Monograph:

Jones, R.P. and Owens, D.H. (1980) Linearly Constrained Quadratic Optimisation with Application to Time Delay Systems. Research Report. ACSE Research Report no 125 . Department of Control Engineering, University of Sheffeld, Mappin Street, Sheffield S13JD

Progress in the Dynamic Analysis of

Symmetrical Packed Distillation Column

by

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Research Report No. 107

January 1980

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ABSTRACT

This work is an extension to previous team work carried out on modelling of packed distillation columns, headed by J.B. Edwards (1) in which the author was a team member and had taken part in development of the model. In this work a close examination of the model input-output stability has been made and some of the remarks made in (1) based on open-loop input-output stability assumptions are asserted. The results of computer programmes developed for time simulation and Nyquist diagrams are also examined and their agreement with theoretical deductions checked.

1. Introduction

The model partial differential equations and the equations of boundary conditions for the case studied in (1) are as follows

$$\dot{y} = y_e - y - \frac{\partial y}{\partial h} - \frac{G}{V} v$$

$$\dot{y}_e = - y_e + y + \frac{\partial y_e}{\partial h} + \frac{\alpha G \ell}{V}$$

$$\dot{x}'_e = x' - x'_e - \frac{\partial x'_e}{\partial h} - \frac{\alpha G}{V} v \qquad \text{system partial differential equations}$$

$$\dot{x}' = - x' + x'_e + \frac{\partial x'}{\partial h} + \frac{G\ell}{V} \tag{1.1}$$

$$y(o) = x'_e(o) - \frac{\varepsilon}{2}\frac{Gv}{V}$$

feed boundary conditions

$$x'(o) = y_e(o) + \frac{\varepsilon}{2}\frac{G\ell}{V} \tag{1.2}$$

$$\alpha T\, \dot{y}_e(L) = y(L) - \alpha y_e(L)$$

top and bottom boundary conditions

$$\alpha T\, \dot{x}'_e(-L) = x'(-L) - \alpha x'_e(-L) \tag{1.3}$$

These equations using the concept of inverted u tube (i.e. conceptually bending the process into the form of an inverted u-tube and redefining the origin of h now at the reboiler) and defining the following vectors

$$\underline{q} = \begin{pmatrix} y - x' \\ y + x' \end{pmatrix}, \quad \underline{r} = \begin{pmatrix} y_e - x'_e \\ y_e + x'_e \end{pmatrix} \quad \text{and } \underline{u} = \frac{G}{V}\begin{pmatrix} v + \ell \\ v - \ell \end{pmatrix}$$

can now be solved for either of $\underline{q}$ or $\underline{r}$. Anticipating feedback control from $y(o)$ and $x'(o)$, which excludes involvement of terminal capacitances within the control loop, attention was focused on vector $\underline{q}(o,p)$. The solution is as follows:

$$\tilde{q}_1(o,p) = \frac{\{(\alpha-1)(\cosh qL-1)p^{-1}-(1+\alpha)(\sinh qL)q^{-1} - \varepsilon/2\}}{\{(1-h_e\alpha^{-1})(\sinh(qL))qp^{-1}+(1+h_e\alpha^{-1})\cosh(qL)\}}\tilde{u}_1(p) \tag{1.4}$$

$$\tilde{q}_2(o,p) = \frac{\{(\alpha-1)p(\cosh qL-1)q^{-2}-(\alpha+1)(\sinh(qL))q^{-1} - \varepsilon/2\}}{\{(1+h_e\alpha^{-1})(\sinh qL)pq^{-1}+(1-h_e\alpha)^{-1}\cosh qL\}}\tilde{u}_2(p) \tag{1.5}$$

The steady state values of Equations (1.4) and (1.5) for step perturbations of magnitude u_1 and u_2 are

$$q_1(o,o) = \frac{\alpha\{(\alpha-1)L^2 - (\alpha+1)L - \varepsilon/2\}}{2(\alpha-1)L + \alpha + 1} u_1 \tag{1.6}$$

$$q_2(o,o) = -\frac{\alpha\{(\alpha+1)L + \varepsilon/2\}}{(\alpha-1)} u_2 \tag{1.7}$$

2. Open-loop Input-output stability

A test for the system input-output stability is fundamental before transient behaviour of the system to step inputs is simulated on the digital computer. This avoids the confusion between the instability of the system of partial differential equations together with their boundary conditions and their assumed equivalent lumped parameter system of ordinary differential equations, assuming that for the numerical method chosen the criteria for numerical stability is well established. Also since the transfer functions of both $\tilde{q}_1$ and $\tilde{q}_2$ are irrational, Nyquist criterion can be applied to derive the conditions for input-output stability of feedback systems if the open-loop transfer function has no singularities in the closed right half complex-plane* (2). The conventional methods like, Routh-Hurwitz etc. are only for rational transfer functions and cannot be used for this test. Based on modern concepts of mathematics a few input-output stability criteria has, in recent years, been established for fairly general systems, but just to check if the system under study possesses the requirements of any of these criteria and to apply them requires a good background of the mathematics involved in them. Instead the following method was chosen, which seems to fit better in the style of this work. Let us consider the denominator of $\tilde{q}_1(o,p)$ and investigate the possibility of a value for p in the closed right half-complex-plane satisfying it. If so then for the value of p

$$\tanh\,(qL) + \frac{p}{q} \cdot \frac{Tp + (1 + \alpha^{-1})}{Tp + (1 - \alpha^{-1})} = 0 \tag{2.1}$$

Consider the variable $q = \sqrt{p^2 + 2p}$ first. It can easily be shown that the roots of any complex number are obtained from the following formula.

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* then the mapping lemma remains valid for irrational transfer functions

$$\sqrt{u_r + jv_r} = X + jY$$

where
$$X = \pm\sqrt{\frac{u_r + u_r + jv_r}{2}} \tag{2.2}$$

$$Y = \frac{v_r}{2X} \tag{2.3}$$

the two roots are of opposite sign. This could also be deduced from the following formula for the roots of complex numbers based on de Moivre's Theorem (3)

$$Z^{1/n} = r^{1/n}\left\{\cos\left(\frac{\theta + 2\pi k}{n}\right) + i\sin\left(\frac{\theta + 2\pi k}{n}\right)\right\}$$

$$k = 0, 1, \ldots, n-1$$

However, in the derivation of transfer functions of q_1 and q_2 in (1), the +ve root of $p^2 + 2p$ **was denoted** q, and therefore here in equation (2.2) only the + ve sign is considered. Since p is the closed right half-complex-plane it must be of the form $p = x_r \pm jy_r$ where x_r and y_r are +ve real figures. Then

$$q = \sqrt{p^2 + 2p} = \sqrt{\underbrace{x_r^2 - y_r^2 + 2x_r}_{u_r} + j\underbrace{\pm 2y_r(x_r + 1)}_{v_r}} \tag{2.4}$$

From equations (2.2) and (2.3) it is evident that when

$p = x_r + jy_r$ $\qquad X > 0$ and $Y > 0$

and when

$p = x_r - jy_r$ $\qquad X > 0$ and $Y < 0$

Therefore the real and imaginary parts of q have the same sign as those of p at all times. Consider now the case when $p = x_r + jy_r$. Let $x_1 = x_r + \frac{1+\alpha^{-1}}{T}$ and $x_2 = x_r + \frac{1-\alpha^{-1}}{T}$ whence $x_1 > x_2$. Substitute for p, q, x_1 and x_2 in the second term of Equation (2.1) i.e.

$$\frac{Tp + (1+\alpha^{-1})}{Tp + (1-\alpha)^{-1}} \cdot \frac{p}{q} = \frac{p + \frac{1+\alpha^{-1}}{T}}{p + \frac{1-\alpha^{-1}}{T}} \cdot \frac{p}{q} \tag{2.5}$$

Then will have the expression

$$\frac{x_1 + jy_r}{x_2 + jy_r} \cdot \frac{x_r + jy_r}{X + jY} = \frac{(x_1 + jy_r)(x_2 - jy_r)}{x_2^2 + y_r^2} \cdot \frac{(x_r + jy_r)(X - jY)}{X^2 + Y^2} \tag{2.6}$$

$$= \frac{\left[(x_1x_2 + y_r^2) - j(x_1 - x_2)y_r\right]}{x_2^2 + y_r^2} \cdot \frac{\left[x_rX + y_rY) + j(y_rX - x_rY)\right]}{X^2 + Y^2}$$

where $y_r X - x_r Y > 0$ since from (2.3) and (2.2)

$$y_r X - x_r Y = y_r X - \frac{x_r y_r (x_r + 1)}{X} = \frac{y_r}{X} \cdot \left[X^2 - x_r (x_r + 1)\right]$$

$$= \frac{y_r}{2X} \left[- x_r^2 - y_r^2 + \sqrt{(x_r^2 + y_r^2)^2 + 4(x_r + 1)\ (x_r^2 + y_r^2)}\right] \qquad (2.7)$$

clearly (2.7) is a + ve value and hence from (2.6) it is evident that the real part of equation (2.5) is always + ve. Now if p were of the form $x_r - jy_r$, then substituting for p,q, x_1 and x_2 in (2.5) will have

$$\frac{x_1 - jy_r}{x_2 - jy_r} \cdot \frac{x_r - jy_r}{X - jY} = \frac{(x_1 - jy_r)(x_2 + jy_r)}{x_2^2 + y_r^2} \cdot \frac{(x_r - jy_r)(X + jY)}{X^2 + Y^2}$$

$$= \frac{\left[(x_1 x_2 + y_r^2) + j(x_1 - x_2)y_r\right]}{x_2^2 + y_r^2} \cdot \frac{\left[(x_r X + y_r Y) + j(x_r Y - y_r X)\right]}{X^2 + Y^2}$$

where $x_r Y - y_r X = - \left[y_r X - x_r Y\right]$ and from (2.7) it must be -ve and therefore again the real part of (2.5) will always remain +ve.

Now let $q = \rho e^{j\beta}$ and examine $\tanh \frac{qL}{2}$

$$\tan \frac{qL}{2} = \frac{1 - e^{-qL}}{1 + e^{-qL}} = \frac{1 - e^{-\rho L\cos\beta}\left[\cos(\rho L \sin\beta) - j \sin(\rho L \sin\beta)\right]}{1 + e^{-\rho L\cos\beta}\left[\cos(\rho L \sin\beta) - j \sin(\rho L \sin\beta)\right]}$$

$$= \frac{1 - e^{-2\rho L\cos\beta} + j2e^{-\rho L\cos\beta}\sin(\rho L \sin\beta)}{1 + e^{-2\rho L\cos\beta} + 2e^{-\rho L\cos\beta}\cos(\rho L \sin\beta)} \qquad (2.8)$$

If the denominator of the above equation is set equal to zero we will have

$$\cos(\rho L \sin\beta) = - \cos h\,(\rho L \cos\beta)$$

The above equality is impossible unless $\beta = \frac{\pi}{2}$ or $- \frac{\pi}{2}$, since only at these values with coth $(\rho L\cos\beta)$ is at its minimum value 1. However β cannot assume the values $\frac{\pi}{2}$ and $- \frac{\pi}{2}$ since then $q = \pm jY$ and X is equal to zero. But for X to be zero from (2.2), we will have

$$u_r < 0 \text{ and } v_r = 0 \qquad (2.9)$$

From (2.4), $v_r = \pm 2y_r(x_r + 1)$ and it can only be zero when $y_r = 0$ in which case $u_r = x_r^2 + 2x_r$ and is always + ve. Therefore the conditions (2.9) will not be met and since the real and imaginary parts of q always have the same sign as those of p,

$$-\frac{\pi}{2} < \beta < \frac{\pi}{2} \tag{2.10}$$

and it is also deduced that the denominator of (2.8) cannot become zero and so it must always be either +ve or -ve. Evaluating its value for any value of p, β and L reveals that it must always be a +ve value. Therefore from (2.8) it is evident that the real part of $\tanh\frac{qL}{2}$ is always +ve and will not vanish to zero. Clearly tanqL in (2.1) will also be the same and hence both terms of (2.1) will always have +ve real parts for values of p in the closed-right-half-complex plane with the real part of tanhqL never vanishing to zero. Therefore (2.1) shall never be possible and $\tilde{q}_1(o,p)$ is open-loop input-output stable. Evidently similar argument is possible for input-output stability of $\tilde{q}_2(o,p)$.

3. Digital Simulation of Transient Response to Step Inputs

There are a number of methods, available to choose for the digital simulation of the system, equations (1.1), each having certain advantages and drawbacks. The simplest method to program is to approximate space and time derivatives of the dependent variables by a simple forward or backward finit difference. That is to assume for example that

$$\left.\frac{\partial y}{\partial h}\right|_h = \frac{y|_{h+\Delta h} - y|_h}{\Delta h} \quad \text{or} = \frac{y|_h - y|_{h-\Delta h}}{\Delta h}$$

However, the nature of boundary conditions (1.2) and (1.3) dictates that time integration of dependent variables in each section of the column may not be performed simultaneously and only after the process of integration of one variable has proceeded from one end of the section to the other, integration of another variable can be started. This feature, depending on the updating procedure taken offers a choice of layouts for integration passes and it is not easy to find a superiority for one layout over another. To avoid this situation after approximating the spatial derivatives, the resulting simultaneous first order equation together with the boundary conditions (1.2) and (1.3) were arranged in the form

$$\dot{\underline{X}} = \underline{A}\underline{X} + \underline{B}\underline{u}$$

where $\underline{A}$ and $\underline{B}$ are only arrays of constants. The state transition matrices of this linear first order equation is only time step dependent. That is

$$\underline{X}\ (t + \Delta t) = \underline{\phi}\ \underline{X(t)} + \underline{\Delta u}$$

Bearing this in mind $\underline{\phi}$ and $\underline{\Delta}$ were computed for a suitably small Δt and integration was progressed using the above formula. As it was discussed in (1) from (1.4) and (1.5), the initial rate of rise may be evaluated as

$$\lim_{t \to o} \dot{\underline{q}}(o,t) = \lim_{p \to \infty} \tilde{\underline{q}}(o,p) = - \underline{I}$$

Now equations (1.6) and (1.7) indicate that the steady state value of $q_2(o,t)$ is always negative, but that of $q_1(o,t)$ is only -ve for short columns and in the case of long columns it may be positive. Therefore the response of $q_1(o,t)$ to step perturbations should behave in a non-monotonic manner. This is the case when $q_1(o,t)$ is non-minimum phase. The complete characterization of non-minimum phase responses in time domain is an unsolved problem (4). This behaviour of $q_1(o,t)$ will be asserted in section 5. The results of simulation for two typical cases of short and long columns are shown in Figure (1) to (4). It can be noticed that the long column has a considerably slower response compared with the short one.

4. Frequency Loci

As it was earlier remarked another benefit of open-loop input-output stability proof is the validity of Nyquist criterion for testing the input-output stability of the feedback system. The Nyquist diagrams are also of use for design of a reduced model to approximate that of the true system. As it will be proven in the followings these loci as p travels on its D contour, will encircle the origin infinitely in clockwise and counter-clockwise direction the net number being zero, due to the fact that the system is open-loop input-output stable. These encirclements impair the ease of establishing the non-minimum phase behaviour of $q_1(o,t)$ from the frequency loci. Equation (1.4) can be written in the form

$$\tilde{q}_1(o,p) = \frac{(\alpha-1)\tanh(\frac{qL}{2})p^{-1} - (1+\alpha)q^{-1} - \frac{\varepsilon}{2}\cdot\frac{1}{\sinh qL}}{(1-h_e\alpha^{-1})qp^{-1} + (1+h_e\alpha^{-1})\coth qL}$$

As $p = Re^{j\theta}$ assumes large values on the D contour ρ in $q = \rho e^{j\beta}$ will also become large in which case the limit of the above equation will become

$$\tilde{q}_1(o,p)_{p\to\infty} = -\frac{\varepsilon}{4}\cdot\frac{1}{\sinh qL} = -\frac{\varepsilon}{2}\cdot\frac{1}{e^{qL} - e^{-qL}}$$

As it was proven before $-\frac{\pi}{2} < \beta < \frac{\pi}{2}$, (2.10), hence the exponential with -ve exponent vanishes. For large values of p, $q = (p^2 + 2p)^{\frac{1}{2}}$ can, using the Binomial expansion be approximated to $q = p+1$ substituting this in the above relation will result in

$$\tilde{q}_1(o,p)_{p\to\infty} = -\frac{\varepsilon}{2}e^{-qL} = -\frac{\varepsilon}{2}e^{-(p+1)L} = -\frac{\varepsilon}{2}e^{-L}\cdot e^{-LR\cos\theta}\left[\cos(LR\sin\theta) - j\sin(LR\sin\theta)\right] \qquad (4.1)$$

From (4.1) it is clear that the Nyquist locus of $\tilde{q}_1(o,p)$ when p assumes values on the semi-circle of the D contour will encircle the orgine with a radius of $r \ll 1$ infinite number of times. Also when p travels along the imaginary axis, there will be infinite encirclements of the orgine after its value exceeds a certain amount. In this case $\theta = \frac{\pi}{2}$ or $-\frac{\pi}{2}$ and the radius of the limit encirclements is equal to

$$\frac{\varepsilon}{2}e^{-L} \qquad (4.2)$$

similar arguements apply to $q_2(o,p)$ which can easily be checked. Figures (5) to (15) show direct and inverse loci for the examples of section 3 . In Fig. (5) the size of the radius of encirclements is large enough for them to be clearly observed on the direct loci. From the inverse loci of Fig. (9) it may also be checked that the radius of encirclements has almost approached its limit value of 14.78 evaluated from (4.2). For the long column the radius of encirclements as may be seen from Fig. (10) are too small to be clearly seen in the direct plot. However, inverse loci of Fig. (11) offers a clear indication of existance of such encirclements. From Figs. (5),(6),(10) and (11) it can also be noted that the gain margin of long column is considerably smaller than that of short column, one of the limitations imposed by the undesirable non-minimum-phase effect. Figs. (12) to (15) show the direct and inverse loci of $\tilde{q}_2(o,p)$ for short and long columns which show that their closed loop systems have a very large gain margin.

5. Non-minimum-phase Behaviour

The following proof of existance of non-minimum-phase effect in $\tilde{q}_1(o,p)$ for long columns is another possibility, relying on the open-loop input-output stability. Since knowing this the transfer function of $\tilde{q}_1(o,p)$ can be written in the form

$$\tilde{q}_1(o,p) = \frac{K_1 N\tilde{q}_1}{\prod_{i=1}^{N} (\alpha_i + p)} \qquad 1 < N < \infty \tag{5.1}$$

where $N\tilde{q}_1$ is the numerator of $\tilde{q}_1(o,p)$ and α_i are finite positive real numbers or complex numbers with positive real part in which case for each factor $(\alpha_i + p)$ there should be another factor $(\alpha_j + p)$ with α_j equal to conjugate of α_i, since complex roots can only exist as conjugate pairs. Now $N\tilde{q}_1$ cannot also be written in this way since if this was possible then $\tilde{q}_1(o,p)$ could have been written as

$$\tilde{q}_1(o,p) = \frac{K \prod_{i=1}^{M} (\beta_i + p)}{\prod_{i=1}^{N} (\alpha_i + p)} \qquad 1 < M < \infty \tag{5.2}$$

and since

$$\lim_{t \to o} \dot{q}_1(o,t) = \lim_{p \to \infty} p\, \tilde{q}_1(o,p) = -1 \tag{5.3}$$

this will require K to be a negative value. However for a long column for which

$$\lim_{t \to \infty} q(o,t) = \lim_{p \to o} \tilde{q}_1(o,p) > o \tag{5.4}$$

this will not be possible if $\tilde{q}_1(o,p)$ is of the form (5.2). Now if there were at least one factor in the numerator of (5.2) of the form $(-\gamma_i + p)$ where γ_i is a positive real number then clearly both (5.3) and (5.4) are satisfied. Therefore (5.1) must at least have one real root in the closed right half-complex plane and hence the non-minimum-phase effect should be existant.

6. References

1. 'The analytical modelling and dynamic behaviour of a spatially continuous binary distillation column', J.B. Edwards, 1979, Research Report No. 86, University of Sheffield.

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3. 'Mathematics of Dynamical Systems', H.H. Rosenbrock and C. Storey, 1970, Nelson, U.K.

4. 'Computer-aided control systems design', H.H. Rosenbrock, 1974, Academic Press, London, U.K.

7. List of Symbols

α	- initial slope of equilibrium curve approximation
β	- plase angle of the complex variable q
θ	- phase angle of Laplace variable p.
ω	- frequency of sinusoidal inputs
ω_T	- interval of frequency marks on Nyquist diagrams
ρ	- magnitude of the complex variable q
$\tilde{}$	- superscript denoting Laplace transforms w.r.t normalised time
h	- normalised distance
$h_e (= \frac{1}{TP+1})$	- transfer function of accumulator and reboiler
$\underline{I}$	- unit diagonal 2 x 2 matrix
j	- $(-1)^{\frac{1}{2}}$
K	- transfer function d.c. gain
ℓ	- small changes in molar flow of liquid in rectifier or stripper
L	- normalised length of entire rectifier or stripper
p	- Laplace variable w.r.t normalised time.
q	- $(p^2 + 2p)^{\frac{1}{2}}$
$\underline{q}$	- vector difference of total of vapour and liquid composition changes
$\underline{r}$	- vector of associated equilibrium values
$\underline{u}$	- vector of total and difference vapour and reflux rate changes
v	- small changes of molar flow of vapour in rectifier or stripper
x,x'	- small changes in liquid compositions in rectifier and stripper
x'e	- y'/α
y,y'	- small changes in vapour composition in rectifier and stripper
y_e	- x/α
T	- normalised time - constants of accumulator and reboiler

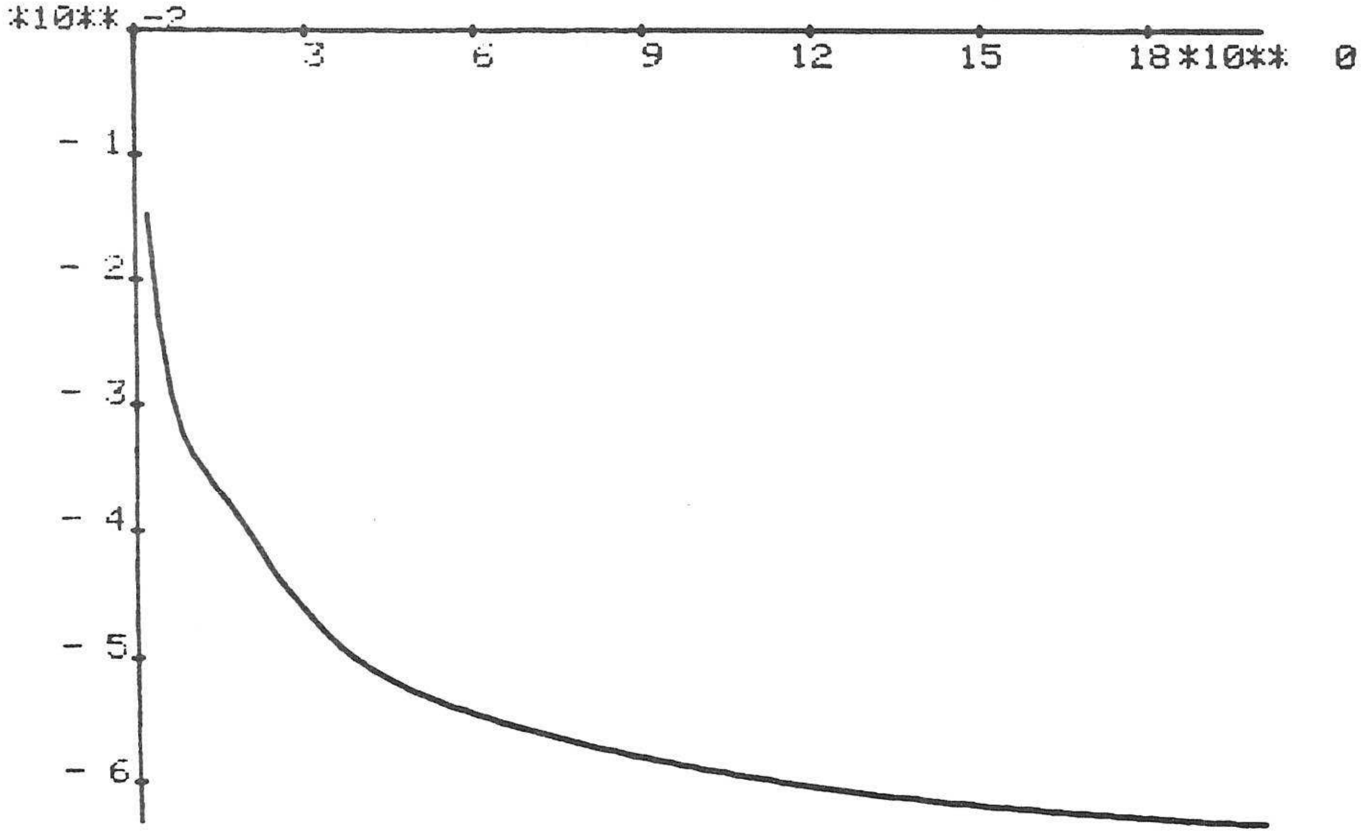

Fig. (1) Step response of $q_1(o,t)$ for a short column ($L=2$, $\varepsilon=1$, $T=5.$)

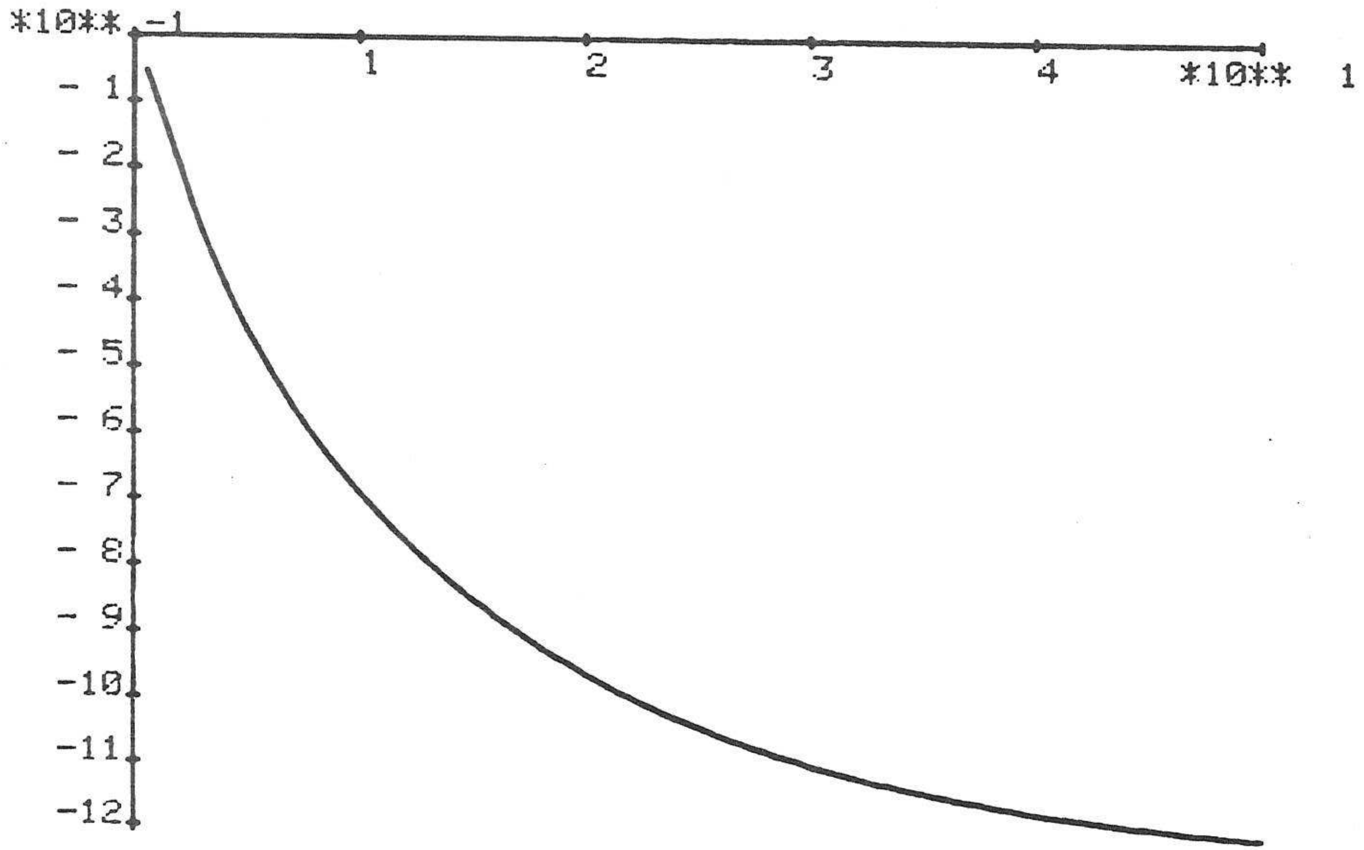

Fig.(2) Step response of $q_2(o,t)$ for a short column ($L=2$, $\varepsilon=1$, $T=5$).

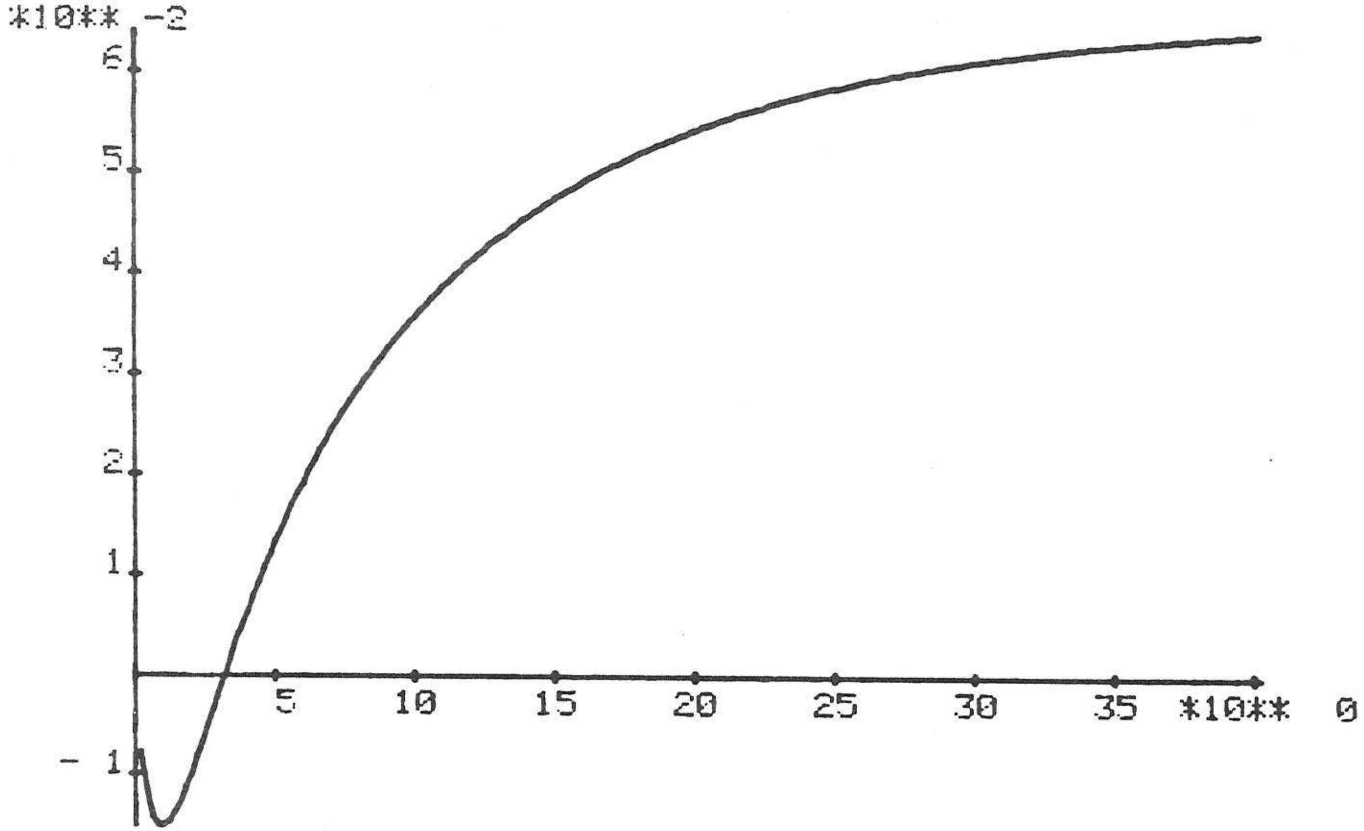

Fig. (3) Step response of $q_1(o,t)$ for a long column ($L=5$, $\varepsilon=1$, $T=5$)

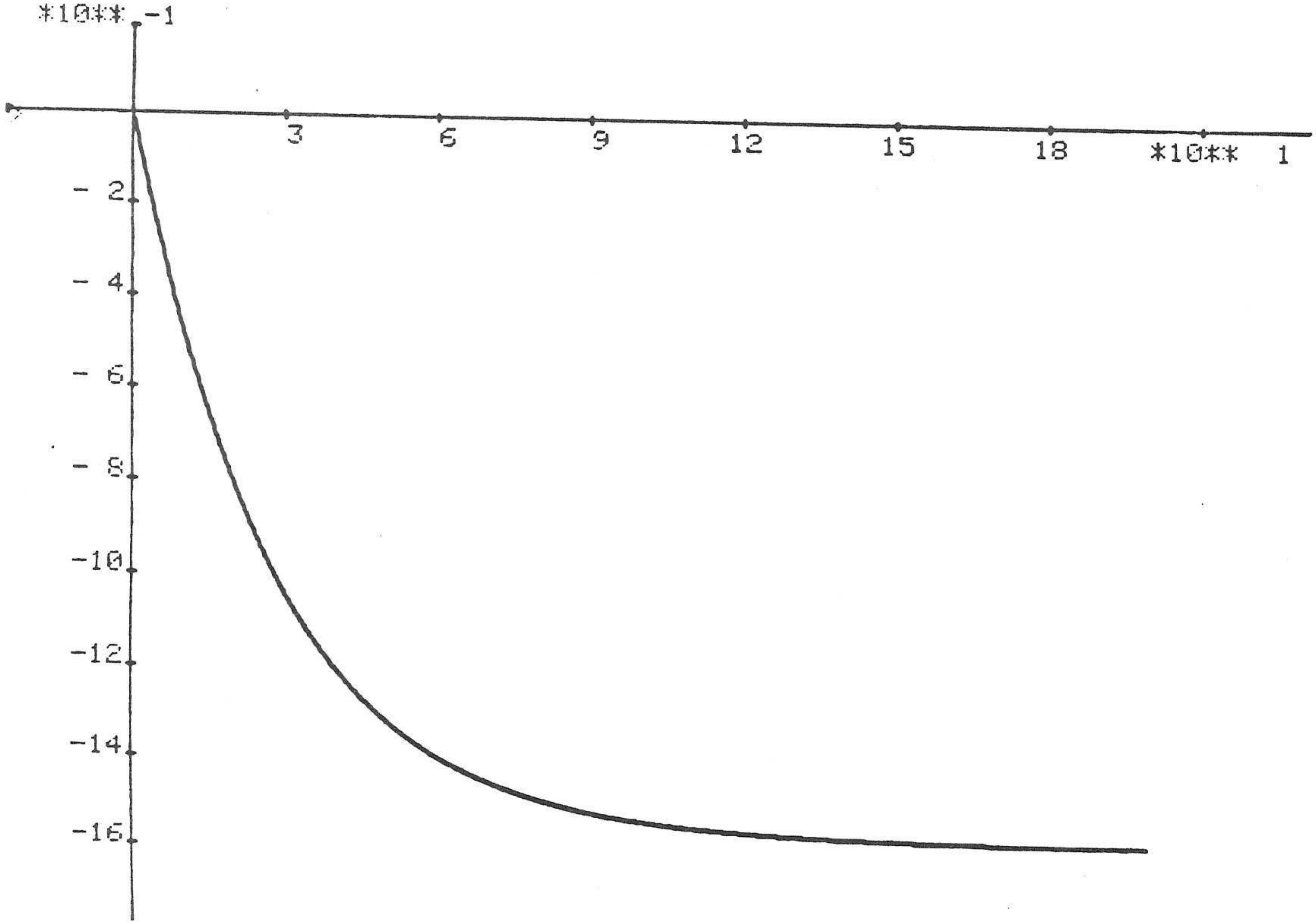

Fig. (4) Step response of $q_2(o,t)$ for a long column (L=5, ε=1, T=5)

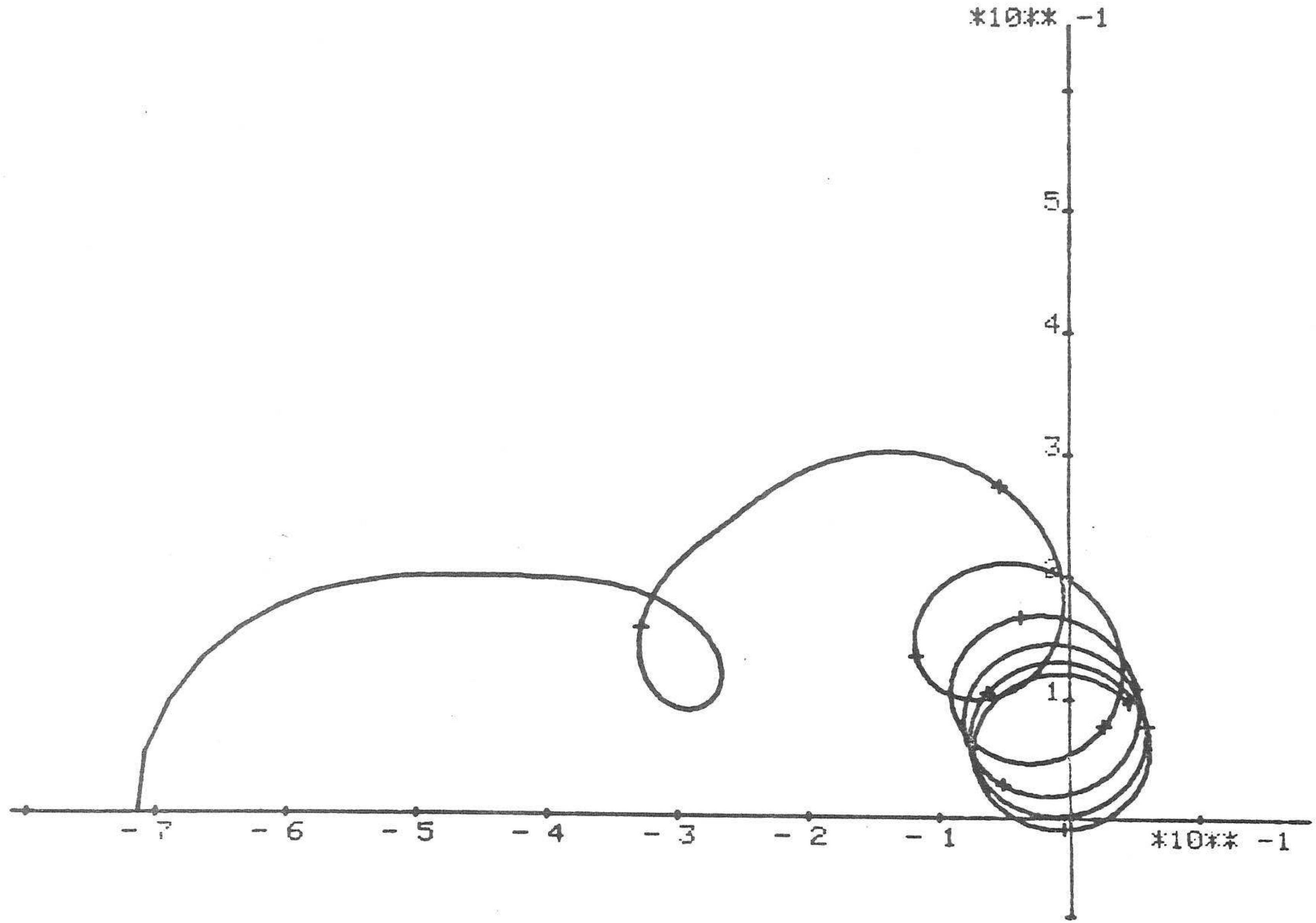

Fig. (5) Direct Nyquist diagram of $q_1(o,p)$ for a short column
($L=2$, $\varepsilon=1$, $T=5$, $o < \omega < 20$, $\omega_T=2$)

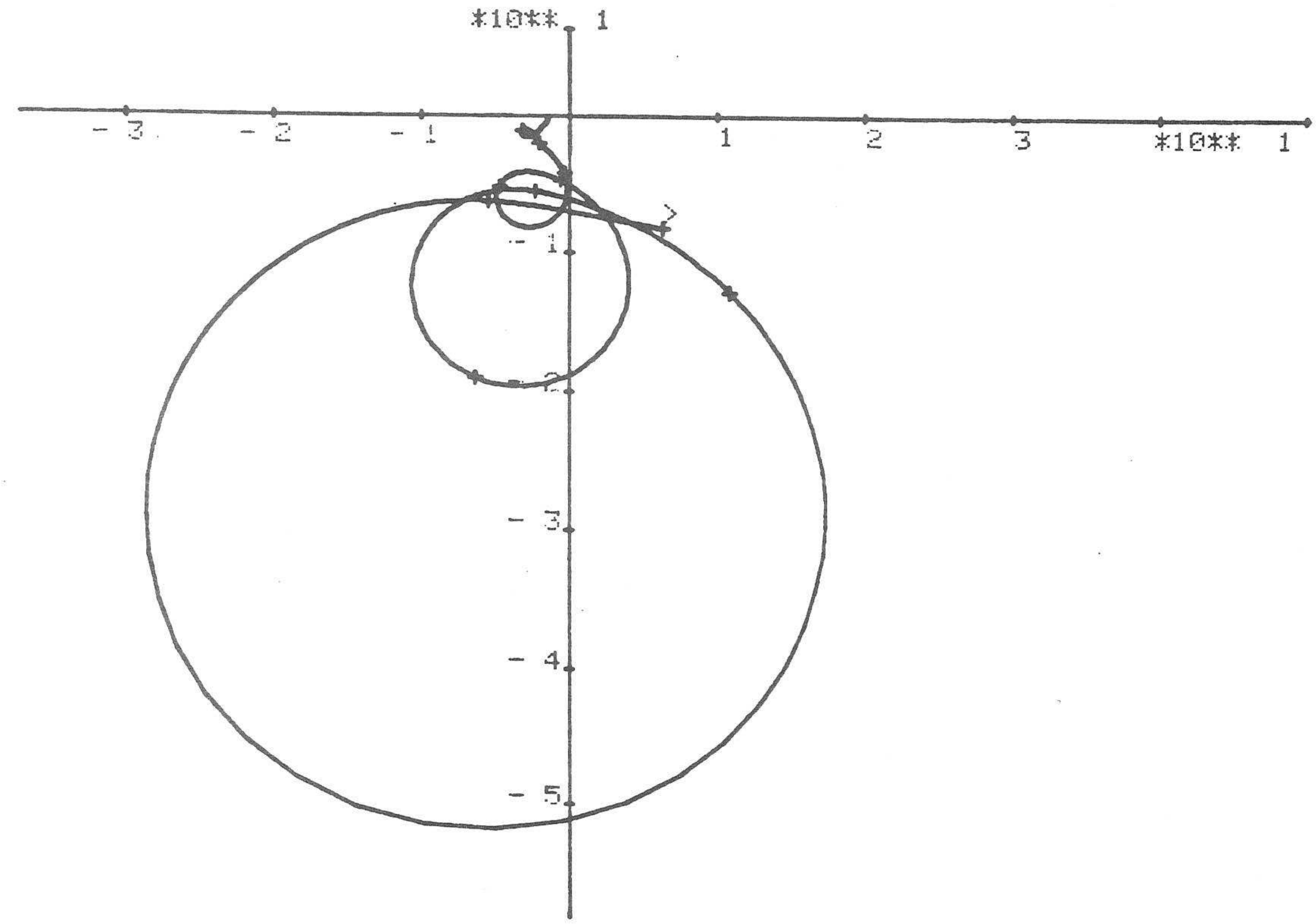

Fig. (6) Inverse Nyquist diagram of q_1 (o,p) for a short column (L=2, ε=1, T=5, o < ω < 14,ω_T =1.4)

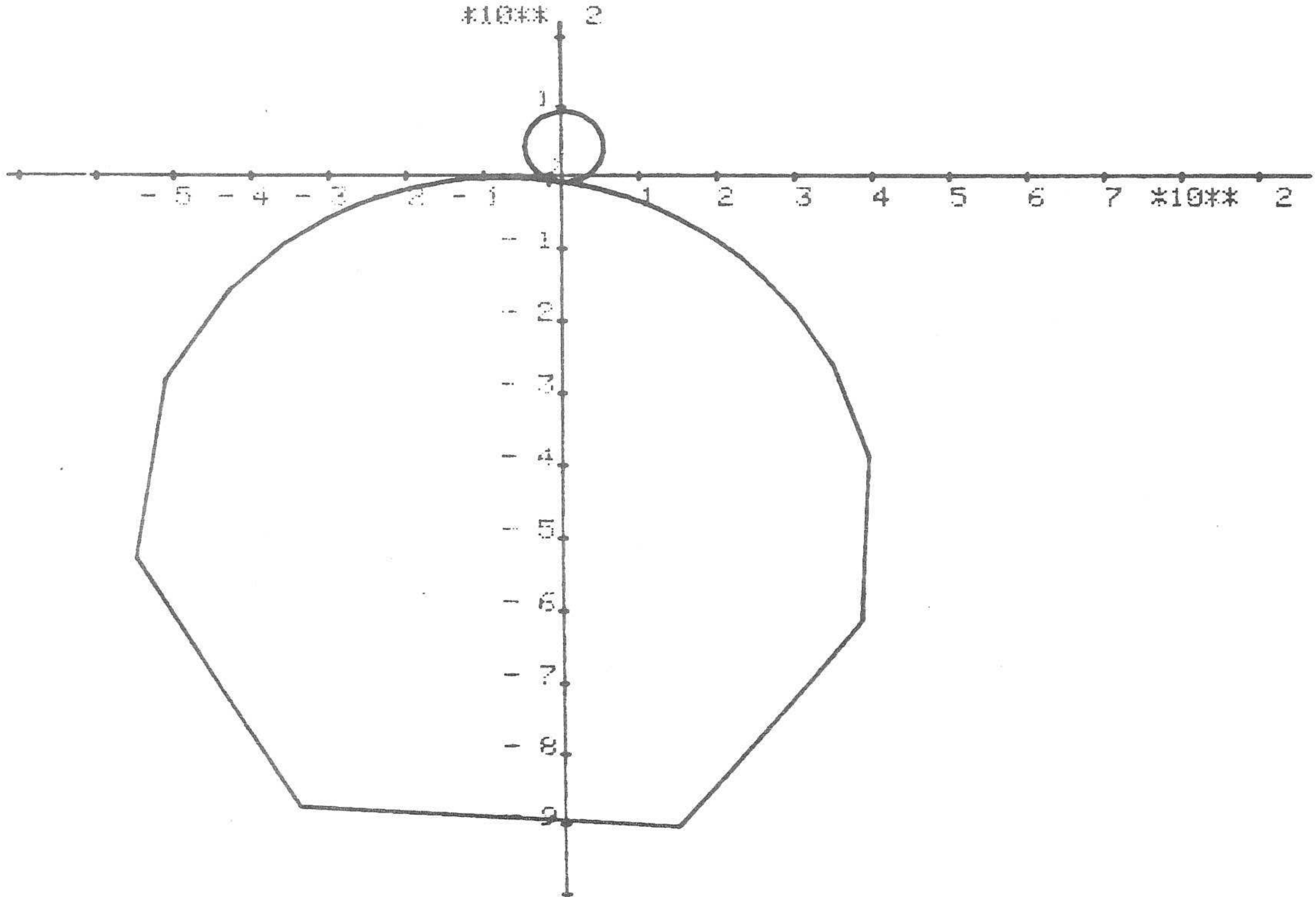

Fig. (7) Continuation of inverse Nyquist diagram of Fig. (6) for $14 < \omega < 18$

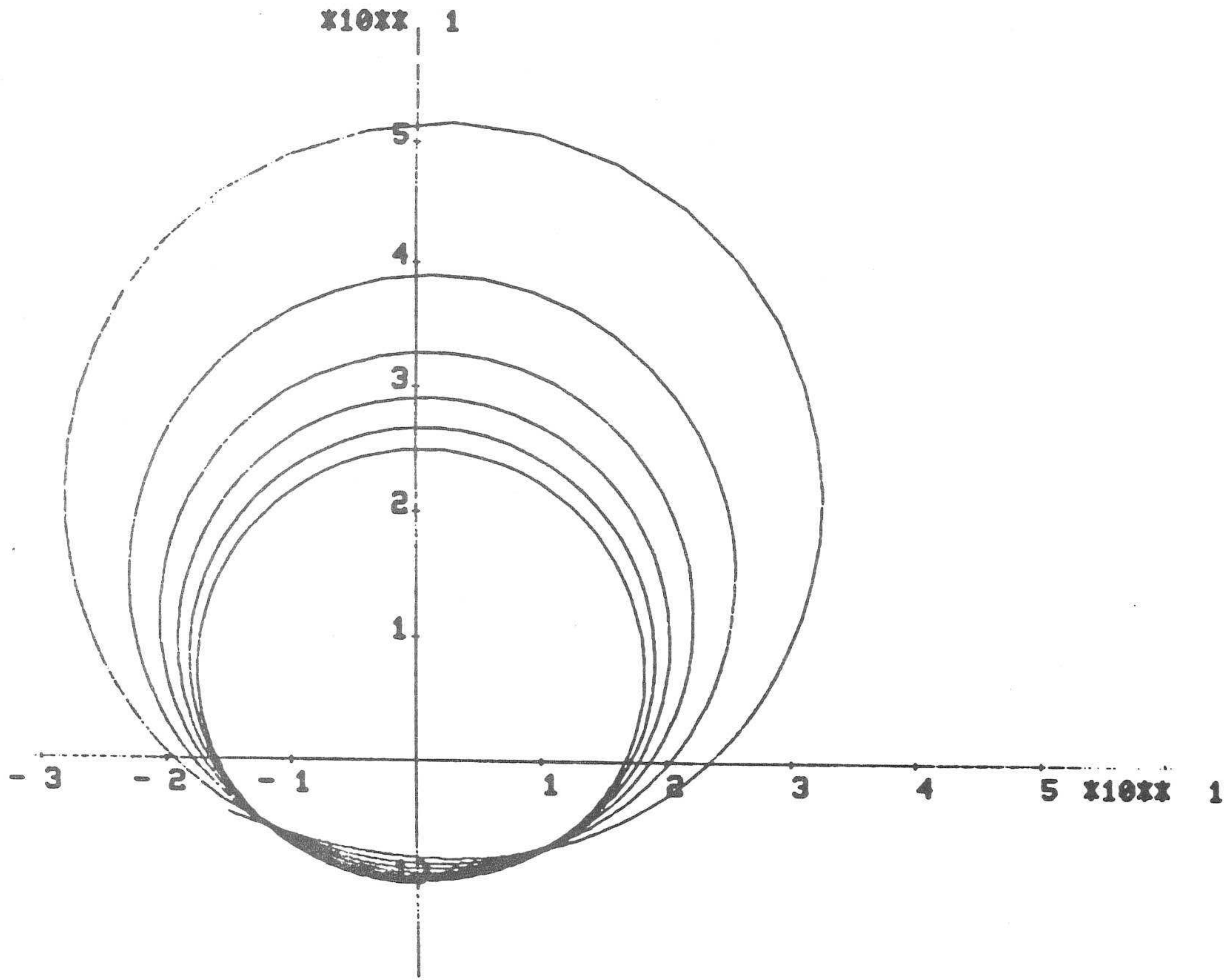

Fig. (8) Continuation of inverse Nyquist diagram of Fig. (7) for $14 < \omega < 40$

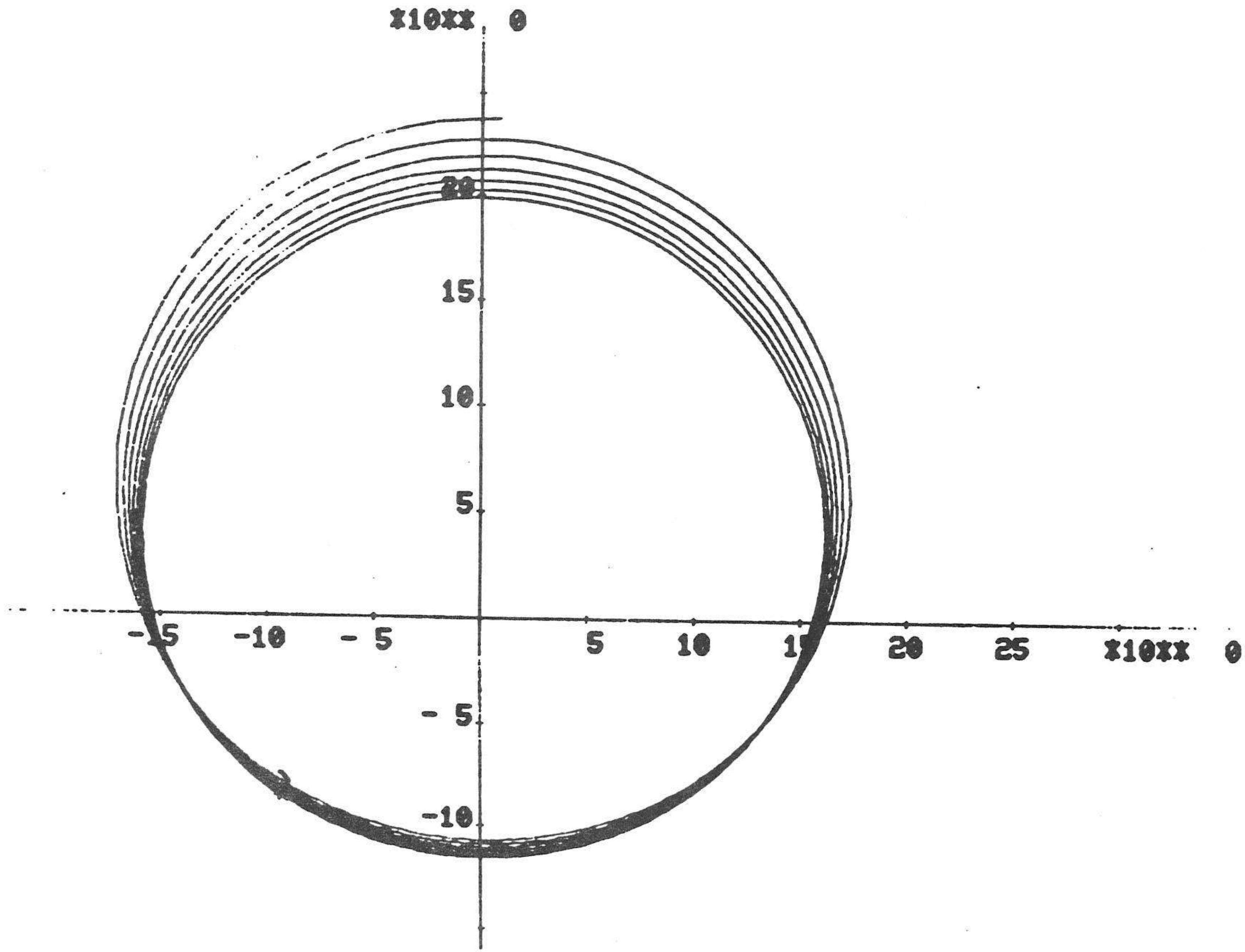

Fig. (9) continuation of the inverse diagram of Fig. (8) for $40 < \omega < 60$

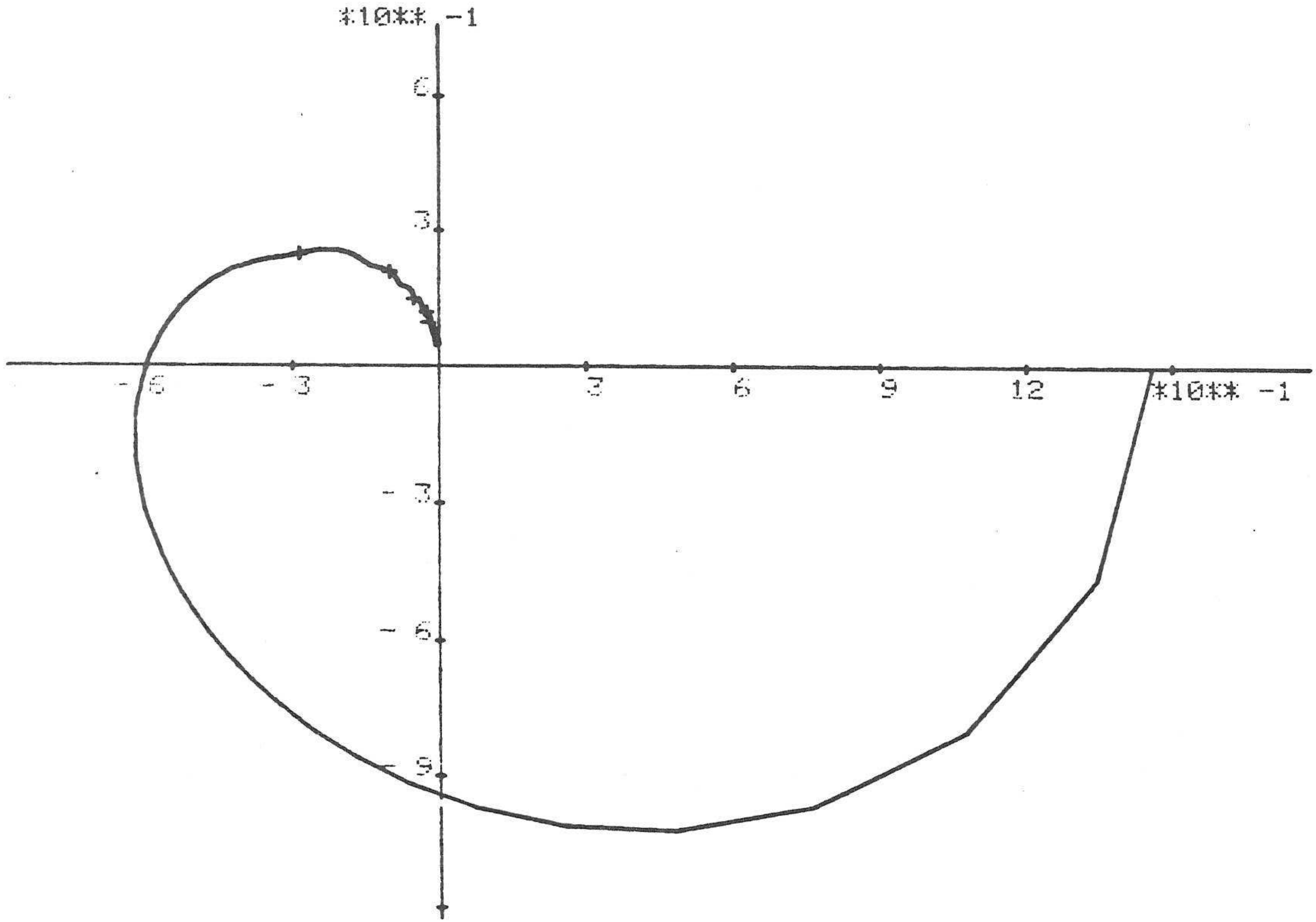

Fig. (10) Direct Nyquist diagram of $q_1(o,p)$ for a long column ($L=5$, $\varepsilon=1$, $T=5$, $0 < \omega < 20, \omega_T = 1$)

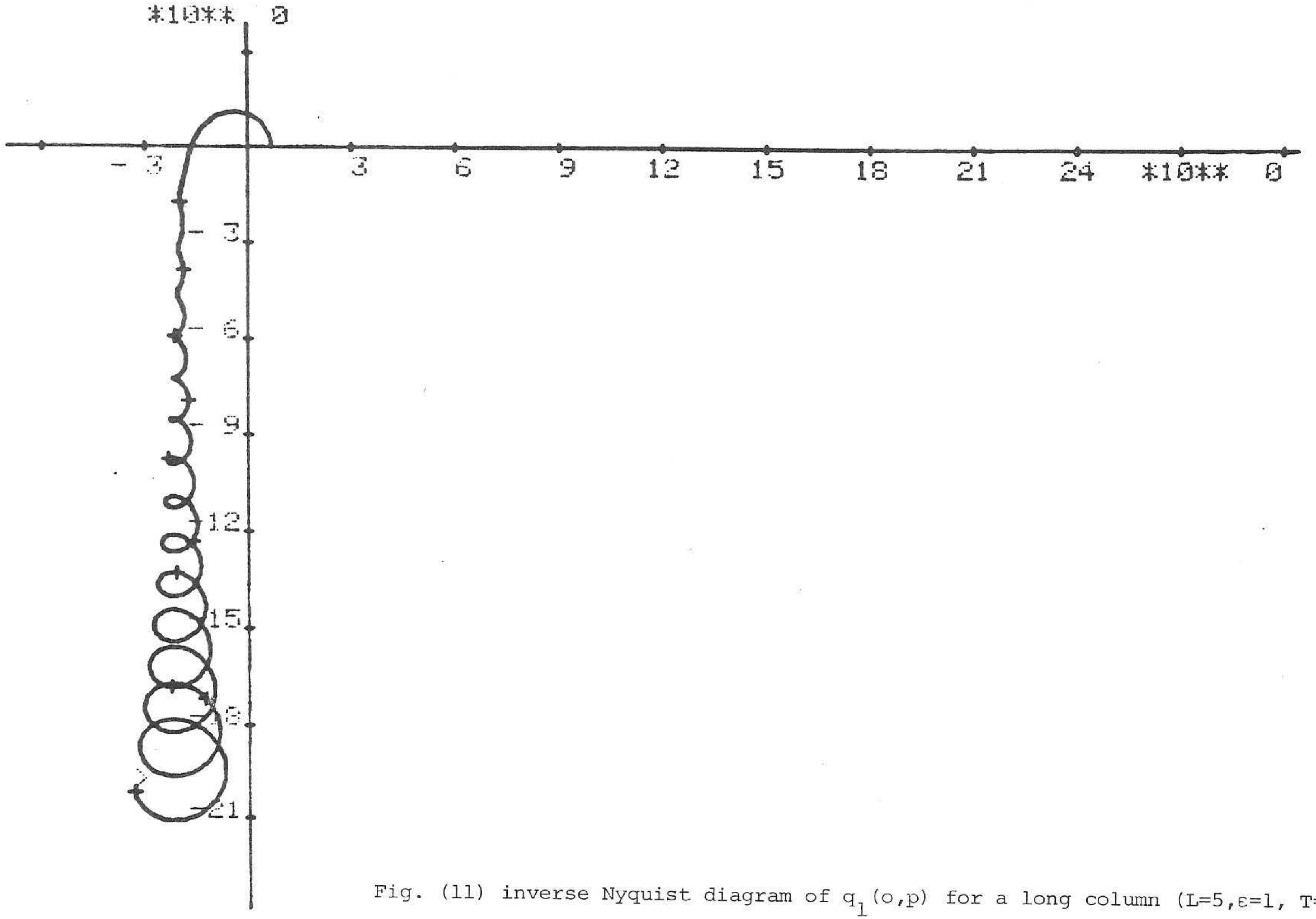

Fig. (11) inverse Nyquist diagram of $q_1(o,p)$ for a long column ($L=5, \varepsilon=1$, $T=5$, $0 < \omega < 20, \omega_T=2$)

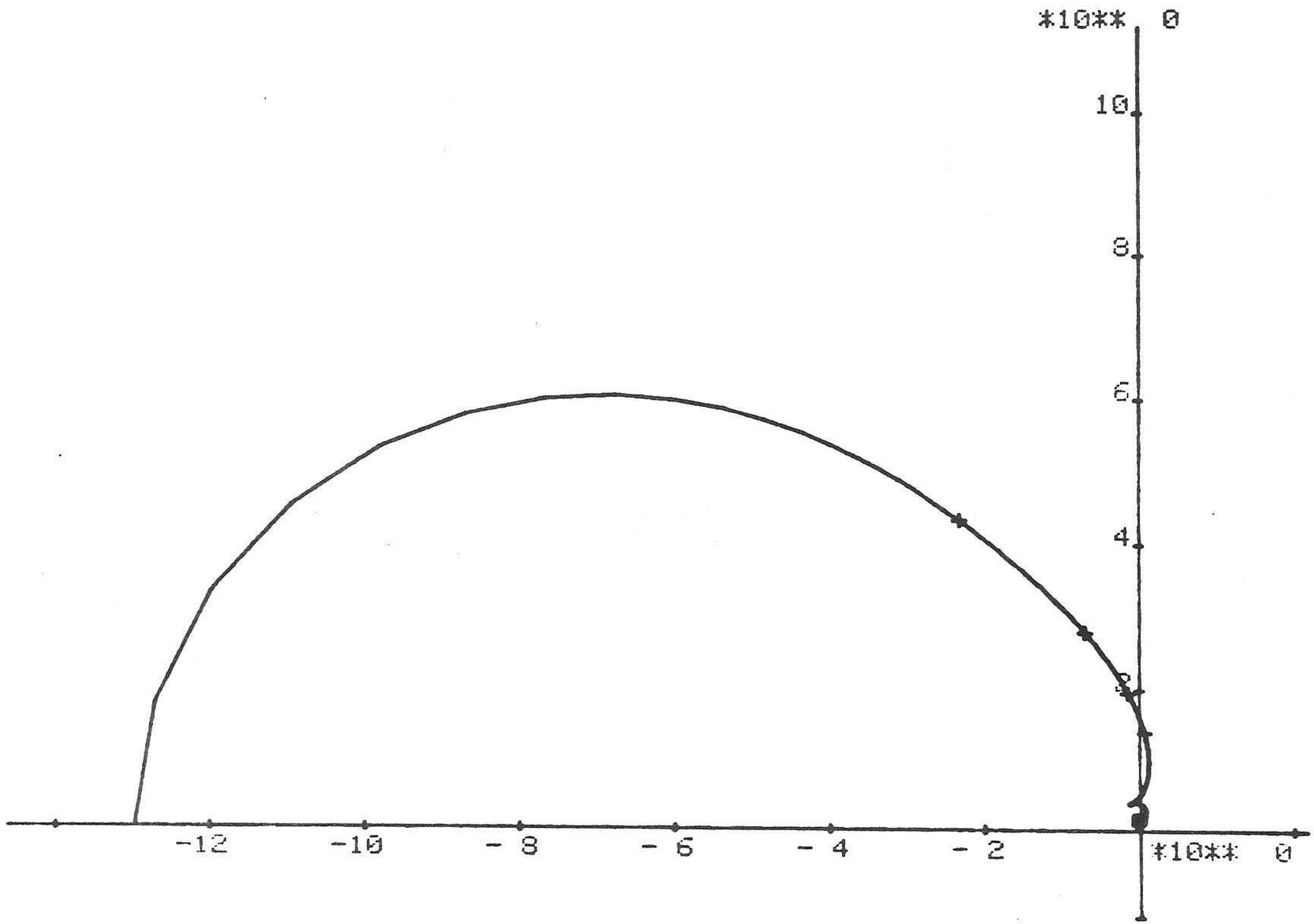

Fig. (12) direct Nyquist diagram of $q_2(o,p)$ for a short column ($L = 2$, $\varepsilon = 1$, $0 < \omega < 10$, $\omega_T = .2$)

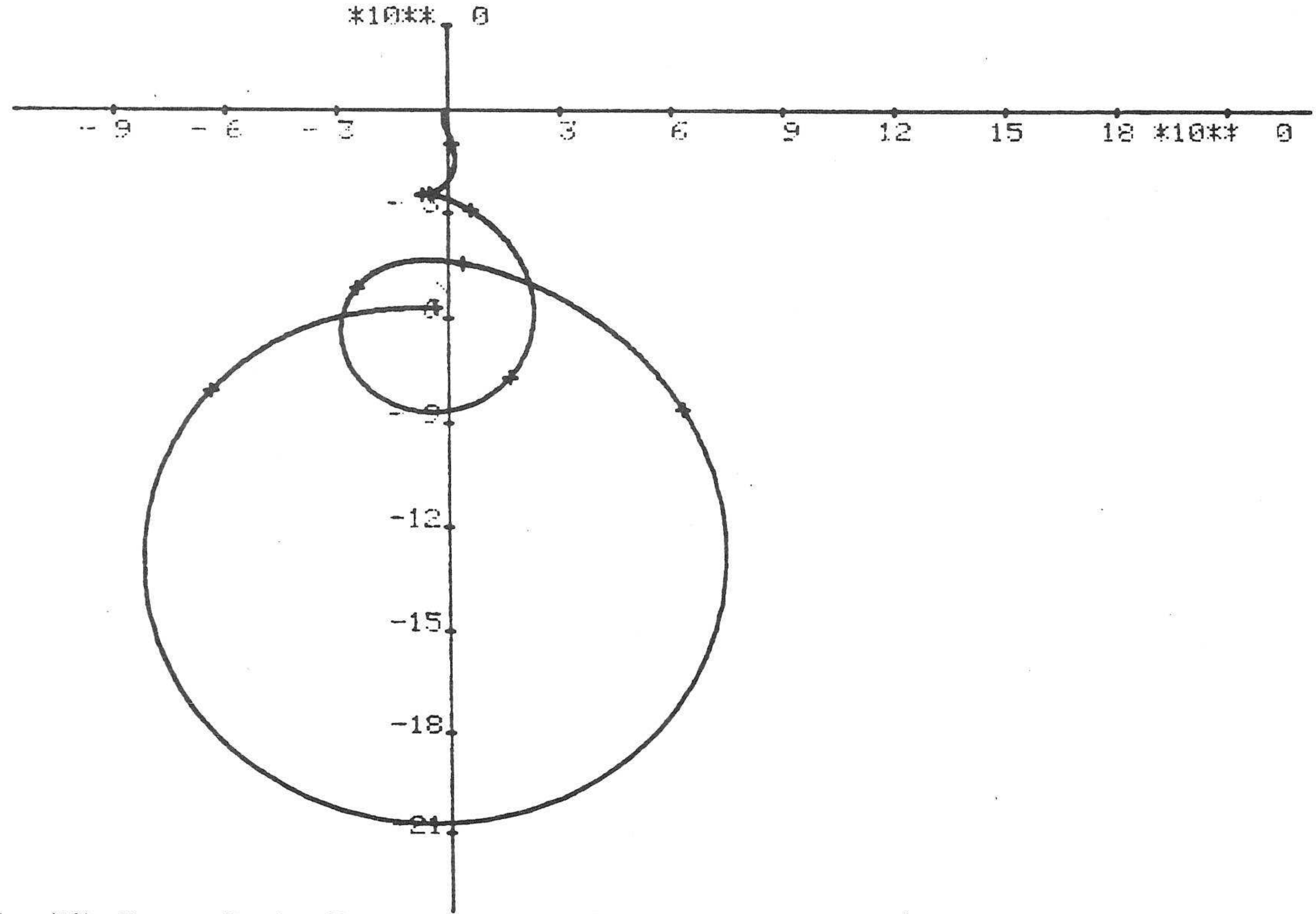

Fig. (13) Inverse Nyquist diagram of $q_2(o,p)$ for a short column ($L = 2, \varepsilon = 1$, $T = 5$, $0 < \omega < 10$ $\omega_T = 1$)

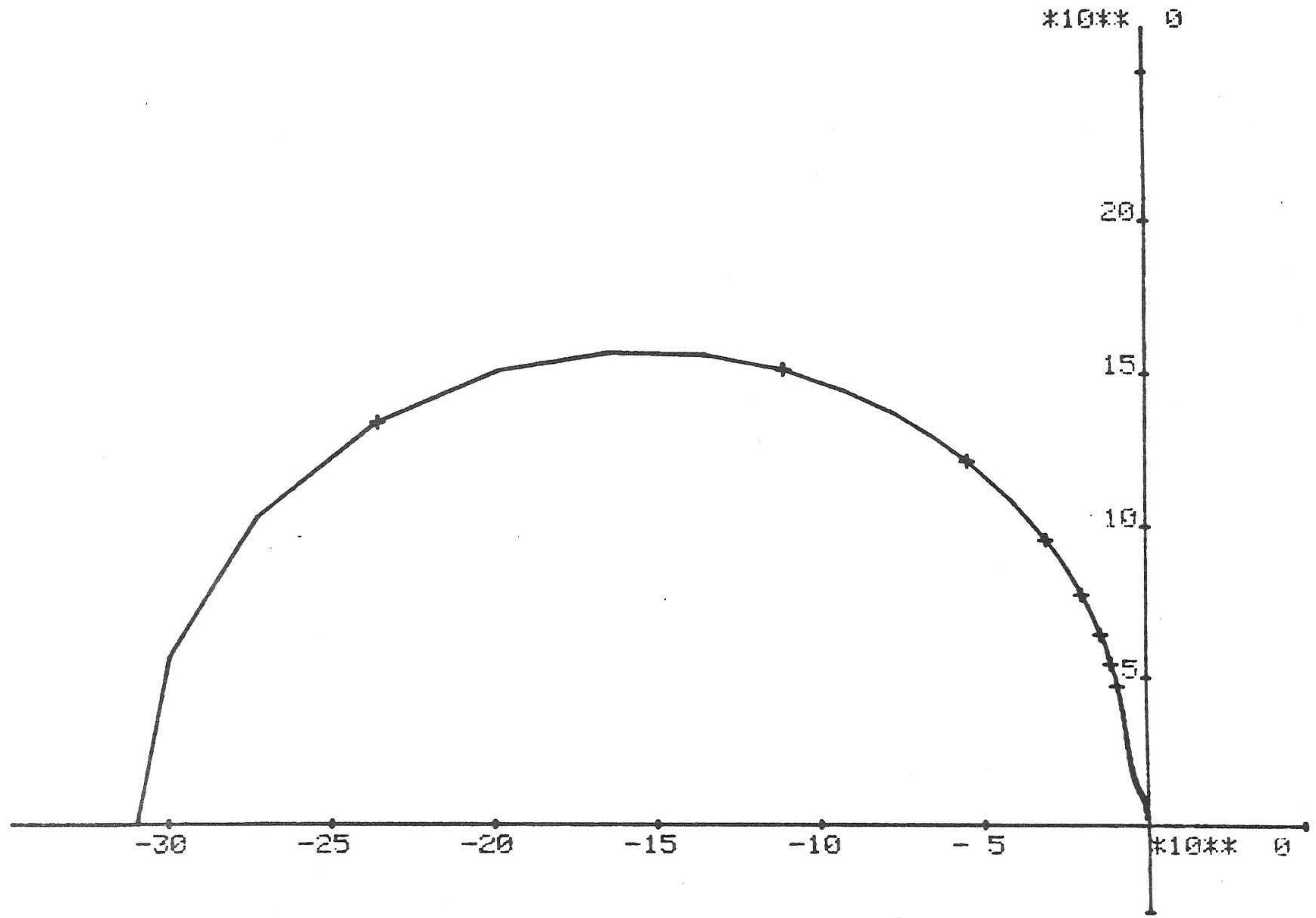

Fig. (14) direct Nyquist diagram of $q_2(o,p)$ for a long column ($L=5$, $\varepsilon=1$, $T=5$, $0 < \omega < 5$, $\omega_T = 0.2$)

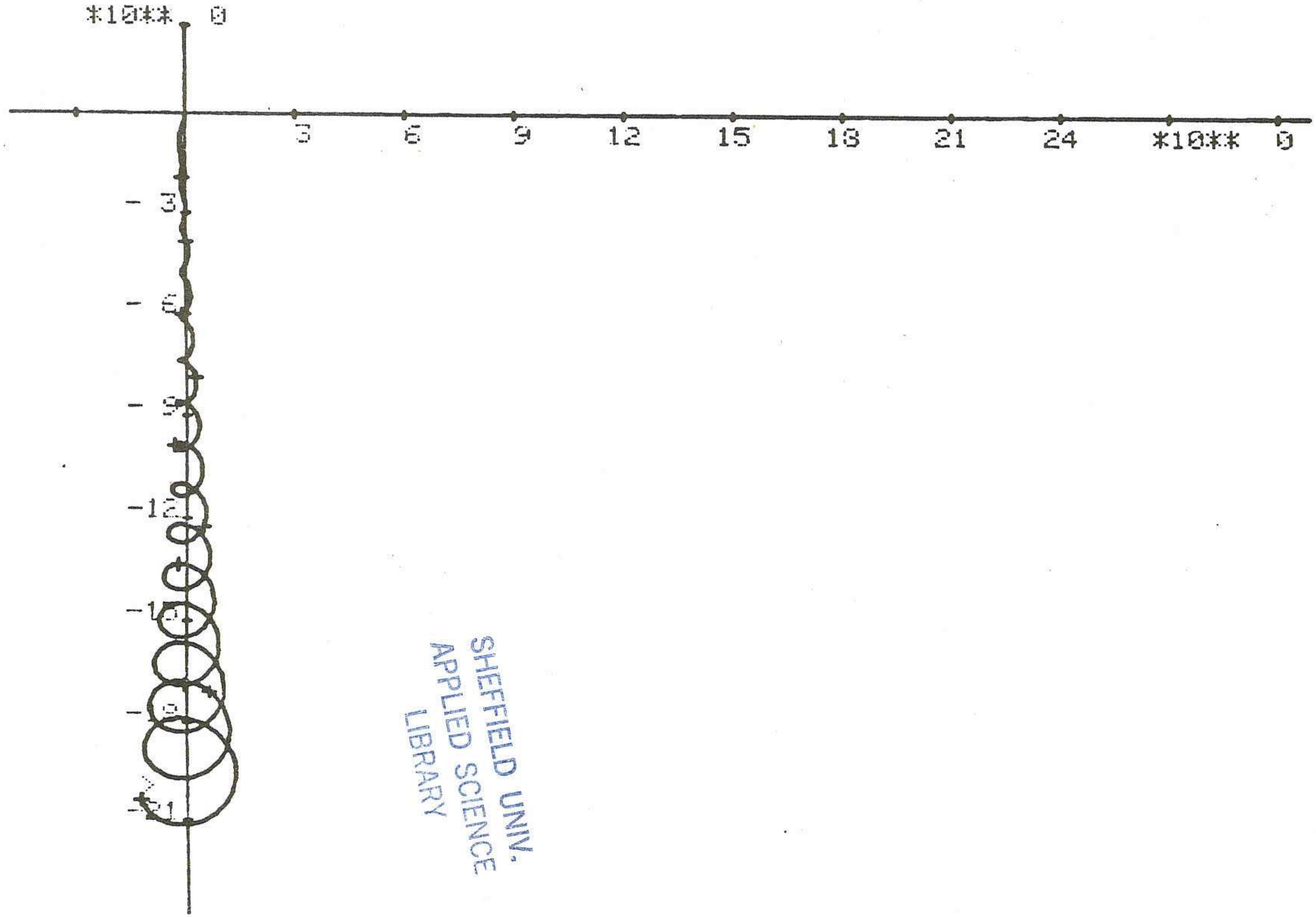

Fig. (15) Inverse Nyquist diagram of $q_2(o,p)$ for a long column ($L=5$, $\varepsilon=1$, $T=5$, $0 < \omega < 20$, $\omega_T = 2$)