

DYNAMICAL SYSTEMS THAT MIMIC FLOW TURBULENCE

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ABSTRACT

The relevance of recent developments in nonlinear dynamical systems towards understanding the onset of turbulence in open flows has often been questioned as the behaviour in all such systems studied to-date is fundamentally different in several respects from that of strong turbulence. In particular, such systems exhibit only slow chaos, which furthermore is not persistent as the control parameter is continuously varied beyond the value critical for onset of chaos. Based on physical considerations of the dynamics of interacting large and small eddies, we devise here a nonlinear system which mimics the strong, fast turbulence characteristic of open shear flows, revealing the possibility of establishing closer connections between dynamical chaos and turbulence.

1. INTRODUCTION

RECENT developments in the theory of dynamical systems exhibiting chaotic behaviour (summarized for example in ref. 1) have raised the question whether turbulence in fluid flows could be understood as dynamical chaos. Several proposals on possible routes to chaos have been made²⁻⁴, and these have found some support from observations in bounded flows such as convection in a box⁵ or Taylor-Couette flow⁶. However, the existence of any connection between the "dynamical chaos" exhibited by such systems and turbulence in *open* flows like boundary layers, jets, etc. has often been questioned. It is generally felt^{4,7} that the chaotic phenomena observed in dissipative systems governed by nonlinear ordinary differential equations may be relevant only to the onset stage of turbulence, i.e. to "weak" turbulence.

More specifically, there are at least three issues that need to be faced⁷.

(i) Chaotic dynamical systems do not exhibit a strong cascade process, of the kind generally considered an essential feature of turbulence⁸, where energy put in at low wave numbers or frequencies produces strong fluctuations at very high wave numbers or frequencies. The spectrum in the dynamical systems studied to-date (e.g. the Lorenz equations⁹) tends to fill up at low (rather than high) frequencies by period-doubling or other similar mechanisms: i.e. the chaos is 'slow'.

(ii) In fluid flows, especially those that are open (e.g. boundary layers), the critical value of a control parameter like the Reynolds number at onset of turbulence is *not* unique (even for a given flow), but

depends strongly on environmental disturbance, levels¹⁰.

(iii) For values of the control parameter beyond the critical value, turbulence invariably persists in the flow, whereas in dynamical systems chaos and order often alternate in narrow windows, and indeed chaos eventually tends to disappear as the control parameter is increased (once again, the Lorenz system is a good example⁹).

The question that arises is whether the above criticisms apply only to systems considered to-date or whether other systems exist that more closely mimic the essential characteristics of 'strong' flow turbulence listed above. The present work is an attempt to devise the simplest possible systems that exhibit the generic behaviour of strong turbulence.

2. GENERAL CONSIDERATIONS

The idea underlying the present models is to treat turbulent flow as interaction between motions at different scales: the emphasis is not on any particular flow such as that over a flat plate or behind a cylinder, but rather on general physical arguments valid for a wide class of turbulent flows. For this purpose we divide spectral (or wave number) space into two broad regions, one where nonlinearity and external disturbances play the major role, representing the so-called large scale or large eddy motion, and the other where viscous dissipation is dominant, representing small or Kolmogorov scale motion. These two scales are coupled by a nonlinear energy transfer mechanism often called the cascade process, schematically illustrated in figure 1 (see e.g. discussion in reference 8).

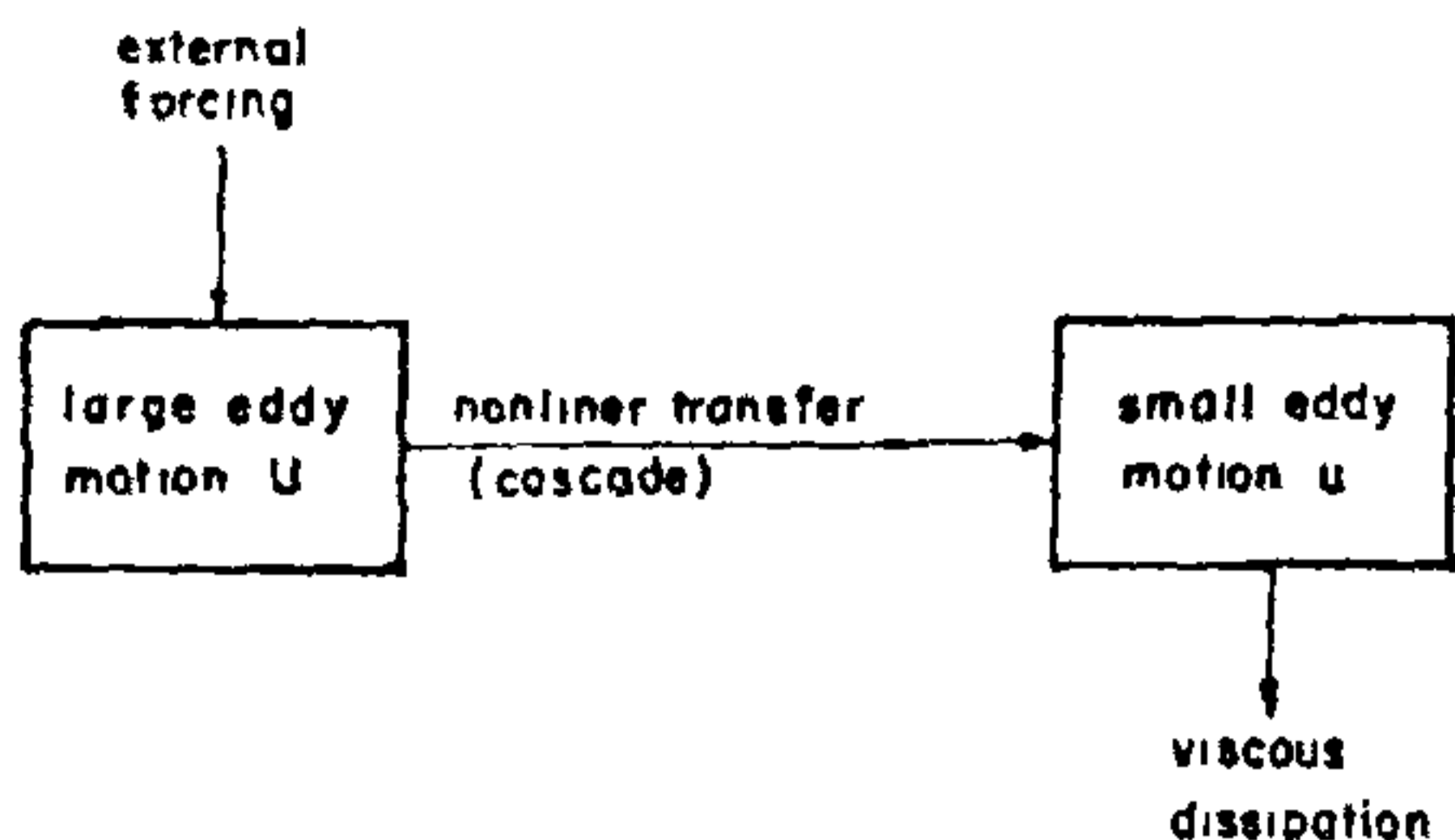


Figure 1. Schematic diagram of energy processes in a turbulent flow.

The first question to be faced is how many and what type of equations should be considered. Dynamical systems that exhibit chaos need at least three degrees of freedom. Since the presence of external disturbances is essential to reproduce (ii) above, their inclusion in the system provides one degree of freedom. The simplest system for our purpose would then consist of two coupled nonlinear ordinary differential equations subject to forcing. Referring to figure 1, we introduce two variables U and u , representing respectively large and small eddy variables. These variables may be thought of as representing slowly varying velocity amplitudes, the actual velocity being a linear combination like

$$aU(t)\exp i\omega_1 t + bu(t)\exp i(\omega_2 t + \phi), \quad (1)$$

where a and b are weighting functions representing the spread in wave number space of the concerned motions, and $\omega_1, \omega_2 (\gg \omega_1)$ are characteristic large and small eddy frequencies. In adopting this approach we make a significant departure from earlier studies, typified by the Lorenz system, where only the lowest few modes are selected for describing the dynamics.

Certain physical considerations may be used to suggest possible forms for the model. We propose that models that mimic turbulence should contain the following features.

(i) The large scale variable U must be governed by a control parameter that plays the role of Reynolds number (denoted by R say), whose variation changes overall system behaviour.

(ii) There must be a critical value R_c of this parameter such that for $R < R_c$ the motion is stable, and for $R > R_c$ the system exhibits linear instability.

(iii) For $R > R_c$, the growth of U because of linear instability will eventually be checked by nonlinearity and saturate at some finite maximum at high values of R .

(iv) The value of R at which onset of chaos will occur, say R_t , will in general be higher than R_c and depend on a forcing $q(t)$ (which may be deterministic).

(v) The small-eddy motion u will gain energy from the large-eddy motion U by nonlinear interaction.

(vi) Energy at the small scales is lost due to direct viscous action.

Several nonlinear models may be written down that are generally consistent with the features listed above. A typical form would be the following.

$$\begin{aligned} dU/dt = & \alpha(R) U & (U_{\max}^2(R) - U^2) \\ & \text{(linear instability)} & \text{(saturation)} \\ & -Ku^2 & + q(t) \\ & \text{(small-eddy damping)} & \text{(external disturbance)} \end{aligned} \quad (2)$$

$$\begin{aligned} du/dt = & kUu & + \varepsilon U & - \delta(R^*)u \\ & \text{gain from large eddies} & \text{large eddy forcing} & \text{viscous dissipation} \end{aligned} \quad (3)$$

Each of the terms here has the physical significance shown underneath. The second term in (2) represents the loss of large-eddy energy to small eddies. The second term in (3) ensures that large-eddy motion always forces *some* small-eddy motion [otherwise $u = 0$ would always be one solution of (3)]. In the last term represents viscous damping that depends on a *local* Reynolds number R_* , which has to be distinguished from the *large-scale* (or overall) Reynolds number R . As Kolmogorov scale motions always have a Reynolds number of order unity⁹, we expect $R_* = O(1)$.

We shall discuss two models belonging to this class, to explore whether such simple nonlinear dynamical systems can be constructed, following the above guidelines, to mimic the observed behaviour of open shear flows.

3. SYSTEM 1

The equations proposed here are

$$dU/dt = U(1 - \nu - U^2) - Ku^2 + q(t), \quad (4)$$

$$du/dt = kU(u + \varepsilon) - \nu_* u, \quad (5)$$

where k and K represent nonlinear transfer coefficients. The parameter ν in (4) plays the role of

viscosity or inverse Reynolds number. The first term in (4) is the nonlinear generation term which, for $\nu < 1$, enables U to grow when it is small but saturates it at a value that depends on ν . (Clearly $\nu = 1$ corresponds to the critical Reynolds number R_c .) For small ν , viscous dissipation in U will be negligible, and $\nu \rightarrow 0$ is like the limit Reynolds number $\rightarrow \infty$ in a flow. At the small scales, direct viscous dissipation is always dominant, so the parameter $\nu_* = O(1)$. To ensure that u will always be excited in the presence of large-eddy motion, a small multiple of U is included in (5) through the parameter ϵ .

Apart from forcing, the model has five parameters. To make things simpler we have put $k = K$ in all cases, but this assumption is not crucial as we shall show later. The parameter ϵ is assigned the small value of 0.05 in all the present computations. With these choices, only three parameters are left open, i.e. ν , ν_* and k .

Extensive exploratory numerical studies using the integration code given in ref. 11 have been made of the nature of the solutions of the system as the major control parameter ν is varied for different combinations of k and ν_* ¹². It has been found that, to preserve the general character of the solutions, in particular in the all-important "high Reynolds number" limit $\nu \rightarrow 0$ mentioned in (iii) of § 1, a special relation between ν_* and k has to be obeyed. This relation is approximately given by

$$\nu_* = -0.050644 + 0.662272 k - 0.0367497 k^2 \tag{6}$$

for $1 \leq k \leq 3$,

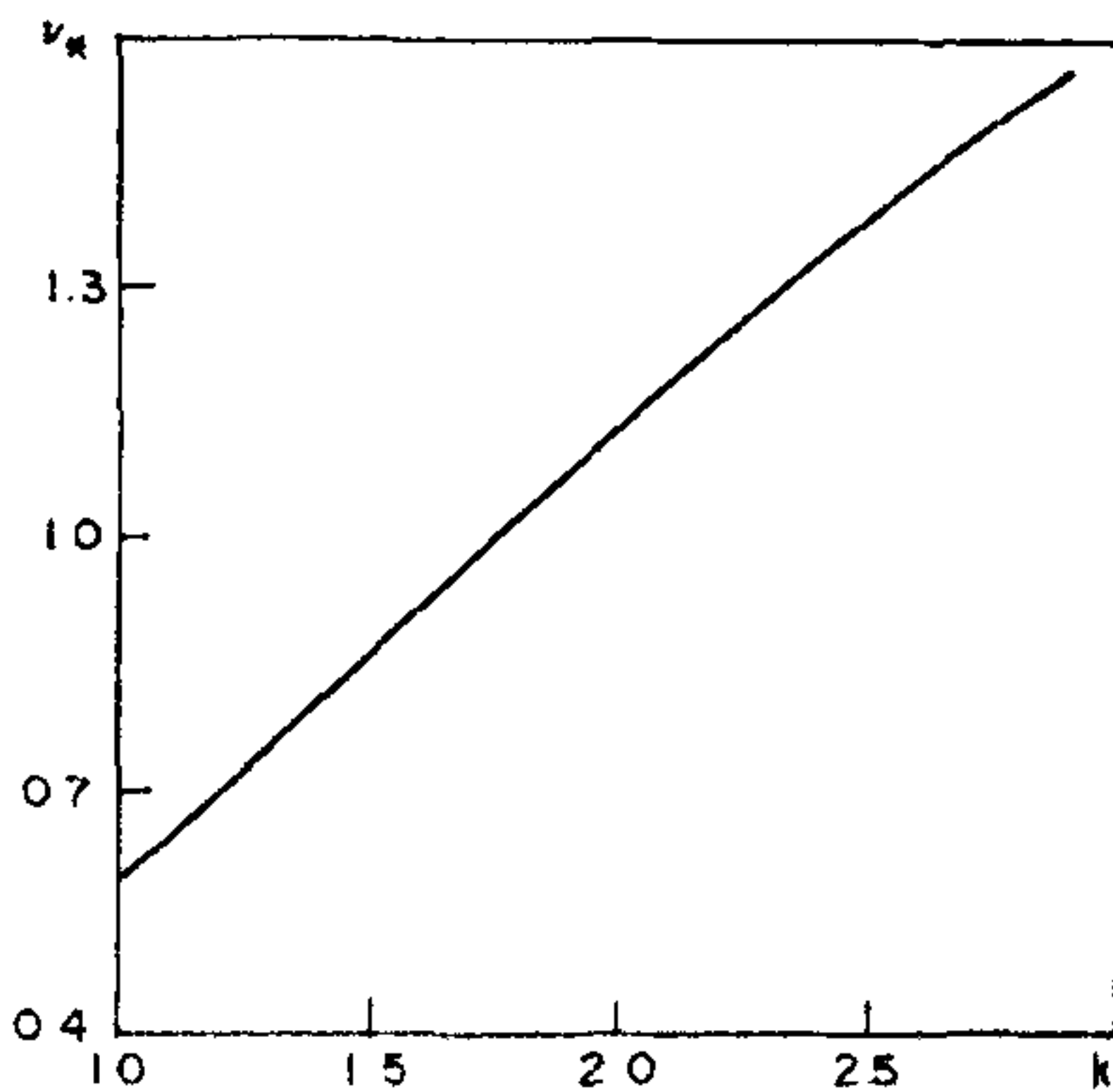


Figure 2. Relation between k and ν_* that preserves the general behaviour of Systems 1 and 2 in the limit of vanishing large scale viscosity.

and is shown in figure 2: its significance in terms of the singularities of the system will be discussed elsewhere. A relation of this type is not difficult to understand physically: a balance between k and ν_* ensures that dissipation equals energy transfer, which in the Kolmogorov theory of turbulence is achieved by an adjustment of the small scales of motion.

To give a feel for the nature of the solutions as the control parameter ν is varied, we now present some with $k = 2.3$ and $\nu_* \approx 1.28$ (these values being consistent with (6)). External forcing is taken to be periodic with

$$q(t) = \bar{q} \cos \omega t. \tag{7}$$

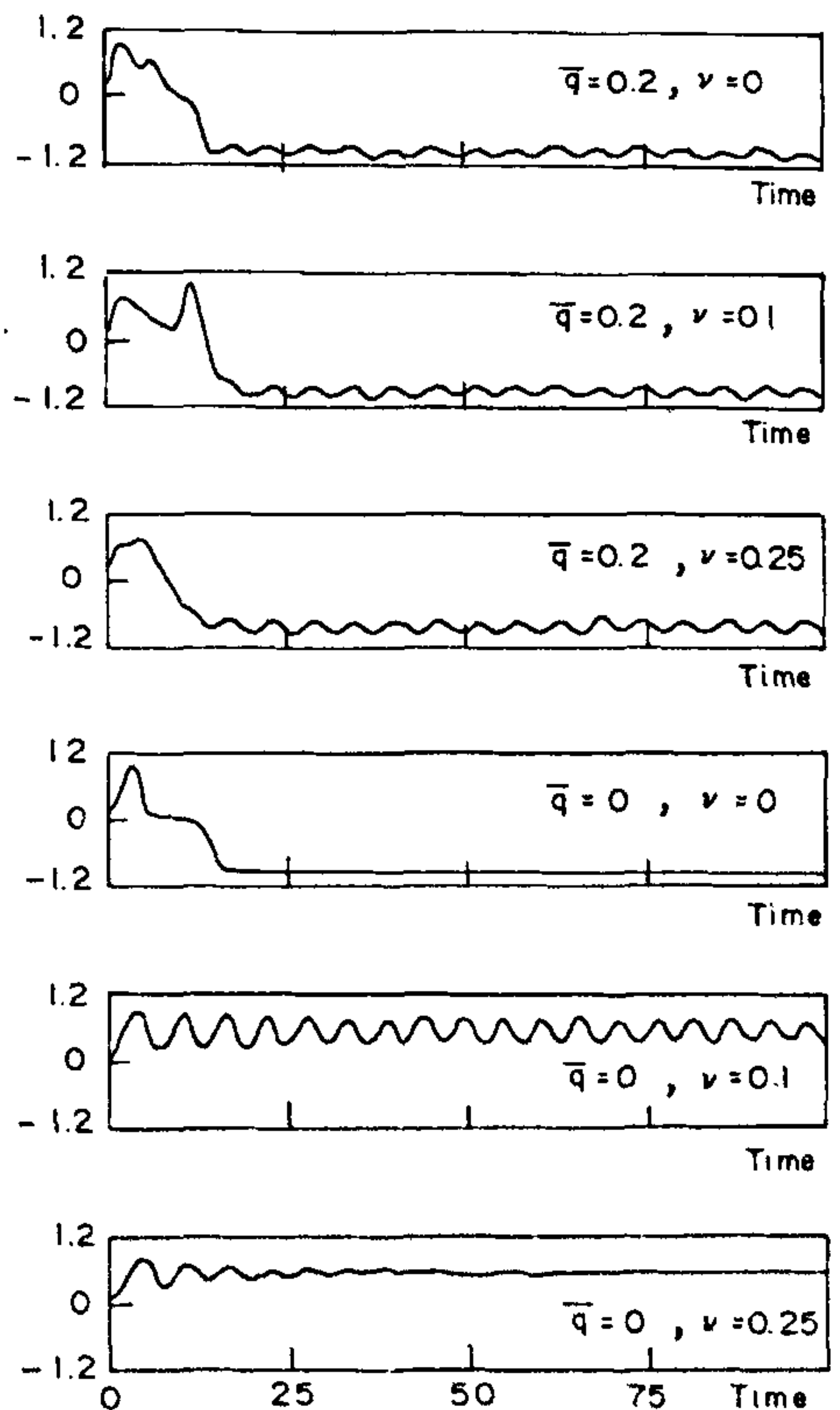


Figure 3. U component of typical unforced and forced solutions of System 1 as the control parameter ν is changed. Other parameters are $k = 2.3$, $\epsilon = 0.05$, $\nu_* = 1.27956$, $\omega = 1.1$. Note that eventually all forced solutions oscillate with negative amplitudes.

Figure 3 shows time traces of U with and without external forcing. Unforced solutions tend to be steady but non-zero when ν is relatively large. As ν decreases, the system shows continuous oscillations of increasing amplitude. However, for values of ν very close to 0, most solutions eventually tend to a steady (negative) state. When a small forcing is applied, the long time behaviour of most solutions is a forced periodic oscillation, with U remaining negative (especially for $q \leq 0.3$). However, with non-negative forcing of large amplitude, it is possible to get chaotic solutions¹². The system however does not have the desirable property that forcing should trigger an inherent instability in it. For this reason further studies of the properties of System 1 are not described here.

4. SYSTEM 2

The equations considered here are

$$dU/dt = U(1 - \nu - U^2) - Ku|u| + q(t), \quad (8)$$

$$du/dt = kU(|u| + \varepsilon) - \nu_* u. \quad (9)$$

Note the great similarity to System 1: the only difference is that the absolute value sign has been introduced at two places; this permits nonlinear energy transfer from large to small eddies and vice versa, depending on the sign of U and u . (It may be noted here that in spite of the cascade process already mentioned, no unique direction for turbulent energy transfer in spectral space can be proved⁸: it is likely that while such energy transfer can and does take place in both directions, that from low to high wave numbers is in general dominant.) Otherwise the meaning of different terms and parameters in (8), (9) remains the same as in (4), (5), and as before we have assumed $k = K$ and $\varepsilon = 0.05$.

Also, as before, we fix the values $k = 2.3$, $\nu_* = 1.28$, and take the external forcing to be periodic. Figure 4 shows typical unforced and forced solutions. For $\nu > 0.125$, the unforced solutions are fixed points, and for $\nu < 0.12$ they are continuous oscillations (limit cycles), whose amplitude increases as $\nu \rightarrow 0$.

The nature of the forced solutions depends upon ν , \bar{q} and ω . When ν is not very small (e.g. 0.25) only periodic solutions are obtained for small forcing amplitudes. As ν decreases, the system becomes sensitive to the forcing and chaotic-looking solutions are obtained. The presence of chaos is inferred in the present work by (a) the appearance of non-repeating time series (visual observation), (b) de-

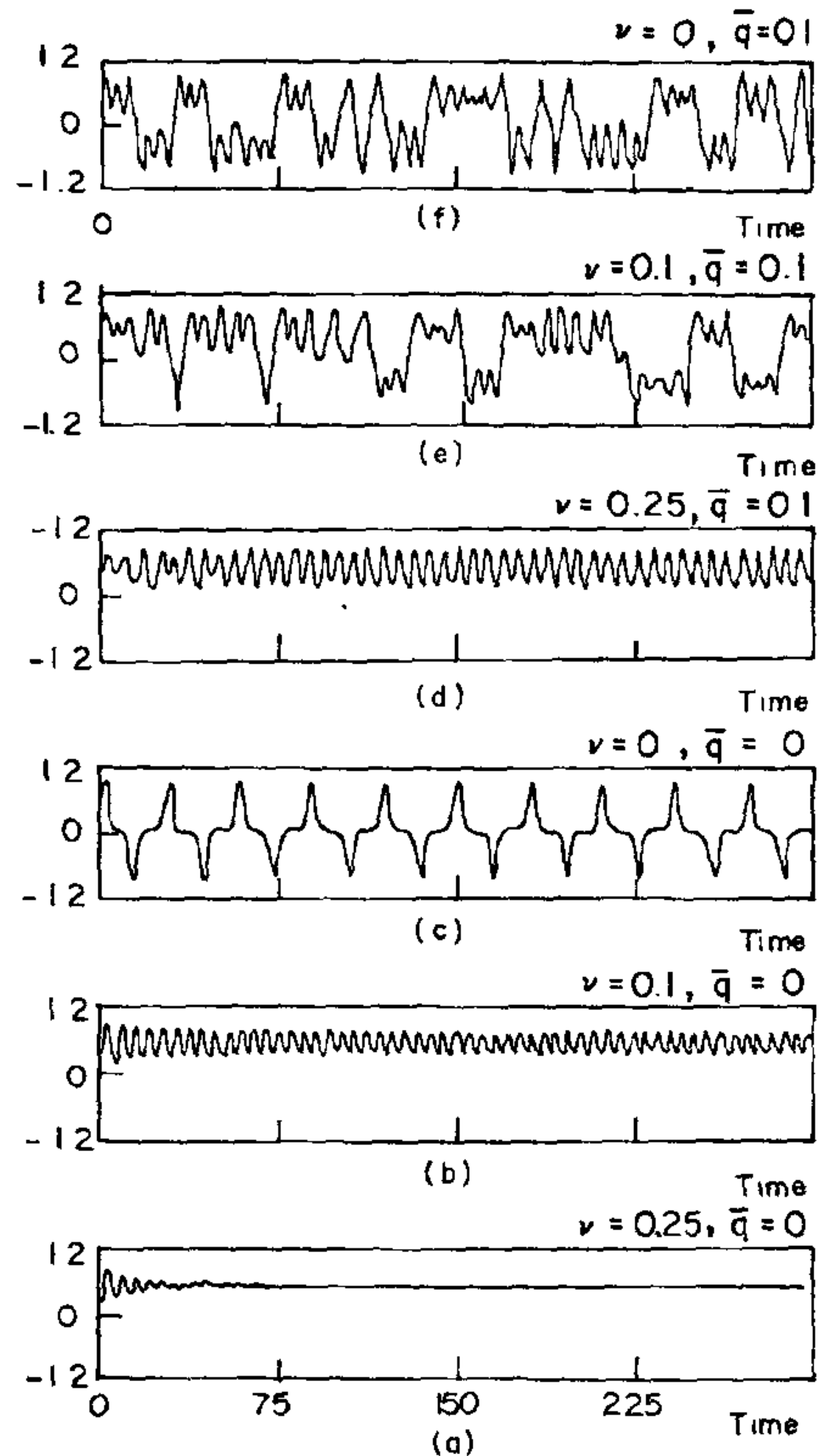


Figure 4. U component of typical unforced and forced solutions of System 2 as the control parameter ν is varied. Other parameters are, $k = 2.3$, $\varepsilon = 0.05$, $\nu_* = 1.27956$, $\omega = 1.0$. At $\nu = 0.25$ forced solution is periodic while for $\nu = 0.1$ and 0, solutions appear random.

caying correlation coefficients for large time lags, and (c) wide-band spectra. From figure 4, it is seen that the forced solutions at $\nu = 0.1$ and $\nu = 0$ appear to be nonrepeating, indicating chaos. The increasing sensitiveness of the system response to external forcing as $\nu \rightarrow 0$ is brought out more clearly in figure 5 where the correlation coefficients for $\nu = 0$ and $\nu = 0.1$ are plotted. The unforced solutions show a correlation coefficient that returns to unity periodically, indicating strong periodicity. The forced solutions show a decaying correlation coefficient depending upon ν and \bar{q} . While the system is chaotic at $\bar{q} = 0.0025$ when $\nu = 0$, it requires

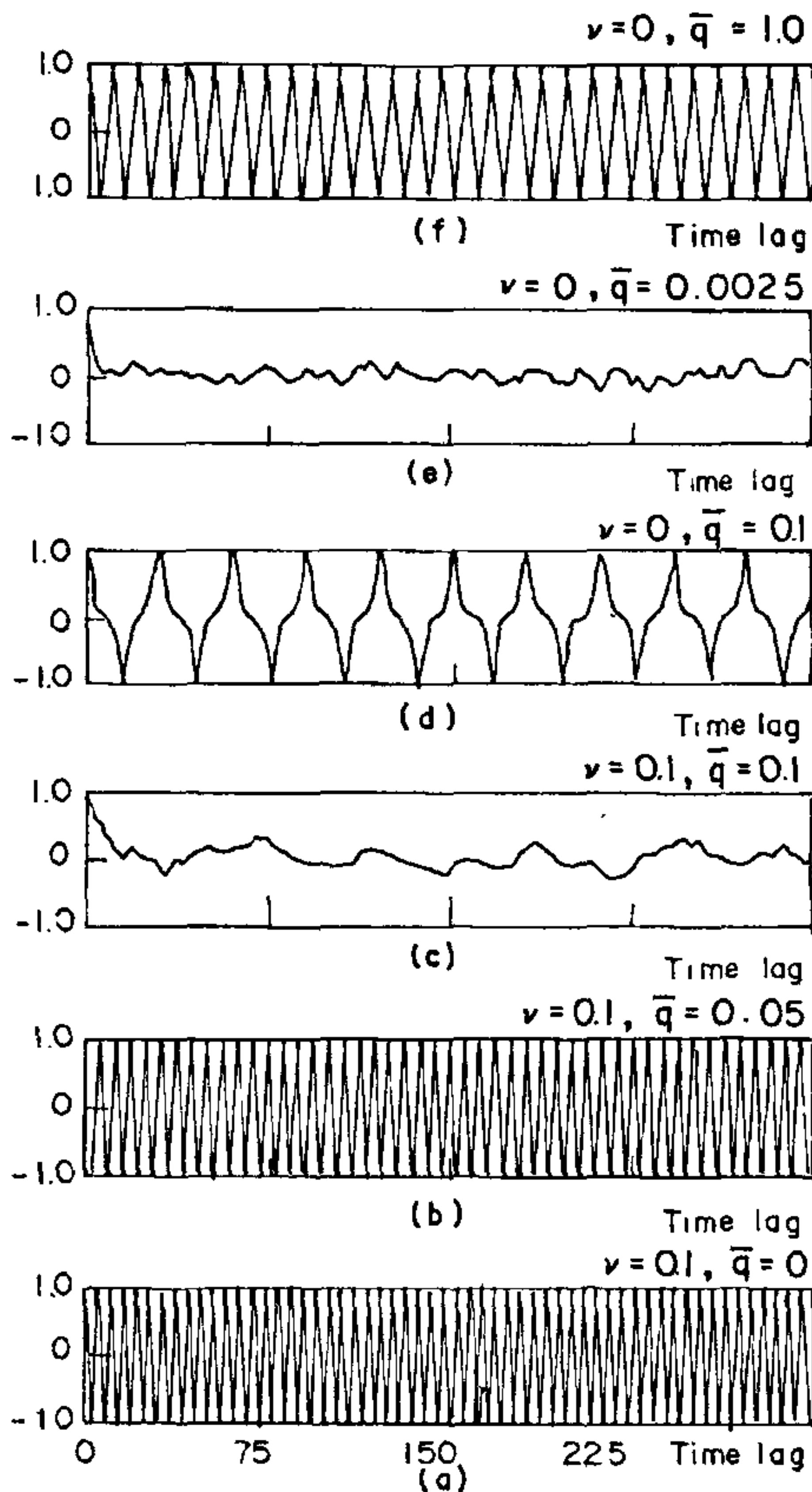


Figure 5. Autocorrelation coefficient of U of System 2 with changing ν and forcing. Fixed parameters are $k = 2.3$, $\epsilon = 0.05$, $\nu_* = 1.27956$. For $\nu = 0.1$, $\omega = 1.0$ and for $\nu = 0$, $\omega = 3.0$. Autocorrelation coefficient returning to unity means strong periodicity; rapid decay in (c) and (e) implies chaotic behaviour. Note (e) is chaotic at very small forcing amplitude.

$\bar{q} > 0.05$ when $\nu = 0.1$. Figure 5 also shows that at $\bar{q} = 1$, the solution is again periodic but now at the forcing frequency; this seems to be true for sufficiently high forcing at all ν . A point to which attention must be drawn is that the forcing frequencies used are different for $\nu = 0$ and 0.1. It was found that the sensitivity of the system varies with forcing frequency for any ν ; the values selected here are in the frequency bands to which the system is most sensitive.

Figure 6 shows spectra for two cases. Periodic

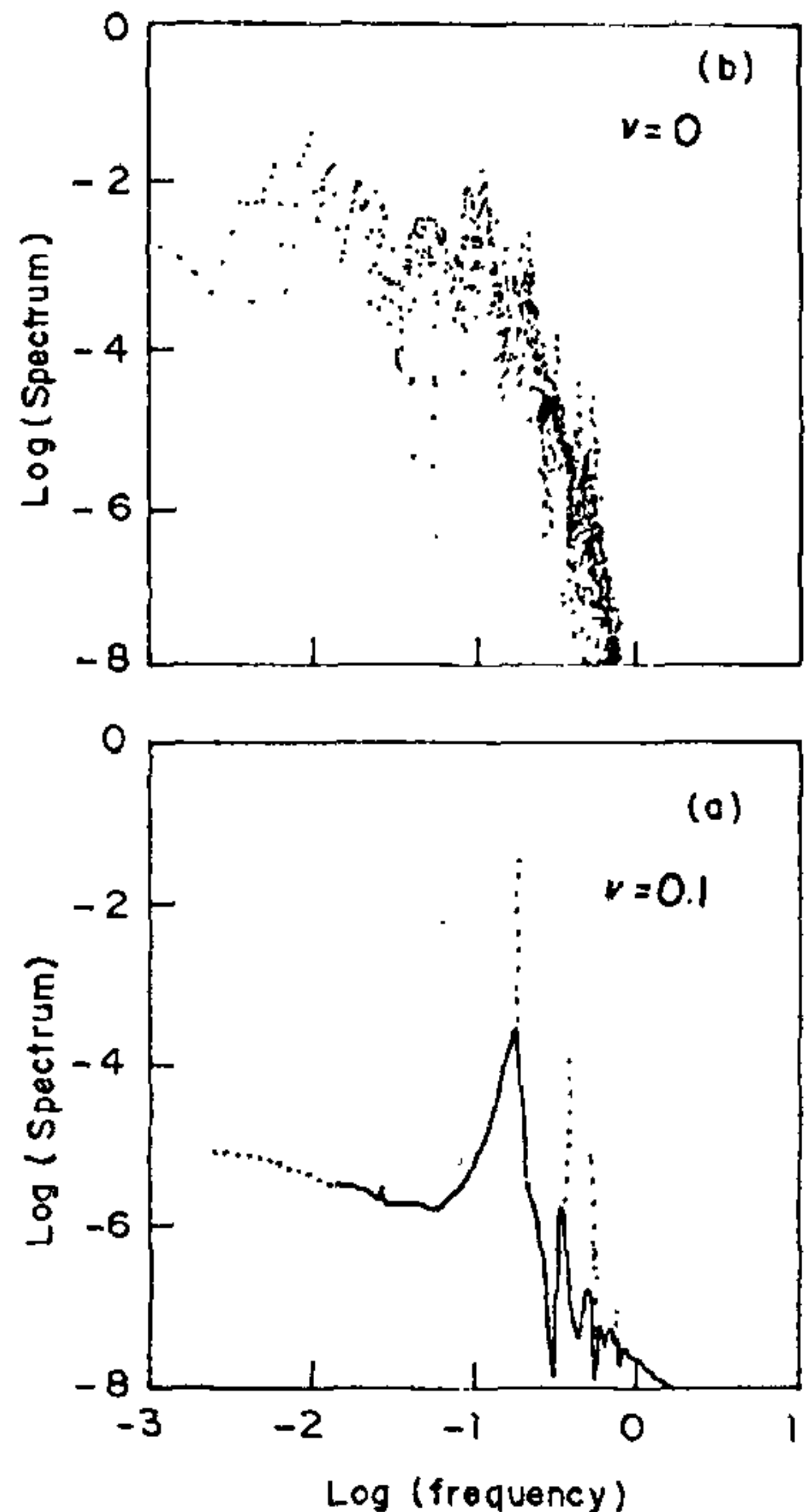


Figure 6. Spectra of U of System 2. Number of data points used is 4096 at a sampling time of 0.2. Parameters are, $k = 2.3$, $\epsilon = 0.05$, $\nu_* = 1.27956$, $\bar{q} = 0.01$, $\omega = 3.4$. While (a) shows narrow peaks (b) has wide-band spectrum indicating chaotic behaviour.

solutions are characterized by narrow band spectra while chaotic solutions show broad-band spectra.

By varying q for a given ν , it is possible to map the boundary between regular and chaotic behaviour. Such a boundary, determined from examination of time traces, correlations and spectra of U , is shown in figure 7. An important feature of this diagram is that as $\nu \rightarrow 0$, the system becomes increasingly sensitive to external disturbances, and even a very small disturbance is enough to induce chaos. As ν increases, larger forces are required to trigger chaos, and there is a limit ($\nu \sim 0.7$, not shown in the figure) beyond which there is no chaos at any forcing amplitude and the system is in forced oscillation. This behaviour is similar to the dependence of flow type on Reynolds number familiar in fluid mechanics¹⁰.

A more detailed mathematical study of System 2 will be reported separately.

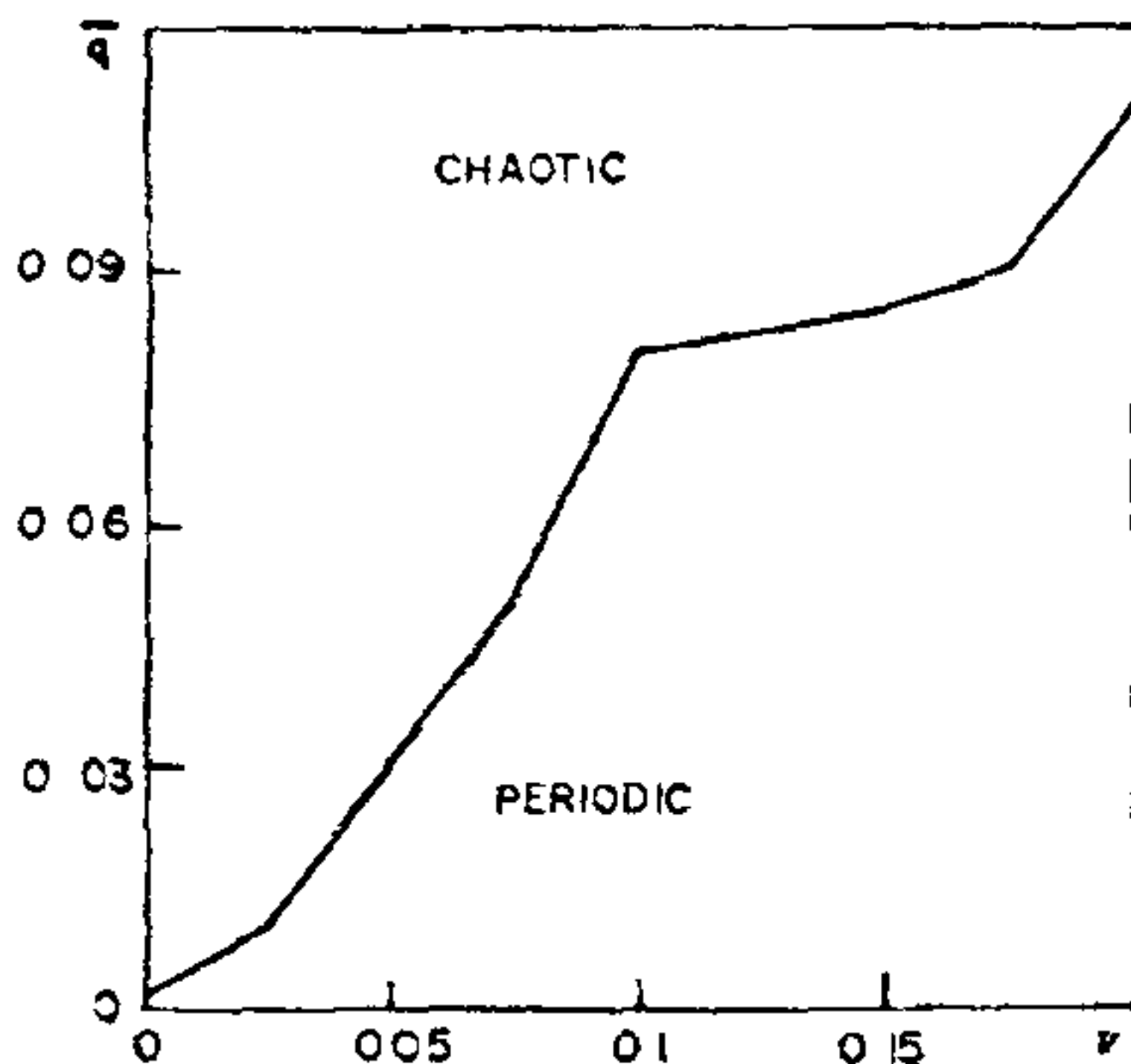


Figure 7. Rough boundary separating periodic from chaotic regimes. Other parameters are $k = 2.3$, $\epsilon = 0.05$, $\nu_* = 1.27956$.

We conclude by showing, in figure 8, typical samples of the complete velocity traces from a linear combination of large- and small-eddy motions as in (i); the resemblance to velocity fluctuations in turbulent flow is evident.

CONCLUSIONS

We report here a new nonlinear dynamical system which has many properties characteristic of open shear flows. Chaos in this system is triggered by

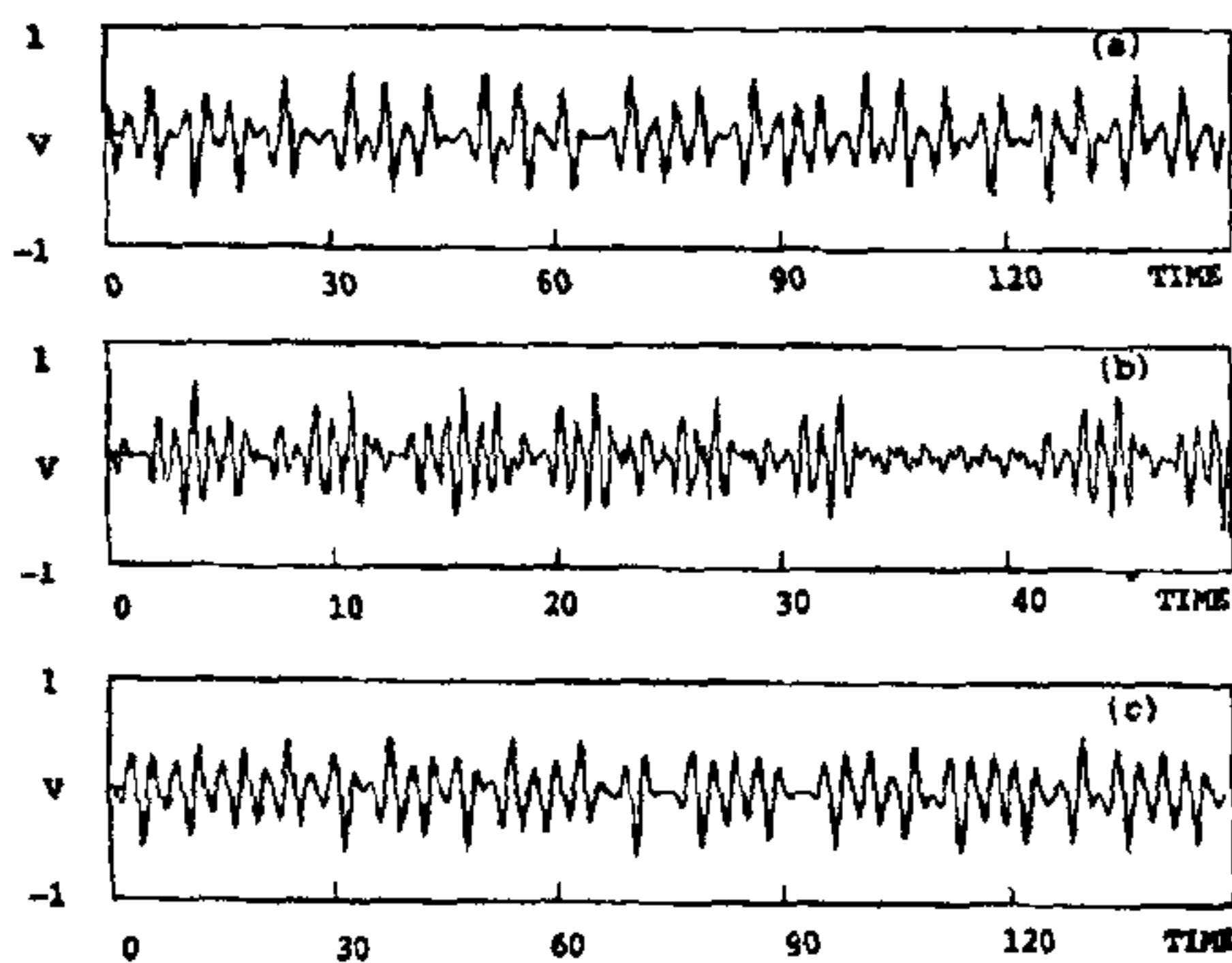


Figure 8. Three examples of actual velocity traces using a linear combination of large- and small-eddy motions as in (1), with $a = 0.5$, $b = 0.25$, $\omega_2 = \sqrt{11001.19}$. (a) $\nu = 0$, $\omega = 1$, $\bar{q} = 0.1$; $\omega_1 = 2.1$. (b) $\nu = 0$, $\omega = 3.5$, $\bar{q} = 1$; $\omega_1 = 8.1$. (c) $\nu = 0.1$, $\omega = 1$, $\bar{q} = 0.1$; $\omega_1 = 2.1$.

(deterministic) forcing, whose values at onset of chaos decrease with a viscosity-like parameter in the model. This mimics the known dependence of Reynolds number on environmental disturbance in a boundary layer¹⁰. Furthermore, chaos persists as the viscosity tends to zero, i.e. in the high Reynolds limit. Extremely high forcing, however, produces forced oscillations. The model therefore promises to throw much light on the nature of transition and turbulence in open fluid flows, and may serve to establish stronger connections between dynamical chaos and flow turbulence.

ACKNOWLEDGEMENT

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SYNTHESIS AND ANTIMICROBIAL ACTIVITIES OF SOME NEW 4-ARYLAMINO ISOXAZOLO [5,4-d] PYRIMIDINE DERIVATIVES

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ABSTRACT

Twentyone new substituted arylamino isoxazolo [5,4-d] pyrimidines have been synthesized from (un)substituted benzaldehydes. The structures of these compounds have been established by elemental and spectral analyses. The compounds were subjected to *in vitro* antibacterial screening against pathogenic strains and antifungal testing against fungi. Some of the compounds exhibit promising results.

INTRODUCTION

ISOXAZOLO [5,4-d] pyrimidine derivatives have been reported to exhibit antibacterial^{1,2}, miticidal³ and analgesic⁴ activities. As anilino group is an important pharmacophore in many antimalarials⁵, antimycobacterial⁶, antibacterial⁷⁻⁹ and antifungal¹⁰ agents, a series of new 4-arylamino-3-substituted isoxazolo [5,4-d] pyrimidines have been synthesized. It is hoped the presence of arylamino moiety in this class of compounds might give improved therapeutic results. The new compounds were evaluated for antibacterial and antifungal activity using standard methods.

MATERIALS AND METHODS

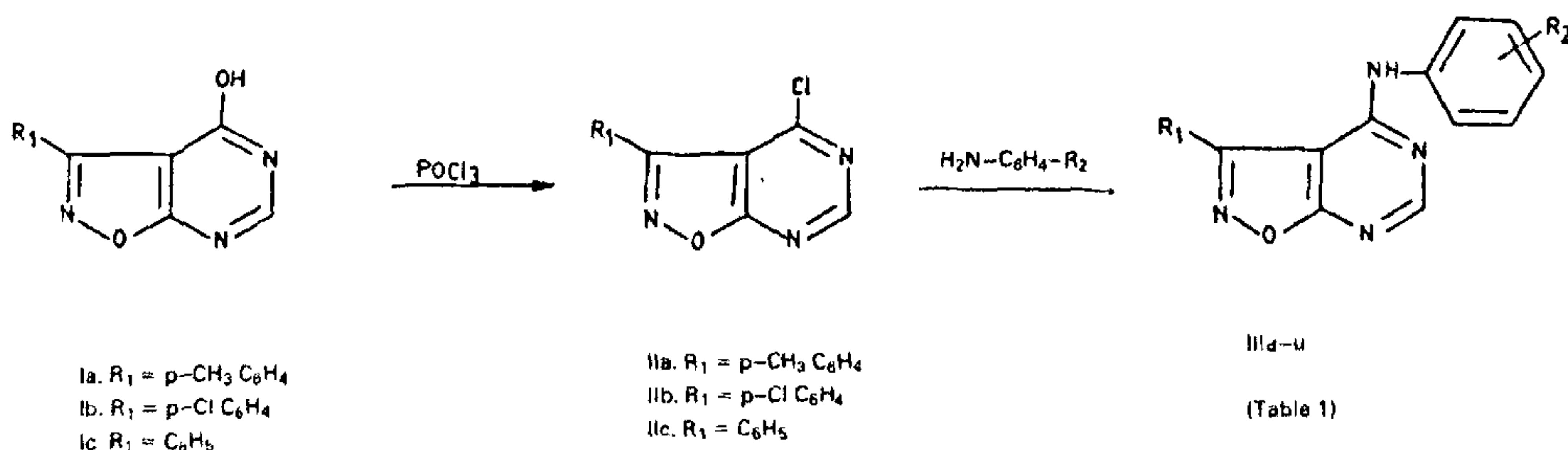
The compounds were synthesized as shown in scheme 1.

The required 4-hydroxy-3-substituted isoxazolo [5,4-d]-pyrimidines (I) were synthesized from (un)-substituted benzaldehydes by the reported procedures¹¹⁻¹³ and converted to 4-chloro-3-substituted isoxazolo [5,4-d] pyrimidines (II) by refluxing them in excess of phosphorus oxychloride. The

compounds were synthesized by heating a suspension of II and arylamine in ethanol under reflux temperature for 3-4 h. Their characterization data are summarized in table 1. The structures of new compounds have been authentically established by their correct elemental analyses and spectral studies. All the compounds were evaluated for *in vitro* antibacterial activity against five pathogenic microorganisms viz. *Escherichia coli*, *Proteus vulgaris*, *Proteus aurigasa*, *Klebsiella pneumoniae* (all gram-negative) and *Staphylococcus aureus* (gram-positive) by the disc diffusion method^{14,15}. They were also subjected to antifungal screening against three fungi viz. *Aspergillus niger*, *Candida albicans* and *Aspergillus flavus* by turbidity method¹⁶. The results, subjectively graded, are presented in table 2 along with results obtained for standards i.e. sulphanylamide and phenol in antibacterial screening and salicylic acid in antifungal testing.

RESULTS AND DISCUSSION

The formation of 4-(*p*-acetylphenylamino)-3-*p*-chlorophenylisoxazolo [5,4-d] pyrimidine (III m) from the corresponding 4-chloro derivative was



Scheme 1.