posssible given the constraints of the method and resolution, and is somewhat indicative of what could be expected with a more effective method, especially for short times.

BIBLIOGRAPHY

BIBLIOGRAPHY

1859 1. A. Clebsch, "Ueber die Integration der hydrodynamischen Gleichungen", Journal fuer die reine und angewandte Mathematic 57, 1-10.

1932 1. H. Lamb, Hydrodynamics, Dover, New York, 239-240

1953 G.K.Batchelor, "The Theory of Homogeneous Turbulence", Cambridge Science Classics, Cambridge England

1954 1. C. Truesdell, The Kinematics of Vorticity, Indiana University Press, Bloomington.

1968 1. R.L. Seliger and G.B. Whitham, F.R.S., "Variational principles in continuum mechanics", Proc. Roy. Soc. A. 305, 1-25.

1969 1. H.K. Moffatt, "The degree of knottedness of tangled vortex lines", J. Fluid Mech., 35, part 1, 117-120

2. S.A. Orszag, "Numerical Methods for the Simulation of Turbulence", Phys. Fluids Supp. II, 250-257.

1971 1. S.A. Orszag (a), "Numerical Simulation of Incompressible Flows Within Simple Boundaries. I. Galerkin (Spectral) Representations", Stud. Appl. Math., L, #4, 293-326

2. S.A. Orszag (b), "Numerical simulation of incompressible flows within simple boundaries: accuracy", J. Fluid Mech., 49, part 1, 75-112

3. G.S. Patterson, Jr. and S.A. Orszag, "Spectral Calculations of Isotropic Turbulence: Efficient Removal of Aliasing Interactions", Phys. Fluids, 14, 2538-2541.

1974 1. V.I. Arnol'd, "The asymptotic Hopf invariant and its applications", Proc. Summer School in Differential Equations, Armenian SSR Academy of Science, G. Wilson, trans.

2. S. Grossmann, Phys. Rev., A11, 2165-2169.

3. E.C.G. Sudarshan and N. MuKunda, Classical Dynamics: A modern perspective, Wiley, New York, 420-438.

1976 1. Grossmann and E. Schnedler, "Fluctuation Corrections of the Turbulence Spectrum by Renormalization Group Methods", Z. Physik B, **26**, 307-317.

1978 1. H.K. Moffatt, Magnetic field generation in electrically conducting fluids, Cambridge University Press, Cambridge

1979 1. E. Kreyszig, Advanced Engineering Mathematics (fourth ed.), John Wiley & Sons, New York.

1980 1. O. Buneman, "Ideal gas dynamics in Hamiltonian form with benefit for numerical schemes", Phys. Fluids, **23**, 1716-1717.

2. E.A. Kuznetsov and A.V. Mikhailov, "On the Topological Meaning of Canonical Clebsch Variables", Phys. Let., **77A**, 37-38.

1981 1. E. Levich, "The Hamiltonian Formulation of the Euler Equation and Subsequent Constraints on the Properties of Randomly Stirred Fluids", Phys. Let., **86A**, 165-168.

2. H.K. Moffatt, "Some developments in the theory of turbulence", J. Fluid Mech., **106**, 27-47.

1982 1. A. Frenkel, E. Levich and L. Stilman, "Hamiltonian Description of Ideal MHD Revealing New Invarants of Motion", Phys. Let., **88A**, 461-465.

2. F.S. Henyey, "Hamiltonian description of stratified fluid dynamics", Phys. Fluids, **26**, 40-47.

3. E. Levich, "Nonlocal Invariants of the Euler Equations as Constraints on the Large-Scale Properties of Turbulent Motion", Phys. Let., **87A**, 461-464.

1983 1. D.D. Holm and B.A. Kupershmidt, "Non-canonical Hamiltonian Formulation of Ideal Magnetohydrodynamics", Physica, **7D**, 330-333.

2. D.D. Holm and B.A. Kupershmidt, "Poisson Brackets and Clebsch Representations for Magnetohydrodynamics, Multifluid Plasmas, and Elasticity", Physica, **6D**, 347-363.

3. G.A. Kuz'min, "Ideal Incompressible Hydrodynamics in Terms of the Vortex Momentum Density", Phys. Let., **96A**, 88-90.

4. E. Levich and A. Tsinober (a), "On the Role of Helical Structures in Three-Dimensional Turbulent Flow", Phys. Let., **93A**, 293-297.

5. E. Levich and A. Tsinober (b), "Helical Structures, Fractal Dimensions and Renormalization-Group Approach in Homogeneous Turbulence", Phys. Let., **96A**, 292-298.

6. J. Marsden and A, Weinstein, "Coadjoint Orbits, Vortices, and Clebsch Variables for Incompressible Fluids", Physica, **7D**, 305-323.

7. H.K. Moffatt, "Simple Topological Aspects of Turbulent Vorticity Dynamics", Turbulence and Chaotic Phenomema in Fluids, Proc. Int. Symposium on Turbulence and Chaotic Phenomena, T. Tatsum ed.

1984 1. M.A. Berger and G.B. Field, "The topological properties of magnetic helicity", J. Flued Mech., **147**, 133-148.

2. A.B. Nassar and S.J. Putterman, "Simplified action priciple formulation of the magnetohydrodynamic equations", Phys. Fluids, **28**, 1001-1002.

3. P.M. Oppeneer, "Variational Principle for Ideal MHD", Phys. Let., **104**, 207-211.

1985 1. R.M. Kerr, "Higher derivative correlations and the alignment of small-scale structures in isotropic numerical turbulence", J. Fluid Mech., **153**, 31-58.

1986 R. Pelz., L. Shtilman and A. Tsinober, "The Helical Nature of Unforced Turbulent Flows" Phys.Fluids 29 (11),

1987 1. W.A. Cassidy and A.L. Frenkel, in preparation.

2. E. Levich and L. Shtilman "Scaling Fractals and non-Linear Variability in Geophysics", Reidel