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THE USE OF SPECIAL PURPOSE COMPUTERS

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## NUMERICAL CALCULATION OF THE CONDUCTIVITY OF PERCOLATION CLUSTERS AND THE USE OF SPECIAL PURPOSE COMPUTERS

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### Abstract

Electrical conductivity diffusion or phonons, have an anomalous behaviour on percolation clusters at the percolation threshold due to the fractality of these clusters. The results that have been found numerically for this anomalous behaviour are reviewed. A special purpose computer built for this purpose is described and the evaluation of the data from this machine is discussed.

### 1. DYNAMICAL SCALING OF PERCOLATION

Percolation [1] has been a model for disordered systems, like porous media, random mixtures of conductors and insulators and gels. It is usually defined on a  $d$ -dimensional regular lattice on which sites (or bonds) are occupied with a probability  $p$  and empty with probability  $1 - p$ . Occupied nearest-neighbors belong to the same cluster. At a critical value  $p_c$  clusters of all sizes are present, particularly also arbitrarily large clusters. These large clusters are fractals, i.e., their density  $\rho$  decreases with their linear size  $L$  with a powerlaw  $\rho \sim L^{d_f-d}$  where  $d_f$  is called the fractal dimension ( $d_f = 91/48$  in  $d = 2$  and  $d_f \approx 2.5$  in  $d = 3$ ).

A consequence of fractality is that the cluster is less connected on larger length scales, it is actually only singly connected on a number of bonds  $n_r$  that grows like  $n_r \sim L^{d_r}$  ( $d_r = 3/4$  in  $d = 2$  and  $d_r \approx 1.14$  in  $d = 3$ ). Due to this unusual decrease in connectivity many fundamental physical laws are different on these fractal clusters from the corresponding

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law on an Euclidean lattice [2]. So, the well known diffusion law,  $R \sim N^{1/2}$ , where  $R$  is the average distance a diffusing particle has from its origin after  $N$  jumps, changes on a fractal to

$$R \sim N^{1/d_w} \quad (1)$$

which is called the ‘‘anomalous diffusion’’ law. The exponent  $d_w$ , the fractal dimension of the trace of the particle on the fractal cluster, is larger than 2 due to the weak connectivity mentioned above.

Another physical law that changes on a fractal is the size dependence of the electrical conductance  $\sigma$ . On an Euclidean lattice it goes like  $\sigma \sim L^{d-2}$ , on a fractal cluster like

$$\sigma \sim L^{-\zeta} \quad (2)$$

where

$$\zeta = 2 - d + \tilde{t}$$

and  $\tilde{t} > 0$ . This effect has actually been measured for instance for Pb on thin Ge and Au films [3]. Electrical conductivity and diffusion are related to each other via the Einstein relation and one can show [4] that

$$\zeta = d_w - d_f \quad (3)$$

The phonon spectrum  $\rho(\omega)$  usually behaves for small frequencies  $\omega$  like  $\rho(\omega) \sim \omega^{d-1}$ , on a fractal one has instead  $\rho(\omega) \sim \omega^{d_s-1}$ , where the spectral dimension  $d_s$  is also related to the previous exponents [5] via  $d_s = 2d_f/d_w$ .

Intrigued by the question if it is possible to relate this critical exponent to usual static critical exponents, particularly to  $d_f$ , several conjectures have been proposed. The most serious ones were

$$d_w = d_f + 1 \quad (4a)$$

(proposed first for  $d = 2$  in Ref [6]),

$$d_w = \frac{3}{2}d_f \quad [5] \quad (4b)$$

(called the Alexander-Orbach conjecture) and for  $d = 2$  only

$$d_w = 2(d_f - 1 + d_f^{-1}) \quad [7] \quad (4c)$$

For  $d = 2$  they give in the same order  $\tilde{t} = 1, 0.948$  and  $0.951$ . Finally it was also proposed that  $d_w = d_f + 1$  for  $d_f \leq 2$  and  $d_w = \frac{3}{2}d_f$  for  $d_f > 2$  [8]. It became clear very soon that none of these relations has a validity for arbitrary fractals as was thought for a moment since they clearly do not work for Sierpinski gaskets or lattice animals [2]. Neither is any

of these conjectures able to reproduce the  $\varepsilon = 6 - d$  expansion [9] even in lowest order in  $\varepsilon$ . On the other hand new arguments favouring some of these conjectures came up [10].

## 2. NUMERICAL METHODS

To shed light upon the question raised by the various conjectures it is necessary to make numerical high-pressure calculations. This can be done via diffusion or via the electrical conductivity. The largest effort done by averaging over many diffusion trajectories gave in  $d = 2$ ,  $\bar{t} = 0.960 \pm 0.015$  [11] which is not very conclusive. More efficient was the evaluation of the probability cloud, i.e., on each site the value of the probability that the diffusing particle is there after  $N$  time steps provided it was at the beginning on the origin with probability one. This method automatically averages over all trajectories and  $\bar{t} = 0.97 \pm 0.01$  [12] was obtained from graphs as shown in Fig.1.

The calculation of the electrical conductivity of percolation clusters can also be done in different ways. Using star-triangle transformations it is possible to reduce the conductance of any  $2d$  network to that of one bond [13] and this method, pushed to systems of size 1000, yields [13]  $\bar{t} = 0.977^{+0.003}_{-0.010}$ . The other way to calculate the conductance is adding bond after bond to the cluster; to do so one has to use a strip geometry.

This method, often called strip method, was introduced in Ref. [14]. Top and bottom of the strip have a fixed potential (fixed boundary condition in the longitudinal direction). If the strip has width  $n$  one defines by  $I_i$  and  $V_i$  the current and potential drops at the end of each of the  $n$  lines and the conductance matrix  $\sigma_{ij}$ , given through

$$I_i = \sum_{j=1}^n \sigma_{ij} V_j \quad (5)$$

is updated via

$$\sigma'_{ij} = \sigma_{ij} - \sigma_{i\alpha} \sigma_{\alpha j} r / (1 + \sigma_{\alpha\alpha} r) \quad (6a)$$

if a longitudinal bond is added at line  $\alpha$  and via

$$\sigma'_{ij} = \sigma_{ij} + (\delta_{\alpha j} - \delta_{\beta j}) \times (\delta_{\alpha i} - \delta_{\beta i}) / r \quad (6b)$$

if a transversal bond is added between lines  $\alpha$  and  $\beta$  where  $r$  is the resistance of the bond. The statistical fluctuations become very small for long strips and the extrapolation to infinite width is just given by

$$\sigma_{11} \sim L n^{-\bar{t}} \quad (7)$$

This method gave [15]  $\bar{t} = 0.973 \pm 0.005$  in  $2d$ .

Instead of having a conductor on each occupied bond and an insulator on each empty bond one can put a superconductor ( $r = 0$ ) on each occupied bond and a normal conductor on each empty bond. In this new problem also a new, independent exponent,  $\bar{s}$ , appears.

It happens, however, that in  $d = 2$  one has  $\bar{s} = \bar{t}$  from duality [16]. Calculating this superconductor problem via the strip method [17] has the advantage over the normal conductor problem of the previous paragraph that one can have periodic (instead of fixed) boundary conditions in the longitudinal direction which considerably reduces the finite size effects. One considers now the resistance matrix  $R_{ij}$ , defined through

$$V_i = \sum_{j=1}^n R_{ij} I_j \quad (8)$$

and updates this matrix via

$$R'_{ij} = R_{ij} - r\delta_{i\alpha}\delta_{\alpha j} \quad (9)$$

if a longitudinal bond at line  $\alpha$  is added and via

$$R'_{ij} = R_{ij} - (R_{i\alpha} - R_{i\beta})(R_{\alpha j} - R_{\beta j}) / (r + R_{\alpha\alpha} + R_{\beta\beta} - R_{\alpha\beta} - R_{\beta\alpha}) \quad (10)$$

if a transversal bond between lines  $\alpha$  and  $\beta$  is added. For large widths one has

$$R_{11} \sim Ln^{-\bar{s}} \quad (11)$$

and

$$\bar{t} = 0.977 \pm 0.010 \quad (12)$$

was obtained with a moderate effort ( $\approx 5$ h Cray 1) [17] as seen in Fig. 2.

In  $d = 3$  the up to now most precise values for the exponents were obtained with the strip method and they are  $\bar{t} = 2.2 \pm 0.1$  [18] and  $\bar{s} = 0.85 \pm 0.05$  [17]. They exclude most of the conjectures but not the Alexander-Orbach conjecture. We note however, that recent [19] diffusion simulations found  $\bar{t} = 2.8 \pm 0.3$  in disagreement with previous work.

### 3. BUILDING A SPECIAL PURPOSE COMPUTER

In order to get the exponents with a significantly higher precision much more computer power has to be inverted. For this purpose the most efficient method, namely that of Ref [17] was chosen and a special purpose computer (SPC) was build to implement this method in hardware.

Isn't it much more comfortable to write a Fortran program and execute it on the next available general supercomputer (like a Cray XMP, an IBM 3090, a Cyber 205, etc...)? Several reasons have led people to do it the hard way:

First of all, general computers must usually be shared with many other users, so one will have access to a restricted number of hours, several hundred hours per year at best. An SPC is available every day of the year, 24 hours a day (except during blackouts).

There also is an important financial aspect: A grant proposal asking for  $2 \times 10^7$  US dollars for a Cray 2 is likely to be rejected. The chances, however, to get  $5 \times 10^4$  US dollars for tools and components to build an SPC are considerably better.

Finally there is speed! Supercomputers are famous for being very fast (that is what makes them price-efficient compared to smaller general computers). Now, however, there exist on the market highly integrated ultrafast chips. If, in addition, one arranges these chips inside the SPC in such a way that many of them work simultaneously (doing the same thing (parallelism), or doing different things (vectorization)) the SPC can be as fast or even faster than a supercomputer. Technologically speaking, this is the reason why SPC's are mainly a development of only the last couple of years.

All these reasons in favour of SPC's have to be counterbalanced by the fact that the building of an SPC involves an enormous amount of work in a field that usually has to be learned from scratch.

Since the building of an SPC is a non-negligible enterprise one should first consider carefully if one has chosen the right problem. There are certain general criteria:

- The problem one wants to solve should be sufficiently fundamental and sufficiently difficult that after two years - which is about the average time one needs to get results from an SPC - the scientific community is still interested.

- The algorithm one uses must be relatively simple, so that the SPC won't get too complex and its construction time too long.

- The method to solve the problem should involve a huge repetition of identical steps (typically  $10^8$  to  $10^{10}$ ) so that one can run the SPC for many days without intervening.

The algorithm and the evaluation of the data should have had extensive previous testing on general computers and one should be so sure about the procedure that one is willing to fix in a definitive way what calculations one will perform. It is usually very difficult to change an SPC once it is built.

Once one has chosen the algorithm for which one wants to build the SPC there are certain necessary conditions required before construction can start: One needs the financial support to buy the hardware components and electronic equipment (like an oscilloscope or a logic analyzer). An enthusiastic team willing to work hard must be formed. At least one person with a solid experience in electronics must belong to the team. Finally one has to find an electronics lab willing to put a reasonable infrastructure at your disposal.

#### 4. THE SPC IN SACLAY

In the following I will briefly describe some aspects of the construction of the SPC that was build in Saclay [20] by M. Hajjar and J.M. Normand to calculate the electrical conductivity of percolation clusters using the strip method.

The first, and most creative step is the design of the architecture of the SPC. One has to try to decompose the algorithm into the largest possible number of elementary calculations that can be performed simultaneously. Some calculations are completely independent from the rest, like the generation of random numbers, and can therefore be

executed by a processor of its own (MIMD = multiple instruction multiple data arrangement), so they are implemented on a separate electronic board.

For the part of the calculation that will be executed the most one has to construct a "pipeline". In our case the main calculation is the updating of a matrix  $R_{ij}$  following eq. (10):

$$R'_{ij} = R_{ij} - R_{i1} - V_i * V_j, \quad (13)$$

where  $V_i$  is a vector and all operations are in 64 bit floating point arithmetic. In fig.3 we see a simplified diagram of the data flow. Like on a car assembly line the first subtraction of eq. (13) is performed for one matrix element while the second subtraction of eq. (13) is done for another matrix element (MISD = multiple instruction single data arrangement). In order that such a pipeline can work every unit must be finished at the same time. So one has to investigate which chips are available on the market. It happens that the fastest 64 bit multipliers need 480 nsec per multiplication (WTL 1064 of Weitek) while a subtraction can be done in 120 nsec (WTL 1065). So one has to put four multipliers in parallel as shown in fig. 3 (SIMD = single instruction multiple data arrangement) and one can get a result every 120 nsec.

The design of the architecture is, however, far from being finished! In fig. 3  $R_{ij}$  and  $V_i$  are stored in memories. One needs a device, the address generator, that determines the location of a given matrix element within the memory. Then one needs somewhere to store the "vector-instructions", i.e., the sets of bits that tell each of the chips what function it has to perform. The ensemble of all these vector-instructions is called the microcode. Which instruction is to be applied and how often is managed by a "sequencer". Roughly speaking the sequencer makes the loops and jumps that we are accustomed to use in Fortran programs. All these units must have the same speed as the central processing unit (CPU) of fig. 3, i.e., 120nsec.

Finally a connection to the external world must be established. One needs a host computer, an in-house Motorola 68000 based card in our case, that will receive the data coming from the CPU, evaluate it and store it on a disk. The host computer need not be fast but must be reliable. From time to time it will make a complete backup of the state of the machine and make consistency checks: It is rather complicated to use error correcting codes as those implemented on the big general computers, so if one finds an error during a calculation (due for example to a cosmic ray) it is restarted using the last backup as a starting point.

The host computer will not work with 64 bits and will, since it is slow, not be synchronous to the CPU, so an interface between the two is needed which is built on a separate board. The whole ensemble is sketched in fig. 4.

After the architecture is settled important electronic decisions must be taken: Which technology should be used to build the electronic boards: wirewrap or printed circuits,

or should one even make integrated circuits ? In Saclay, we opted for printed boards in TTL logic. Also one has to choose all the chips out of the data books of the different manufacturers and to compare them one has to carefully study their specifications. Since about 200 different chips were needed this is a major effort.

After all these decisions are made, a detailed layout has to be made for each board. Each pin of each chip must be properly connected and, of course, the chips must fit on the board.

In order that the connections are not too long and do not cross each other too much the placing of the chips on the board and the routing of the connection lines between them has to be done very carefully. CAD (= computer assisted design) programs are commercially available and can be extremely useful for this purpose. CAD programs can write all information concerning the locations of chips and wires on tape. These tapes can be sent to a company that will make the boards for you within several weeks.

In the meantime one orders the chips from the respective manufacturers and builds the backplane into which the boards can be placed. Everything is put together and the SPC is ready for testing. The debugging will take some more months before actual calculations can start.

## 5. RESULTS OBTAINED ON THE SPECIAL PURPOSE COMPUTER IN SACLAY<sup>[21]</sup>

The machine is microprogrammable and turns at 25 Mflops so that for our type of calculation it is about 10 % faster than the vectorized program run on one processor of the Cray X-MP. Memory allows to calculate strips of widths  $n \leq 255$  in two dimensions. Technical details about the machine are given elsewhere [20].

All calculations were done on the square lattice. We considered bond percolation at  $p_c = 0.5$  and site percolation at  $p_c = 0.592745$  (2) [22]. The strips are at least 100 times longer and the statistical error bars at least 10 times smaller than in ref. [17]. One hundred days of CPU time were needed to obtain these data, fifty days alone for the two values for  $n = 40$  since the time required grows with  $n^3$ .

While generating the above data we encountered an unexpected problem that turned out to be due to the random numbers. Random numbers  $X_k$  are generated through the lagged-Fibonacci sequence

$$X_k = (X_{k-r} + X_{k-s}) \bmod 2^{32} \quad (14)$$

Using the generator  $(r, s) = (17, 5)$  of (4), which had been implemented also on an other special purpose computer [32], we observed for bond percolation at  $n = 9$  a spurious deviation of the data from the expected monotonic behaviour by about ten times the size of the error bars (independent of the seed). We also encountered weaker, significant deviations at some other sizes (e.g.  $n = 5$ ) and also for the generators  $(r, s) = (31, 13)$  at

$n = 10$  and  $(r, s) = (55, 24)$  at  $n = 20$ . Although we do not understand the origin of these flaws they are apparently inherent to the family of generators of (14). These problems could only be observed because of the long sequences (up to  $10^{11}$ ) that we generated, still the periods of the three generators are respectively larger than  $10^{14}$ ,  $10^{18}$  and  $10^{25}$ . We note that in other cases where sequences of this length have been used similar problems were observed [28]. Because of this problem we were forced to repeat our calculation for a large part of the values with up to three different generators in order to identify the biased data. So, effectively we spent much more CPU time.

In fig. 5, we show our data multiplied by  $n^{0.98}$  as a function of  $n$  in a log-log plot. Due to universality the curves should become parallel, straight lines of slope  $0.98 - \tilde{t}$  for large  $n$ . Because of the corrections to scaling they are curved, fortunately in the opposite way. So, the bond percolation data imply  $\tilde{t} \leq 0.98$  while the site percolation data imply  $0.96 \leq \tilde{t}$  excluding therefore already both conjectures 91/96 of eq. (4b) and 1 of eq. (4a).

We tried several fits based on the minimalization of the square distance from the individual data points. A logarithmic prefactor fits very badly and can be excluded. Fitting with one powerlaw correction gives leading exponents for site and bond percolation that differ by at least one percent. Fitting a logarithmic correction gives about the same result. The precision of our data should, however, allow for a determination of  $\tilde{t}$  better than one percent.

To better understand the above problem we explicitly imposed that in the relation

$$R_n = n^{-\tilde{t}}(c_1 + c_2 n^{-\omega}) \quad (15)$$

not only  $\tilde{t}$  but also the leading correction exponent  $\omega$  should be universal ( $c_1$  and  $c_2$  are non-universal constants). So we plotted  $R_n n^{\tilde{t}}$  against  $n^{-\omega}$  for different choices of  $\tilde{t}$  and  $\omega$  and tried to find  $\tilde{t}$  and  $\omega$  such that both site and bond percolation data fall on straight lines. This is not possible reflecting the problem found before. For site percolation a straight line can be obtained for reasonable values of  $\omega$  ( $\approx 1.2$ ). For bond percolation the data are never aligned and for the parameters for which site percolation data are straight the bond percolation data line on an  $S$  shaped curve. In fig. 6 we show such a situation. It becomes therefore clear that higher order corrections play an important role in bond percolation. Only for sizes  $n \geq 7$  the leading correction seems sufficient since the data seem to follow a straight asymptotic line (see fig. 6).

We explored for which exponents the data are reasonably consistent with the scenario of fig. 6, i.e. straight lines for all site percolation data and for bond percolation with  $n \geq 7$ . We found

$$\tilde{t} = 0.9745 \pm 0.0015 \quad \text{and} \quad \omega = 1.2 \pm 0.2 \quad (16)$$

The value of  $\tilde{t}$  falls into the error bars of all previous estimates [12,15,17] and its error bar is several times smaller than previous error bars.

Besides the very precise calculation of the dynamical exponent of  $2d$  percolation, which excludes the two conjectures 91/96 and 1, we estimated the leading correction to scaling exponent and found that in the case of bond percolation sizes  $n < 7$  are dominated by even higher corrections. We discovered that random number generation is the most critical numerical difficulty and we believe that for the future of high speed computation it is of fundamental importance to find generators that have no pathologies when one has sequences of the order  $10^{11}$ . Our calculation would not have been possible without the special purpose computer and work calculating  $\bar{t}$  and  $\bar{s}$  in three dimensions is on course.

## 6. A SHORT REVIEW OVER SOME SPECIAL PURPOSE COMPUTERS THAT HAVE BEEN BUILT FOR STATISTICAL PHYSICS

Most of the about twenty SPC's that have been built by physicists in the last five years are related to statistical physics. Their construction time ranges from four months to four years. their price from 200 US dollars to  $2 \times 10^5$  US dollars. About half of the SPC's built are restricted to very specific applications; the others are more general. In addition there are at least 30 projects for SPC's about which I will not talk. A partial list of the more specific existing SPC's that are related to statistical physics is given in table I.

Table I  
Some SPC's built for statistical physics.

Place	Type	Completed	Ref.
M.I.T., USA	cellular automata	1982	23
E.N.S., France	cellular automata	1986	24
Santa Barbara, USA	Ising	1982	26
Delft, Netherlands	Ising	1982	30
Bell Labs, USA	Ising (spin glass)	1984	32
Delft, Netherlands	molecular dynamics	1983	36
Saclay, France	random conductivity	1987	20

Cellular automata have been the cheapest [23] and the shortest times were needed to construct them [24]. Since cellular automata SPC's can visualize their configurations very nicely on a screen, many interesting pictures have been made with them. Quantitative results have, however, been quite rare up to now. This might change in the future if recent ideas by Pomeau and others [25] to model hydrodynamic flow through cellular automata are exploited.

SPC's of the Ising type have been more successful in yielding precision data. The Santa Barbara machine [26] held the world record for a while for the speed of simulation of an Ising model with 30 million updates per second. (This record was later broken again

by general computers [27]). It yielded precise values for the critical temperature and the dynamic critical exponent of the three dimensional Ising model making nearly  $10^{12}$  updates [28]. However, more or less at the same time about equally precise estimates were obtained by other methods [29]. Also some incorrect results were produced for certain system sizes which were presumably due to correlations in the random number generator as was suggested for instance by calculations on the DISP [30]. The DISP is an SPC, slower but more versatile than the Santa Barbara machine. Several other calculations have already been performed on it including some that were reported on at this conference [31].

Another successful Ising-type SPC is the spin glass machine [32] built in Bell Labs. They found evidence for a finite transition temperature in the three-dimensional short range Ising spin glass [33]. The same result was also found by other authors at the same time using conventional computers [34]. The machine at Bell Labs was also used to study the random field Ising model [35].

Much more complex than the machines described above are molecular dynamics SPC's since they involve real numbers instead of integers and since they involve long range instead of short range interactions. The first molecular dynamics SPC was built by Bakker [36] in a pioneering effort using fixed point arithmetic. This machine was used to give some evidence that in two-dimensional melting no hexatic phase exists [37] in agreement with work done on conventional computers [38]. Another SPC for molecular dynamics has just been completed in San Jose [38].

Finally a number crunching SPC of equal order of difficulty is the one built in Saclay [20]. Its performance and the results obtained with it have been presented above.

Summarizing, we have described a new effort that has been made in the field of computational physics to overcome usual limitations of general supercomputers. It has to be left to the future to see if this development will survive in the long run or if a new generation of supercomputers will render it obsolete. Some more information about this field can be retrieved from older review articles [39].

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## FIGURE CAPTION

**Fig. 1** - log-log plot of the square distance  $R^2$  as a function of time steps  $N$  for a system  $40 \times 40$  at  $p_c$  averaging over 200 samples. The slope is  $2/d_w$ .

**Fig. 2** - log-log plot of  $n^{91/96}/\Sigma_n$  against  $n$  for  $2d$  bond percolation. The error bars are statistical. If conjecture (4b) were correct one would have asymptotically a horizontal line. Taken from Ref. 17.

**Fig. 3** - Schematic diagram for an architecture to calculate eq. (13). Taken from Ref. 40.

**Fig. 4** - General diagram of the Saclay machine [20]. The parts surrounded by heavy lines are the ones actually built. Taken from Ref. 40.

**Fig. 5** - log-log plot of  $R_n n^{0.98}$  against  $n$  for bond (b) and site (s) percolations. The bond percolation data are multiplied by a factor 2.5 to allow showing all data in one figure. Taken from Ref. 21.

**Fig. 6** -  $R_n n^{0.975}$  against  $n^{-1.3}$  for bond (b) and site (s) percolations. The bond percolation data are multiplied by two to allow showing all data in the same figure. Taken from Ref. 21.

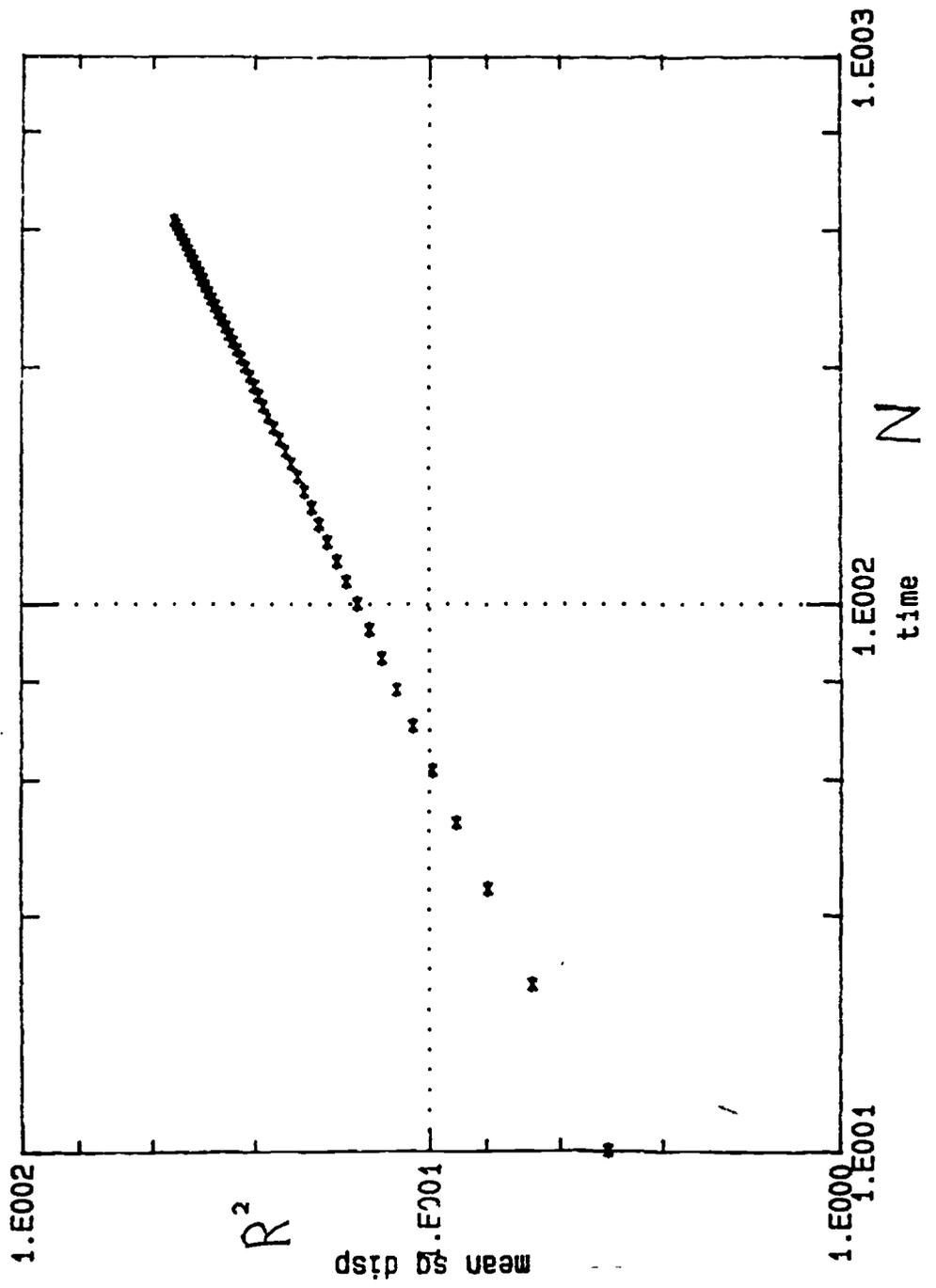


Fig 1

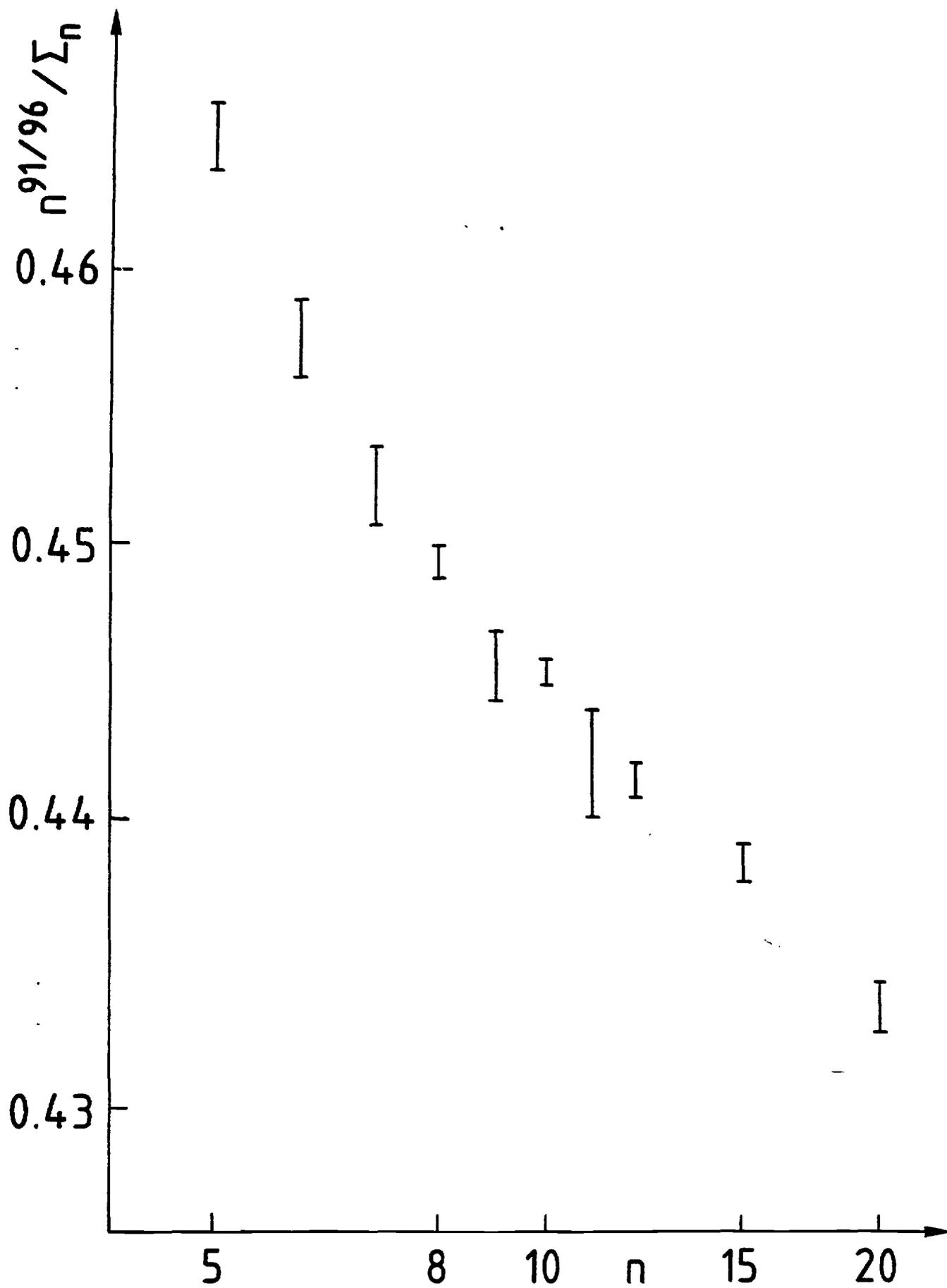
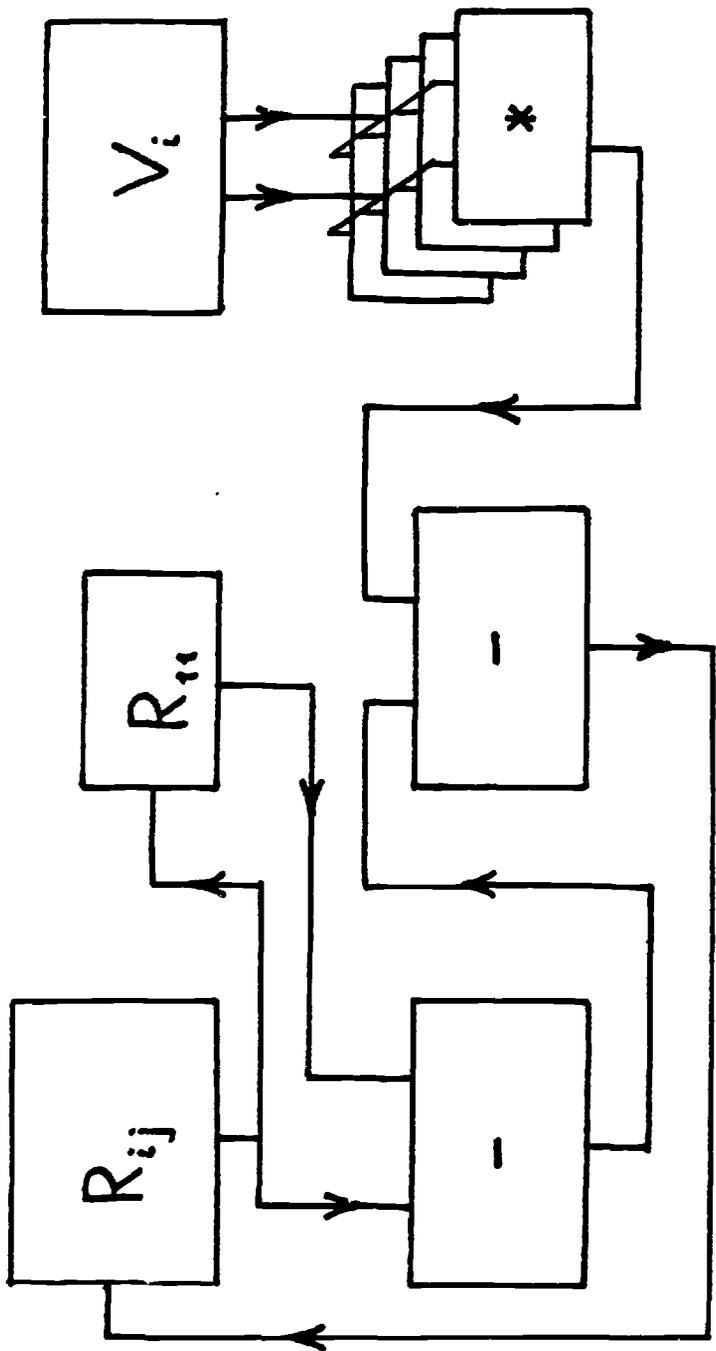


Figure. 2

15



16

Fig. 3

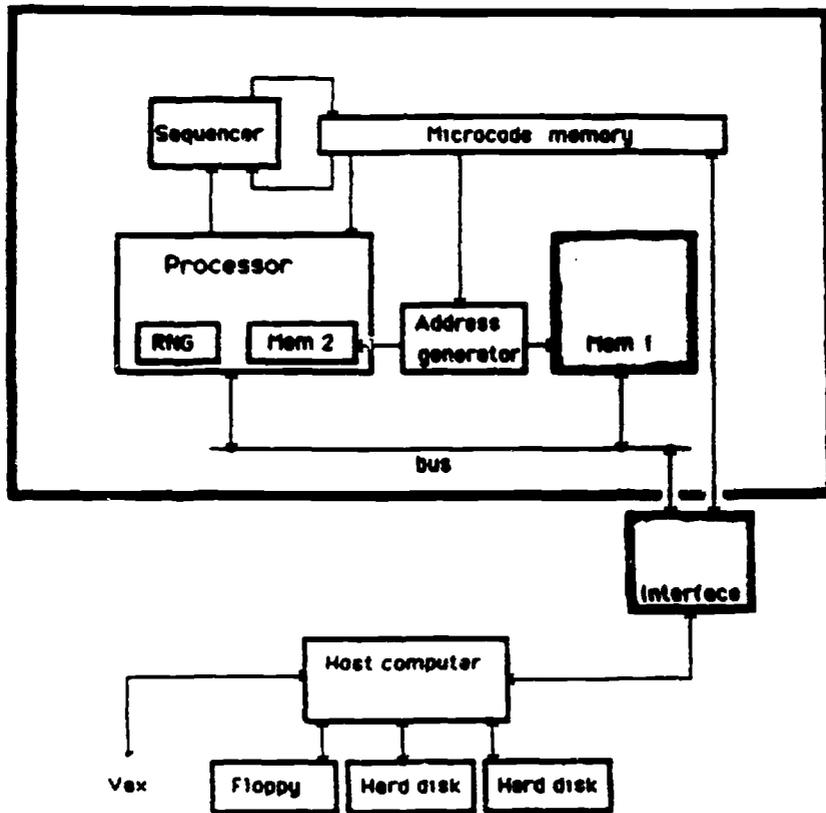


Fig. 4

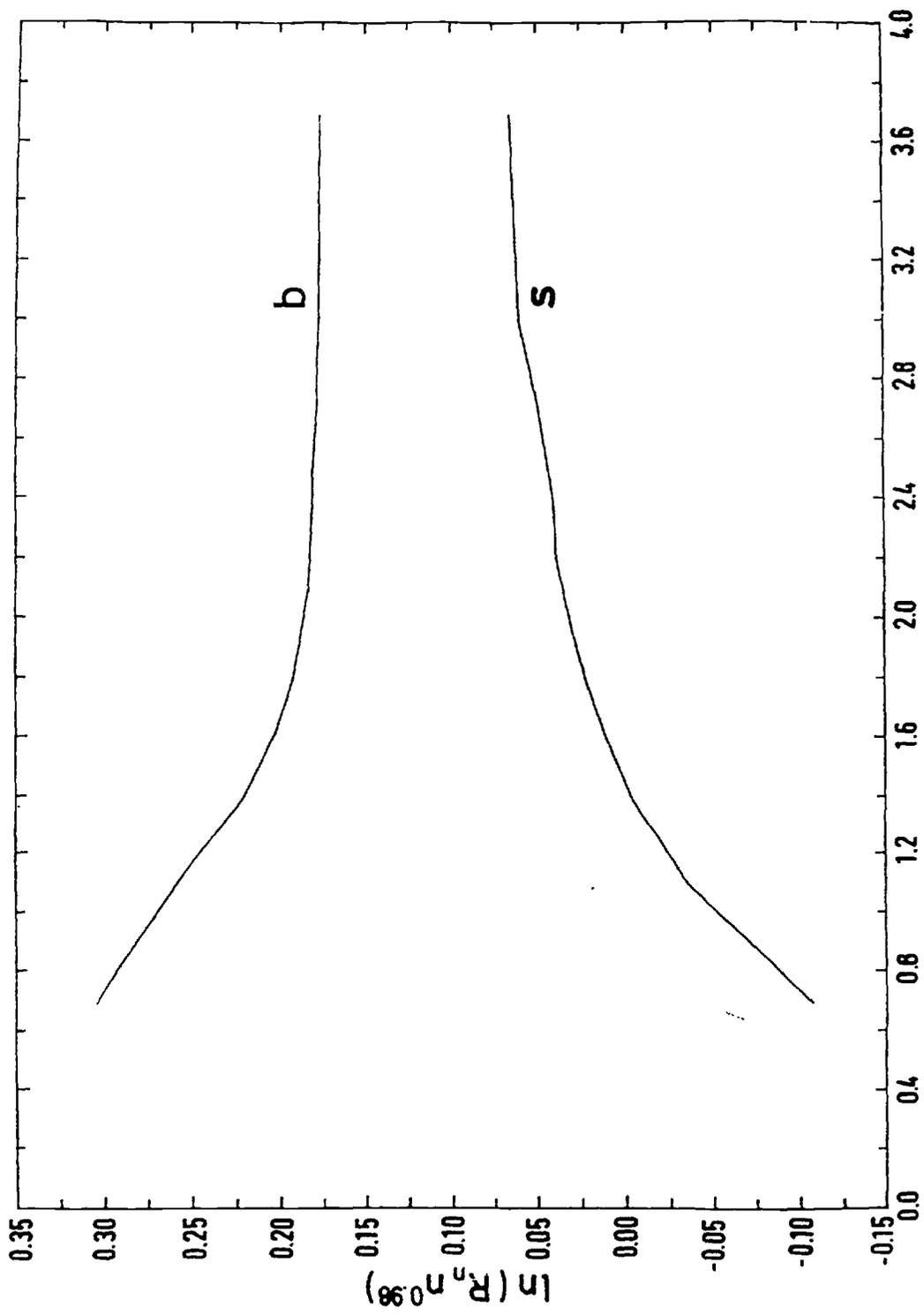


Figure 5

18

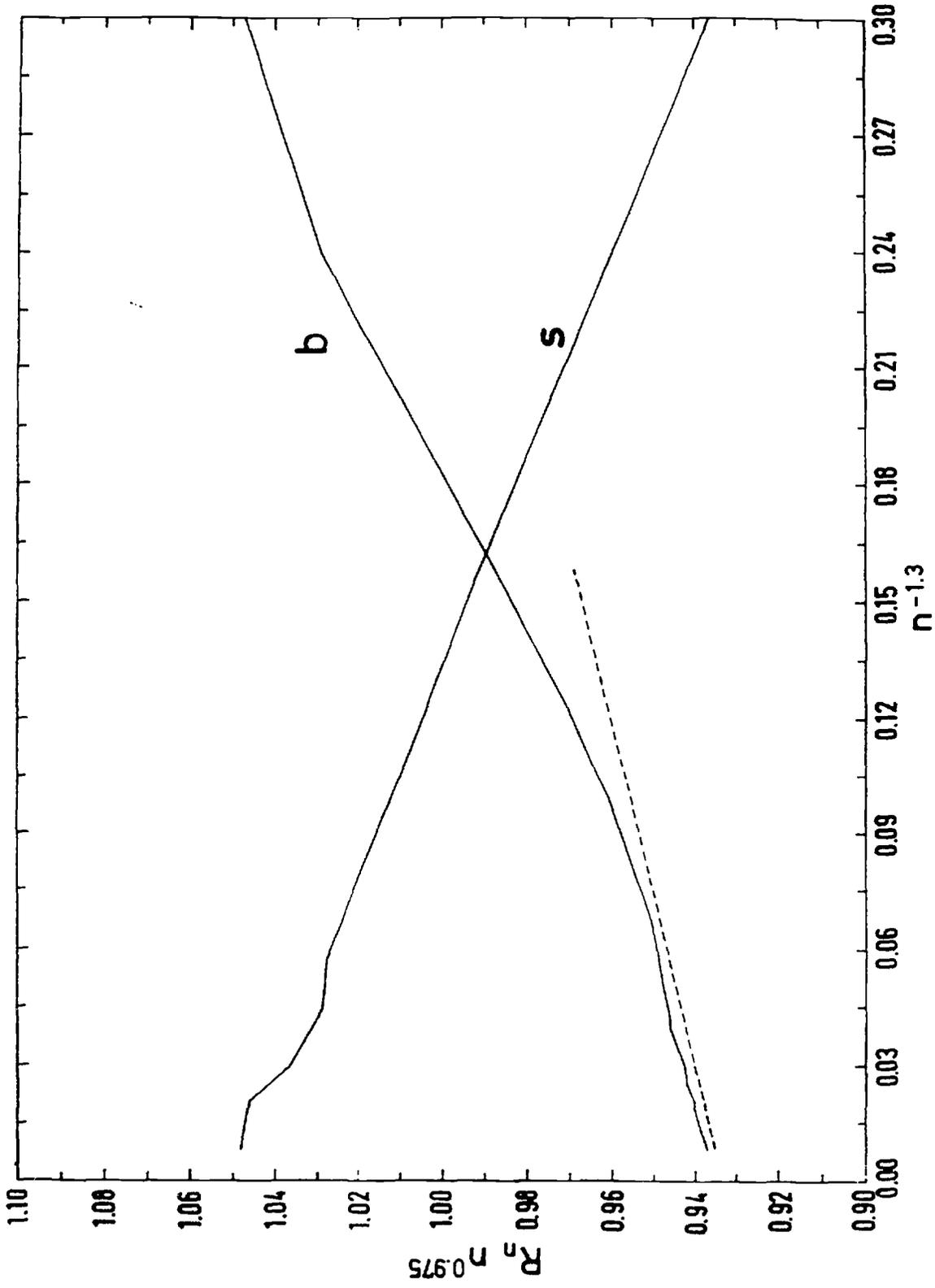


Figure 6

19