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EXPERIMENTAL MATHEMATICS*

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1. INTRODUCTION

The subject of description and discussion in this article is *experimental mathematics.* With this phrase I mean — more or less — using a computer as a mathematical laboratory, in which there can be done experiments for gaining insight and intuition for understanding (mathematical) problems and which can serve to generate ideas for conjectures. Or experiments which can suggest where to find, or how to construct, a counterexample. Or experiments designed to illustrate and modify certain potential routes for proving a conjecture and calculations to test or refine certain, as yet quite vague, conjectures. In brief, I intend to discuss a branch of mathematics which relates to more established mathematical thinking roughly as experimental physics to theoretical physics.

It is a simple fact of observation that computational results may — and very often do — lead to the development of new mathematics, i.e., also conceptual advances; just as observational and experimental results have always done since the time of Archimedes, both in the physical sciences and in mathematics.

Of course experimental mathematics in this sense is not purely a modern phenomenon. It is well known that Gauss did masses of calculations (examples) and derived insights from the results and, e.g., the Littlewood-Richardson rule(1) in the representation theory of the symmetric groups and general linear groups was first observed empirically in 1934, [1], later proved and since has led to a minor industry in combinatorics and representation theory.

However, computers have certainly added a new dimension to the enterprise of experimental mathematics, as if our mathematical laboratory suddenly obtained a new batch of instruments for measuring and exploring a new range of phenomena; also, it may well be that in many fields of mathematics a natural limit for "hand" calculations had been reached. In any case, the last 20 years or so have seen (the beginning of) a remarkable flowering of experimental mathematics, often in the hands of investigators with a physical or engineering background.

My interest here, in this talk, is in experimental mathematics as a tool of discovery. That means that I shall not really talk about scientific computing in so far as that activity is aimed at obtaining numerical answers for problems which are well understood (in principle) and solved, but where actually doing all the calculations is beyond the capacities of a modern human calculator (and even of one of a number of generations ago), irrespective of how much ingenuity and talent is needed to do the job numerically. However, there is no

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sharp boundary between scientific computing and experimental mathematics for several reasons. It may, for instance, very well happen that a computational scheme will suggest conceptual advances (cf. 3.4 below), or be so successful that a mathematical challenge arises: is this merely an unusually successful numerical trick or do we have here evidence for a previously unrecognized "truth" about a certain mathematical physical, chemical, etc. problem(34) (cf. especially 3.13 below and also the later half of note 5). Scientific computing is already a multi-billion dollar industry (with computational fluid dynamics taking care of most of the budget) and well on its way to becoming a separate mathematical discipline — much like, e.g., statistics — , with a methodology and aesthetics of its own. There certainly is something like a beautiful computation, and in that aspect it becomes very close to experimental mathematics which, in my view, will also become — it probably already is — a discipline in its own right.

There is also a second reason why scientific computing, or even just the availability of enormous computing power, stimulates "pure" mathematics. The mere existence of computing power has influence on the kinds of theoretical problems which can be considered and investigated(27). Thus a number of research areas with a fully developed theoretical (or pure, if one wants) component, like, e.g., semi-parametric statistics — I have in mind bootstrap methods and the jackknife statistic [2] — , two and more dimensional statistics (with its heavy dependence on computer graphics) [3](4), and computerized (read: applied) tomography would probably not have existed without very substantial computing power [4]. In this connection, it is interesting to observe that the theoretical problem at the basis of computerized tomography: inversion of the Radon transform was solved in 1917 [5]; as a matter of fact the formula seems to have been known (in dimension 3) to the Dutch physicist Lorentz before 1906 cf. [6, 7], and it has been rediscovered independently a number of times(2). A Nobel prize was given for applying — more precisely: implementing — this formula and, later, these applications generated, and still generate, whole series of new theoretical problems [4, 8].

I shall also not discuss "computer assisted proofs", such as that of the four colour problem, and I shall certainly not say anything about the philosophical implications and questions thereof [9, page 380-386].

Also, these lines are written from the point of view of a user of experimental mathematics but not a doer, and I shall concentrate on three examples where doing experiments (of quite moderate size as such things go) resulted in new unexpected insights, sometimes concerning a topic where nothing really interesting was supposed to happen. And where the mathematical experiments gave rise to new concepts, solution methods, and even whole new areas of inquiry. The examples, which will be discussed briefly and anecdotically below, in general terms, and omitting virtually all hard mathematics, are "the hard hexagon model of lattice statistical mechanics", "chaos and universality for iterated maps", and "integrable systems and the soliton revolution". These three examples are the topics respectively of sections 4, 5, and 6 below. Besides that, a number of other examples will be briefly mentioned in sections 3 and 7.

2. TWO CONTRASTING OPINIONS

Here are two rather opposite opinions

> "As I see it, within another generation, the mainstream of mathematics will not be analysis, number theory and topology but rather numerical analysis, operations research, and statistics. . . . I am not suggesting that the pure areas of mathematics or

for that matter the classical topics in applied mathematics such as transform methods, partial differential equations and approximation theory, will disappear. Instead like Newtonian mechanics, they may move permanently from centre stage in mathematics departments."

J. C. FRAUENTHAL [10]

A rather different opinion is the following

"... by the judicious use of computers we can penetrate into new areas and discover linkages to diverse areas of mathematics unforeseen by our forebears. With insight obtained from numerous solutions, often displayed naturally by graphs and cinemas, we may be liberated from the prejudices of our conservative and sometimes misguided mathematical intuitions."

"Almost everyone using computers has experienced instances where computational results have sparked new insights. The range covered is large: from uncovering mistakes in formal derivations or calculations to suggestions for combinations of parameters with which to make asymptotic expansions and thereby obtain equations which are analytically tractable; and finally to shining the light of inspiration into areas which have been thought devoid of possible new concepts or new fundamental truths."

"Although several pioneering steps have been taken, we are just at the beginning of a mind augmenting revolution that inexpensive and robust computing will allow the prepared investigator."

N. ZABUSKY [11]

This is precisely as John von Neumann expected things to develop. Speaking in 1946, he remarked [12]:

"The advance of analysis is at this moment stagnant along the entire front of nonlinear problems ... not transient ... we are up against an imported conceptual difficulty."

And he was counting on the computer to remedy this situation [ibid.]

"... we conclude by remarking that really efficient high-speed computing devices may, in the field of nonlinear partial differential equations as well as in may other fields which are now difficult or entirely denied of access, provide us with heuristic hints which are needed in all parts of mathematics for genuine progress .... This should lead ultimately to important analytical advances."

Also, one perhaps should reflect that our much vaunted intuition (in mathematics) and feeling for phenomena is maybe overrated. H. HAHN, [13], once described intuition as "force of habit rooted in psychological inertia" (3), and without fresh experience to feed on, one can easily see how this might become so. If, therefore, as seems to be the case, we have indeed, in a number of fields, reached something of a limit in computation by hand, experimental mathematics becomes a must. Quoting Hahn, as above, Zabusky, loc. cit., speaks in this connection of the enriching possibilities of "computational synergetics" and mathematical innovations, given a judious use of computer power.

Below in Sec. 4, 5, and 6 I shall try to describe in more detail how in a few instances interaction of experimental mathematics with theoretical and applied mathematics went, and shall try to point out the synergetic influences. These short descriptions and the section of loose quotes below should suffice to indicate which way things seem to be going.

In addition, it seems worth remarking that in all three of the main examples described below there is a nice mix of pure and applied mathematics (besides experimental mathematics and physics) and not much seems to remain of the supposed gap between the two. This also makes papers dealing with these topics hard to classify, a more and more common phenomenon, which indicates that present day mathematics is more integrated and far less tree-like than would be convenient for bibliographical and information storage and retrieval purposes.

3. QUOTES

As I remarked before, and as Zabusky remarked in the quote above, it is a simple fact of experience that doing mathematical experiments on a computer may easily lead to sudden illuminating (true or false, but stimulating) insights. Let me try to illustrate this by quoting from the more recent scientific literature. Let me also stress that I made no special effort to find such quotes. These are simply the ones I happened to come across since the moment, now about a year ago, when I started thinking about an article on experimental mathematics. There are likely to be many more and it seems clear that the controversy indicated above was in fact already settled long before Frauenthal made his remarks.

3.1. From computational physics in general

> " The goals of computation . . . include the discovery of new simplyfying physical principles by observing the computed behaviour of the model"

D. R. HAMANN [14] (5,6)

To this I would also like to add that computers enable both experimentalists and theorists to explore physical systems in a manner not previously possible (by "real" experiments). For instance, certain parameters can be pushed to unphysical values, or simply to values impossible to realize in an existing laboratory(42). Also, this way experiments can be carried out in sciences where experiments have been said to be impossible; such as economics.

And it is well known that (new) principles often manifest themselves most clearly in some sort of limit, some sort of extreme case. As R. Isaacs remarks in his advice to young applied mathematicians [15]: if you do not understand how something will behave, take an extreme case.

3.2. Concerning Yang-Mills gauge theories

For a quantum field theory of strong interactions based on quarks (interacting by exchanging gluons), one wants both "confinement", wherein an isolated quark would have infinite energy, and asymptotic freedom, which means that the interactions between quarks become weaker as they move closer together. This seems hard to do, and maybe even counterintuitive. However, out of Monte Carlo simulations for studying solutions to interacting quantum fields there came:

> "The main result is that we now have rather compelling numerical evidence that this theory [Yang-Mills gauge theory] can simultaneously give rise to the phenomena of quark confinement . . . and asymptotic freedom . . . ."
>
> M. CREUTZ [16]

3.3. On food webs

A food web is a schematic diagram showing the (who eats whom) relationships among species in a community of plants and animals. Omnivores are animals consuming prey from two or more trophic levels. In simulated webs with Lotka-Volterra interactions between species, long food chains lead to severe population fluctuations that are inconsistent with long-term persistance. Also, numerical studies of the dynamical stability of model webs with Lotka-Volterra interactions predict that the number of omnivores in a real food web is significantly lower than would be found if the connections within the web were made at random. This last fact turned out to be the case, and the first one goes a way towards explaining that, in real food webs, species tend to interact directly only with a handful, four or five or so, of other species regardless of the size of the ecological community. Sources for these remarks are [17] and [18].

3.4. From computational fluid dynamics (CFD)

Computational fluid dynamics (CFD) is the process of solving problems in fluid dynamics (including aerodynamics) on a computer. That is, they basically deal with one particular set of partial differential equations, the Navier-Stokes equations. In spite of that, this is a multi-billion dollar industry which mostly belongs to scientific computing and which is rapidly turning into a discipline of its own (besides applied mathematics, statistics, pure mathematics, experimental mathematics, etc.), with its own aesthetics and paradigms. It has, however, very definite and interesting relations with all three of pure, applied, and experimental mathematics. For example:

> "Some mathematical and CFD developments go hand in hand: Lax's theories of hyperbolic conservation laws and of differencing in conservation form (see [19, 20]) are parts of a single picture."
>
> "A recent example is provided by Glimm's existence proof for nonlinear hyperbolic equations [21], which was loosely suggested by Godunov's computing scheme and has in turn given rise to new algorithms (see [22])."
>
> A. J. CHORIN [23].

3.5. On glassy solids and quench echos

> "When we try to understand atom motion in amorphous solids we face a complicated problem in classical mechanics . . . . Without a periodic crystal lattice to simplify the calculations, we must look for other properties that make things tractable. A

phenomenon recently observed in computer models of many-body systems give us such a simplification, at least in the calculation of a number of properties of glassy solids."

"In spite of their seemingly random motion, atoms in computer-simulated glasses 'remember' the time interval between a pair of freezings, simplifying certain many-body calculations."

S. R. NAGEL a.o. [24].

3.6. From geology

One use of simulation or computer modelling is to find out whether certain accepted axioms of dogmas are indeed tenable. Just as mathematics has often been concerned with the question of whether a certain set of axioms is compatible. Cf. also note 7. From palaeogeomagnetics we have, e.g.:

"Computer models, designed to synthesize palaeosecular variations of the geomagnetic field, cast doubt on some widely accepted palaeo magnetic dogmas."

K. M. CREER [25].

3.7. A chaotic quote

Chaos, in the setting of iterated maps of an interval into itself, will be briefly discussed in Sec. 5 below. Period doubling bifurcations play an important role there. From thermosolutal convection (convection in the presence of a stabilizing concentration of a solute):

"Numerical experiments on two-dimensional convection reveal a transition from periodic oscillations through a sequence of period-doubling bifurcations. . . . . This is the first example of period-doubling in solutions of partial differential equations."

D. R. MOORE a.o. [26].

3.8. From catalytic chemistry

The properties of single atoms (from a chemical point of view) have been known for a long time and also those of bulk substances, but not those of clusters of, say, 2-200 atoms. Especially in connection with catalysis.

"Some preliminary computational studies and complementary model experiments, . . . suggested that some really exciting chemistry could exist in this domain and provided a strong incentive to learn how to make the clusters."

T. H. MAUGH II [27],

3.9. Re phase transitions and the van der Waals picture of liquids

"A remarkable revival of the van der Waals picture of liquids occurred during the last two decades. This renaissance was spurred by the discovery [28, 29, 30] from computer simulations that a system of hard spheres (impenetrable 'billiard balls') has a first order fluid-solid transition that is intimatedly related to the freezing and melting transitions of real materials . . . ."

D. CHANDLER a.o. [31].

3.10. Re planet formation

One possible model for the formation of the planets of our solar systems involves the idea of lots of small pieces which, when they collide, may, under the right conditions, adhere to one another. This idea was computer-simulation tested by G. W. Wetherill with spectacular results as the pictures below will testify.[36] The first picture refers to the initial state with a hundred planetesimals, the second depicts the situation after a long time interval with about 20 "small planets" and the third depicts the result a really long time later with just five planets left.

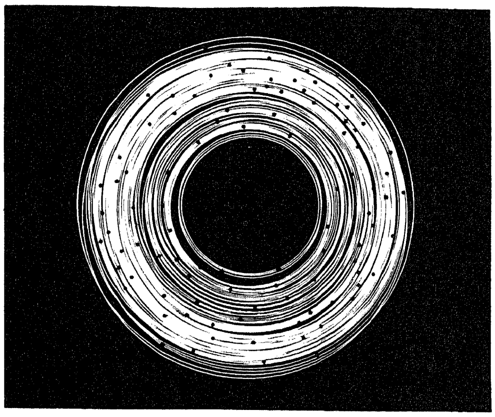


Fig. 1. (from [32])

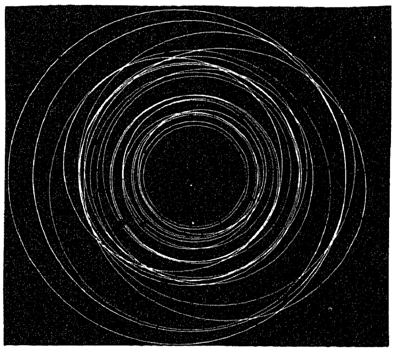


Fig. 2. (from [32])

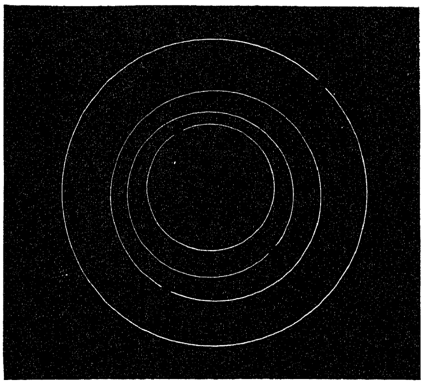


Fig. 3. (from [32])

3.1. From cosmology

> "Take a mixture of gas and dust, cook it appropriately with the aid of a large computer and a galaxy may emerge. That, at least, is the dream of astronomers who study the most remote galaxies."
>
> J. SILK [33]

Besides that, it has become clear that the universe contains very

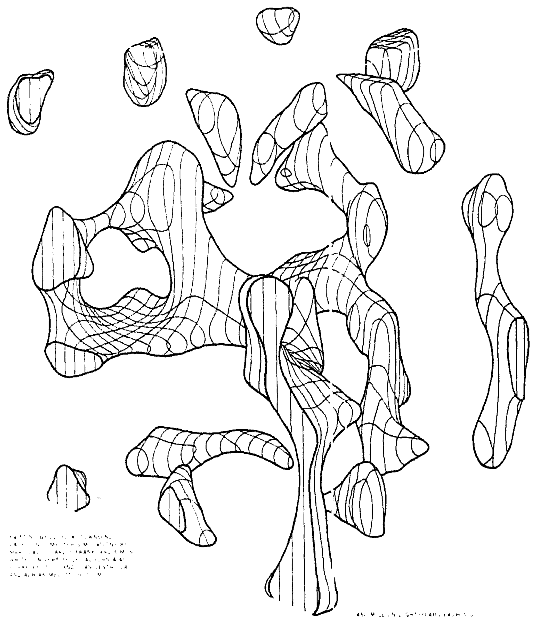


Fig. 4. (from [34])

large, indeed unusually large, voids; it is not at all homogeneous with galaxies or clusters of galaxies, or superclusters randomly distributed. Instead, it is very clumpy. It thus becomes interesting to test whether various candidate cosmogenies predict (or admit) such clumpiness. Computer studies concerning this have, indeed, been carried out, and some of these are reported on in a beautiful report [34] in the National Geographic magazine. An artist's impression of the resulting filimentary structure (caused by clumping of neutrinos) is shown above(8).

3.12. From fluid dynamics (out of equilibrium)

> "Progress [in fluid dynamics] through the years has been uncertain however, with periods of success amid long periods of frustration and fragmentation of effort. But today we are in an upswing. In particular it seems that we may be close to understanding quantitatively why a fluid out of equilibrium can behave as it does - long an intractable problem. Two tools especially have contributed: the laser and computer

simulation. These tools, the one experimental, the other theoretical, yield unambiguous results that allow one to test theories (some of which were proposed long ago) and that suggest paths for further study."

H. J. M. HANLEY, *Physics Today*, Jan. 1984, p. 25

"Computer simulations indicate that simple liquids can display a surprising range of exotic nonequilibrium phenomena, more commonly seen in systems of macromolecules."

D. J. EVANS a.o. [35]

"However computers are prompting important changes within mechanics itself . . . We will see that the effort to model real systems forces us to pay close attention to constraints, in particular, to nonholonomic constraints, which we do not often encounter in textbook problems in classical mechanics.

W. G. HOOVER [36]

3.13. From quantum field theory

Finite element methods are well known in partial differential equations. Basically, one selects a number of functions (often monomials in the variables) and attempts to "approximate" the solution of the PDE by taking linear combinations of these functions. To this end, divide the region into nonoverlapping patches, impose the PDE at one point in every patch and impose conditions of matching (with the functions on a neighboring patch or boundary conditions, as the case may be) at the boundaries of each patch. This gives algebraic conditions for the coefficients.

In principle, one can also take operator-valued coefficients and try to do similar things for the equations of quantum field theory by using, say, a lattice. There arises the extra difficulty of seeing to it that the equal time commutation relations hold (at all times). This turns out to be possible [37, 38]. In other words, the resulting operator difference equations preserve equal-time commutation relations. When the same idea is applied to a free fermion theory, it turns out that the resulting difference equations are consistent with equal-time anticommutation relations, and other nice properties, and, quite surprisingly it turns out that the oft-encountered problem of so-called fermion doubling is avoided. This last fact was a totally unexpected bonus and is remarkable in that there are general theoretical results [39] showing that fermion doubling when taking lattice approximation is difficult to avoid. As Carl Bender recently remarked in a telephone conversation with me:

"It is as if Nature intended us to use finite element methods"

C. M. BENDER, Dec. 1983[9,10]

4. THE HARD HEXAGON MODEL OF LATTICE STATISTICAL MECHANICS[13]

In lattice statistical mechanics models

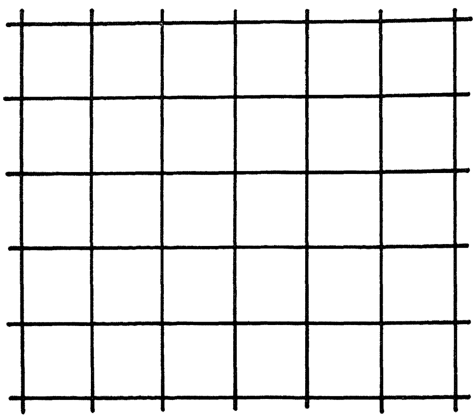


Fig. 5.

one works with a lattice in d-space, for example, a square lattice in two space, as depicted above. Atoms are supposed to be located at some or all of the sites. Each atom can be in several states. To each configuration c there is assigned an energy $E(c)$. For a large chunk of N sites of the lattice now write down the so-called partition function

$$Z_N = \sum_c \exp(-E(c)/kT) \tag{4.1}$$

(where k stands for the Boltzmann constant and T for the temperature. This is *the* basic object of statistical mechanics and from it one calculates various thermodynamically interesting quantities such as the free energy $F=-kT\ln Z_N$, the probability of the system being in state c (i.e. configuration c), the free energy per site in the large N limit $f(t)=-kT\lim_{N\to\infty}N^{-1}\ln Z_N(T)$ (one expects this limit to exist), the internal energy per site $u(T)= -T^2\frac{\partial}{\partial T}(T^{-1}f(T))$, the specific heat per site $c(T)=\frac{\partial}{\partial T}u(T)$, . . . (also all kinds of average and expected values, such as correlations), the partition function per site

$$\kappa = \kappa(T)=\lim_{N\to\infty} Z(T)^{1/N} \tag{4.2}$$

and one is, in particular, interested in finding out whether these functions $f(T)$, $u(T)$, $c(T)$, etc. have singularities at certain values of T (phase transitions). For instance, for the square lattice depicted above, one could be interested in the model where all sites are occupied with an atom at each site i with spin either up ($\sigma_i=1$) or down ($\sigma_i=-1$) and nearest-neighbour-only interaction resulting in an energy function (Hamiltonian)

$$E(\sigma) = -J\sum_{(i,j)}\sigma_i\sigma_j + K\sum_i \sigma_i \tag{4.3}$$

where the first sum is over all pairs of adjacent sites (i,j) and the second one over all sites i. This is the well known nearest neighbour Ising model,

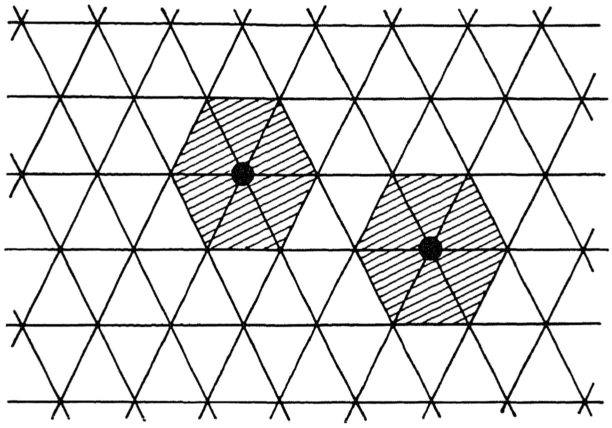


Fig. 6.

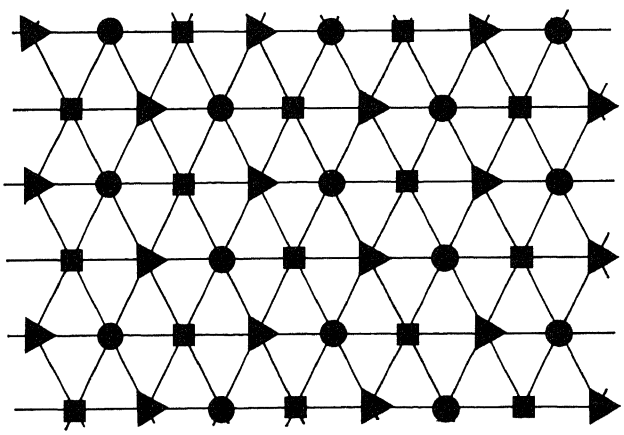
and is not the subject of this section. In the case of the hard hexagon model, one considers a triangular lattice as shown in Fig. 6 above. The possible states at each site are 1 (atom present) and 0 (empty). The energy function (Hamiltonian) is such that the partition function takes the form of the generating function

$$Z(z,N) = \sum_p g(p,N) z^p = 1 + Nz + \frac{N(N-7)}{2} z^2 + \cdots \tag{4.4}$$

where $g(p,N)$ is the number of ways in which p atoms can be distributed over the lattice of N sites such that no two coincide and no two neighbouring sites are occupied. Thus, if a given site is occupied, a whole hexagon of sites is forbidden (cf. Fig. 6), as if we were dealing with a gas of impenetrable hexagonal atoms. Whence the name hard hexagon model [12].

The parameter z in (4.4) has much to do with T in (4.1) and plays the same role. It is called the activity.

Now if there are only a few atoms, say 1, each site has equal probability of being occupied. So for small z one expects the full triangular symmetry to be present. There are three ways of packing very large densities of atoms on the triangular lattice (cf. Fig. 7): either all the rectangular sites are occupied



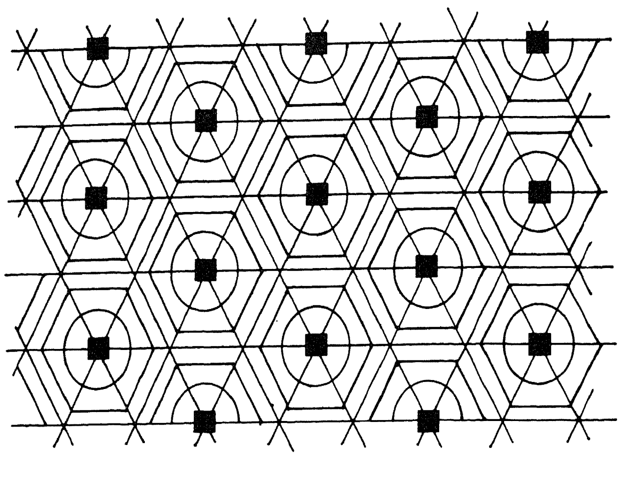


Fig. 7.

(and no others), or all the circular ones, or all the triangular ones. There is loss of symmetry, indicating a phase transition, which is, of course, just the sort of thing one is looking for when constructing such models. Let $\rho_S =$ density on square sites, $\rho_T =$ density on triangular sites, and $\rho_C =$ density on circular sites. Suppose that as z increases the square sites are preferred, then $\rho_S \to 1$, $\rho_T \to 0$, $\rho_C \to 0$ as $z \to \infty$, and if $R = \rho_S - \rho_T$, say, the graph of R as a function of z would look something like that in Fig. 8.

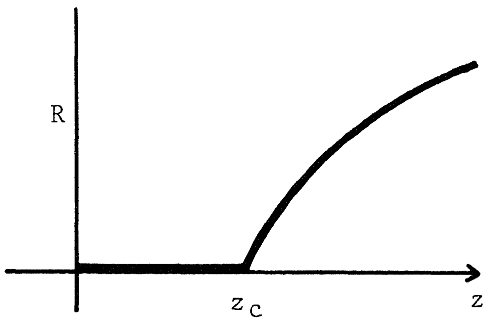


Fig. 8.

I.e. there must be a critical point z_c where R first becomes non-zero. By various numerical calculations (maximum eigenvalue estimates, series expansions in z and z^{-1}), estimates for z_c can be obtained. One such by J. Gaunt in 1967 gave $z_c = 11.05 \pm 0.15$. There is also a nonphysical critical point z_n for which Gaunt, obtained $z_n = -0.0900 \pm 0.0003$. If one is in an experimental mood, one can calculate sum and product of z_c and z_n to find $z_c + z_n = 10.96 \pm 0.15$, $z_c z_n = -0.995 \pm 0.014$ and observe that these are practically integers. This would result in

$$z_c = \tfrac{1}{2}(11 + 5\sqrt{5}) = [\tfrac{1}{2}(1+\sqrt{5})]^5 \tag{4.5}$$

All this was observed by Gaunt, but he did not include the conjecture (4.5) in his paper. Other calculations resulted in a value for $\kappa(1)$ (cf. (4.2) above) of $\ln \kappa(1) = 0.3333 \pm 0.0001$ by Metcalf and Yang in 1978 and they did publish the conjecture that $\ln \kappa(1) = 1/3$.

Around this time Rodney J. Baxter, Canberra, Australia, decided to take up the challenge, convinced that he had devised a class of methods which would yield far more precise numerical results. This method is based on so-called transfer matrices, in this case corner transfer matrices, and it results in the partition function $Z(z, N)$ being written as a trace of the sixth power of an (in principle infinite) matrix

$$Z = Trace\ A^6 \tag{4.6}$$

The power 6 here is important from the numerical point of view, leading, with a bit of luck, to rapid convergence of the series expansion

$$Z = \lambda_1^6 + \lambda_2^6 + \lambda_3^6 + \cdots$$

where $\lambda_1, \lambda_2, \lambda_3, \cdots$ are the eigenvalues of A in descending magnitude. How to actually calculate $\lambda_1, \lambda_2, \cdots$ requires more clever ideas (cf. [40, 41]), but some of the results are

Approximating matrix size	$\ln \kappa(1)$	Error
2×2	0.333 050	1.9×10^{-4}
3×3	0.333 242 657	6.5×10^{-8}
5×5	0.333 242 721 958	1.8×10^{-11}
7×7	0.333 242 721 976 1	4.7×10^{-15}

so that, obviously, $\ln \kappa(1)$ is not $1/3$.

Of course, the λ_i are functions of z, and knowing a small z expansion of $Z(z)$ and $A(z)$, one can write down the leading terms of λ_i in the small z expansion

λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8	λ_9	λ_{10}
1	1	$-z$	z^2	z^2	$-z^3$	$-z^3$	z^4	z^4	z^4

and test various monomials in the λ_i suggested by these leading terms in a search for some kind of regularity. Baxter did just that, and found (for the 7×7 approximation [15]:

$\lambda_4\lambda_3^{-2}$	0.999 999 853
$\lambda_5\lambda_2^{-1}\lambda_3^{-2}$	0.999 999 539
$\lambda_6\lambda_3^{-3}$	0.999 757 797
$\lambda_7\lambda_2^{-1}\lambda_3^{-3}$	0.999 730 684

Thus, it seemed that $\lambda_j = \lambda_2^s x^{n_j}$, $s \in \{0,1\}$, $x = \lambda_3$. Now, Baxter had encountered some such situation before. Namely, when he solved the eight vertex model, and in that case theta functions and elliptic functions had played a fundamental role. So he programmed the computer to calculate the exponents in a product expansion

$$z = -x \prod_{n=1}^{\infty} (1 - x^n)^{c_n}$$

(one of the sorts of thing one naturally thinks of if one has theta functions in mind), and Baxter found 5,-5,-5,5,0, 5,-5,-5,5,0, 5,-5,-5,5,0, 5,-5,-5,5,0, 5,-5,-5,5,0, 5,-5,-5,5,0, ... A most stimulating result. This then provided the starting point for solving the hard hexagon model exactly [41] including that indeed $z_c = \frac{1}{2}(11+5\sqrt{5})$.

The story does not stop here. Far from it. Baxter found that he could make good use of certain (formal) identities of the type

$$\sum_{n=0}^{\infty} \frac{q^{n^2}}{(1-q)(1-q^2)\cdots(1-q^n)} = \prod_{n=1}^{\infty} \frac{1}{(1-q^{5n-4})(1-q^{5n-1})}$$

known as Rogers-Ramanujan identities [42, 43, 44]. These "belong" to the world of theta functions. More precisely, it turned out that there are four regimes for the generalized hard hexagon model. For three of these the identities that Baxter found and could use turned out to be known. For the fourth one he could conjecture (and verify to degree 80) one which turned out to be new, again using computer support. This one was shortly after proved by G. E. ANDREWS [45].

Still the story is not finished. One can consider the "decorated hard hexagon" model in which, instead of two possible states 0 and 1, one has k possible states at each site. This has also been considered by Baxter and Andrews and turns out to involve generalized Roger-Ramanujan type identities in which the magic number 5 is replaced by $2k+1$. And things go on . . . .

All in all there now is a flourishing interdisciplinary area of research between combinatorics and lattice statistical mechanics which arose, to a large extent, from Baxter's work on the hard-hexagon model[11, 14].

5. CHAOS AND UNIVERSALITY FOR ITERATE MAPS OF AN INTERVAL INTO ITSELF

We are interested in a map of an interval into itself. For instance

$$\begin{aligned} &f_\mu(x) = 1-\mu x^2\,, && [0,1]\to[0,1] \\ &f_\mu(x) = \mu x[1-x]\,, && [0,1]\to[0,1] \\ &f_\mu(x) = \mu\sin\pi x\,, && [-1,1]\to[-1,1] \end{aligned} \tag{5.1}$$

And we are especially interested in what happens if the mapping is iterated a large number of times and how this "limit behaviour" changes as the parameter μ changes.

Before I say anything about the phenomenology let me quote something from [46] about the history of the topic

> "The methods used to study smooth transformations of intervals are by and large elementary and the theory could have been developed long ago *if anyone had suspected that there was anything worth studying.* In actual fact, the main phenomena were discovered through numerical experimentation and the theory has been developed to account for the observations. In this respect, computers have played a crucial role in its development."
>
> O. E. LANFORD [46]

A quote which certainly supports the point of view of von Neuman and Zabusky rather than that of Frauenthal [16].

Here is something of the phenomenology observed. For small μ ($\mu<0.75$ for the second of the maps of (5.1)), there is a unique attracting point x_0; that is for almost all x (in fact, all x except $x=0$) the sequence

$$x,\ f_\mu(x),\ f_\mu^{(2)}(x)=f_\mu(f_\mu(x)),\ f_\mu^{(3)}(x),\ \cdots$$

converges to x_0. Then, as μ becomes larger, x_0 splits into an attracting orbit of period 2, that is there are two points, x_1 and x_2, say, such that $f_\mu(x_1)=x_2$, $f_\mu(x_2)=x_1$ and for almost all x, $f_\mu^{(n)}(x)$ comes arbitrarily close to x_1 or x_2 and hops back and forth between the two with each new iteration. For still larger μ (at $\mu_2=1.25\cdots$), an attracting orbit of period 4 appears, which in turn splits into one of period 8 at $\mu_3=1.368\cdots$ etc. It turns out (numerically) that these μ_n have a limit and that

$$\mu_\infty-\mu_n \sim \mathit{const.}(4.6692\cdots)^{-n} \quad \text{as } n\to\infty \tag{5.2}$$

This number 4.6692. . . now turns out to be a universal constant, meaning that the same constant appears for all kinds of different maps, a numerical discovery of M. FEIGENBAUM [47] and COULLET-TRESSER [48]. It is now often known as the Feigenbaum number. There is more. If one plots the position of the attractors of period 1, 2, 4, 8, 16, . . . as they are about the fission, one obtains something like the following picture (Fig. 9).

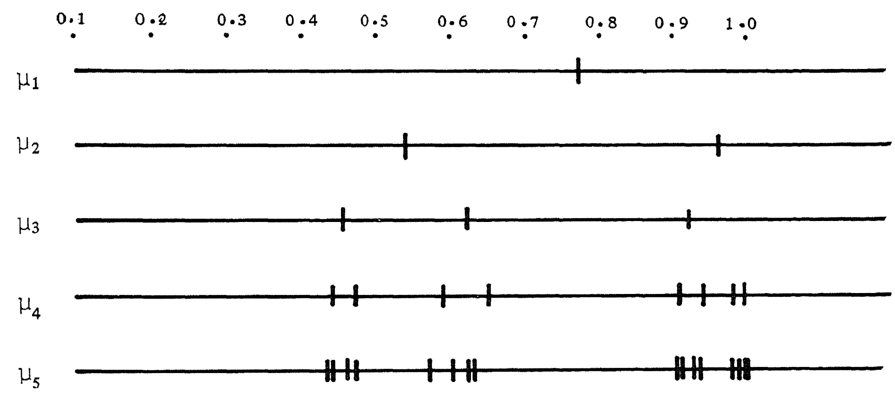


Fig. 9.

One observes that the left half of each line is the mirror image of the line immediately above scaled down by a factor of about 2.5. The precise factor (in the limit) turns out to be $a=2.5092078\ldots$, and again it turns out to be a universal constant.

These numerical observations or discoveries of course simply cry out for an explanation and great progress has been made in the theoretical understanding of why such things happen. Mathematically, the clue lies in the consideration of the nonlinear mapping (of functions into functions) $T: f\to a^{-1}(f\circ f)(ax)$ and to search for a scaling constant a for which this mapping has a fixed point. The fixed point is hyperbolic with one eigenvalue (of its linearization at the fixed point) greater than 1. This eigenvalue is equal to 4.6692. . . .

There also remain lots of open questions. For instance, there is very little known of the solvability of functional equations like $f(x)=a^{-1}(f\circ f)(x)$ and of the properties of the solutions. E.g., does there exist a smooth solution? Another open question concerns the order in which various periodic orbits appear as μ increases. Omitting the periods of order $\geqslant 8$, this sequence is

1,2,4,6,7,5,7,3,6,7,5,7,6,7,4,7,6,7,5,7,6,7

and it also appears to be of a universal nature [49]. This is as yet unexplained and is not understood.

As μ_n reaches its limiting value 1.401. . . and goes past it, the motion of a point becomes chaotic (17) meaning that it is virtually impossible to predict the position of the n-th iterate $f^{(n)}(x)$ for a starting point x; in other words, small differences in starting position rapidly (exponentially fast) become very large differences in the higher iterates. For still larger μ, a measure of more ordered motion may reappear, etc.. We are also as yet quite far from understanding this pattern of reappearance and disappearance of more ordered motion.

Turning to the more dimensional case, there also appear to be universality phenomena for both conservative and dissipative mappings of pieces of planes into themselves which still are ununderstood and provide a fruitful hunting ground for experimental mathematicians [50-54].

Deterministic chaos theory has become a thriving business (18) and has made significant contact with other areas of investigation such as scaling and renormalization (group) theory in physics and theories of turbulence in fluid dynamics.

6. INTEGRABLE SYSTEMS AND THE SOLITON REVOLUTION

Probably the first mathematical experiment on a computer was done in Los Alamos, at the time that the MANIAC, the Los Alamos copy of the Princeton Von Neumann machine, was barely finished. Fermi, Ulam, and Pasta had deliberatedly selected a problem for which the machine would be much more suitable than a human calculator. Here is Stan Ulam on the topic in his autobiography [55].

> "As soon as the machines were finished, Fermi, with his great common sense and intuition recognized immediately their importance for the study of problems in theoretical physics, astrophysics, and classical physics. We discussed this at length and decided to attempt to formulate a problem simple to state, but such that a solution would require a lengthy computation which could not be done with pencil and paper or with the existing mechanical computers. After deliberating about possible problems we found a typical one requiring long-range prediction and long-time behaviour of a dynamical system. It was the consideration of an elastic string with two fixed ends, subject not only to the usual elastic force proportional to strain, but having, in addition, a physically correct small non-linear term. The question was to find out how this non-linearity after very many periods of vibrations would gradually alter the well-known periodic behaviour of back and forth oscillation in one mode; how other modes of the string would become more important; and how, we thought, the entire motion would eventually thermalize, imitating perhaps the behaviour of fluids which are initially laminar and become more and more turbulent and convert their macroscopic motion into heat. . . .
>
> Our problem turned out to have been felicitously chosen. (37) The results were entirely different qualitatively from what even Fermi, with his great knowledge of wave motion, had expected. The original objective had been to see at what rate the energy of the string, initially put into a single sine wave (the note was struck as one

tone), would gradually develop higher tones with the harmonics, and how the shape would finally become a "mess" both in the form of the string and in the way the energy was distributed among higher and higher modes. Nothing of the sort happened. To our surprise the string started playing a game of musical chairs only between several low notes, and perhaps even more amazingly, after what would have been several hundred ordinary up and down vibrations, it came back almost exactly to its original sinusoidal shape. . . .

Another Los Alamos physicist, Jim Tuck(39), was curious to see if after this near return to the original position, another period started again from this condition and what it would be after a second "period". With Pasta and Metropolis, he tried it again and, surprisingly, the thing came back, a percent or so less exactly. These continued and, after six or twelve such periods, it started improving again and a sort of superperiod appeared. Again this is most peculiar."

S. Ulam [55]

Here is picture of the sort of thing which went on (Fig. 10).

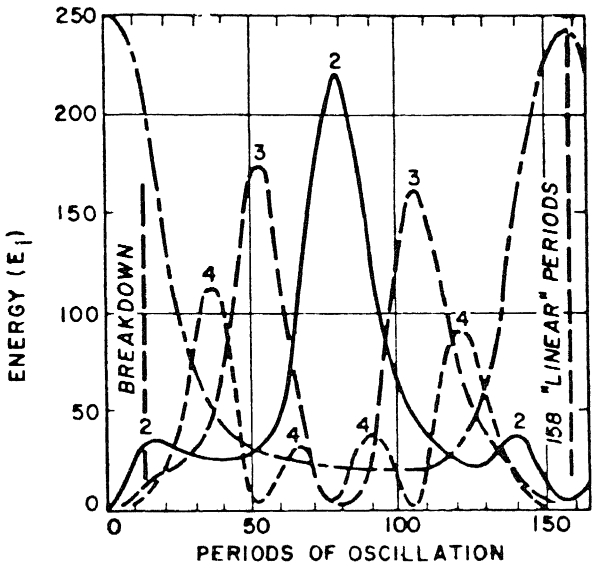


Fig. 10. (from [56])

This, of course, demanded an explanation. It was almost as if there were certain entities wich were stable in time and for which some sort of superposition principle would hold.

These entities were found, they are the so-called solitons, a term coined by Kruskal, Miura, Gardner, Greene, and Zabusky to describe a solitary travelling wave which retains its shape while travelling and with the remarkable stability property that when it encounters another soliton both emerge intact from a temporary messy interference pattern (apart from a phase change). A picture illustrating this behaviour of

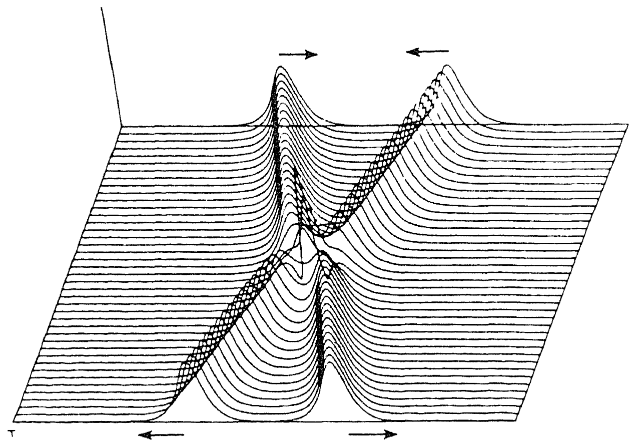


Fig. 11. (from [11])

solitons is Fig. 11. For a lengthy and most thorough account of how the concept of solitons developed initially in the hands of the five persons just named and of how the computer, or more precisely mathematical experiments with the help of a computer, continued to play an important role cf. the review paper [11] by one of those deeply involved, N. Zabusky. Such was the start of the soliton revolution and out of it there came the so-called "inverse spectral transform" method of solving a number of nonlinear equations such as the Korteweg-de Vries equation $u_t + uu_x + u_{xxx} = 0$, the sine- Gordon equation $\phi_{zz} - \phi_{tt} = \omega_0^2 \sin\phi$, the cubic Schrödinger equation, etc., and with it the number of important physical models which can be exactly solved increased from around four to something like thirty. By now the soliton business is booming and both in theory and in applications it accounts for hundreds of papers each year (perhaps more).

Solitons like those depicted in Fig. 11 can, of course, be small, but this does not mean that we can linearize the KdV equation, e.g., to $u_t + u_{xxx} = 0$, or the sine- Gordon equation to $\phi_{zz} - \phi_{tt} = \omega_0^2\phi$. The solitons then disappear, they are truly nonlinear phenomena. Cf. Figs. 12 and 13 below. The top picture of Fig. 12 shows a solution of the linearized sine-Gordon equation (discretized as coupled systems of pendulums). The second picture of Fig. 12 shows a true soliton solution of the sine- Gordon equation. The pictures of Fig. 13 also show such solutions to the sine- Gordon, this time in an application to magnetic systems.

There exists so far no method (algorithm) for determining whether a given system is (completely) integrable, which is the mathematical property lying behind the soliton phenomenon. If a system is suspected of being completely integrable the thing done is, nowadays, to first throw it on a computer (16). The following two sets of pictures may indicate what one looks for in such cases. Figures 14, 15, and 16 depict the orbits of an unequal mass, respectively equal mass, so-called Toda lattice, at higher and higher energies(19). All the dots in the left sides of Figs. 15 and 16 come from a single orbit. The unequal mass Toda lattice of the left exhibits more and more chaotic behaviour with increasing energy: it is not integrable. The equal mass Toda lattice of the right-hand side of the preceding three pictures shows much more regular type behaviour. It turned out to be integrable. It is also a historical fact that the integrability of the Toda lattice was thus discovered by computer experiments [57, 58]. The theoretical proof, by H. Flaschka, followed some years later (28).

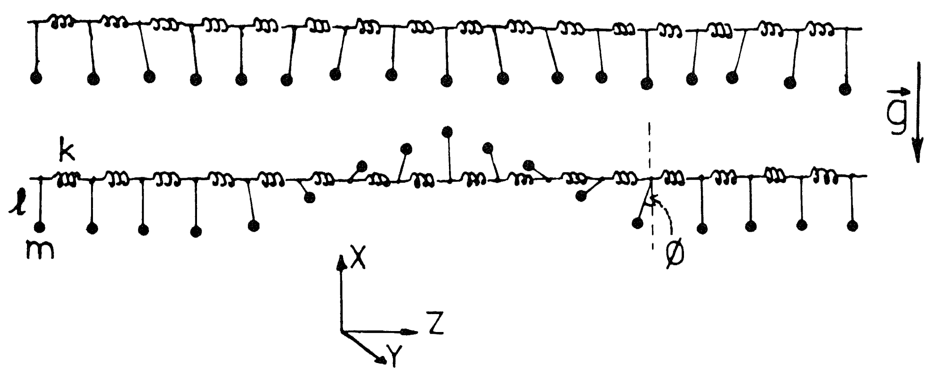


Fig. 12. (from [59])

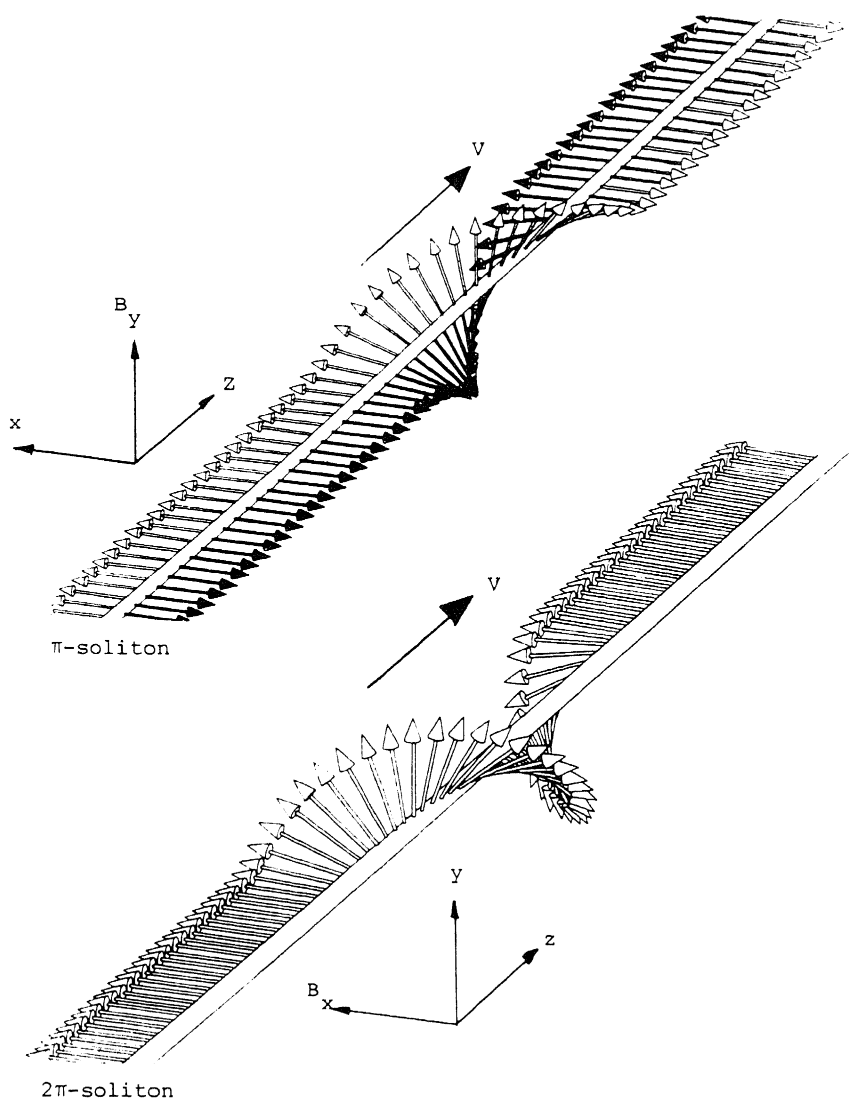


Fig. 13. (from [60])

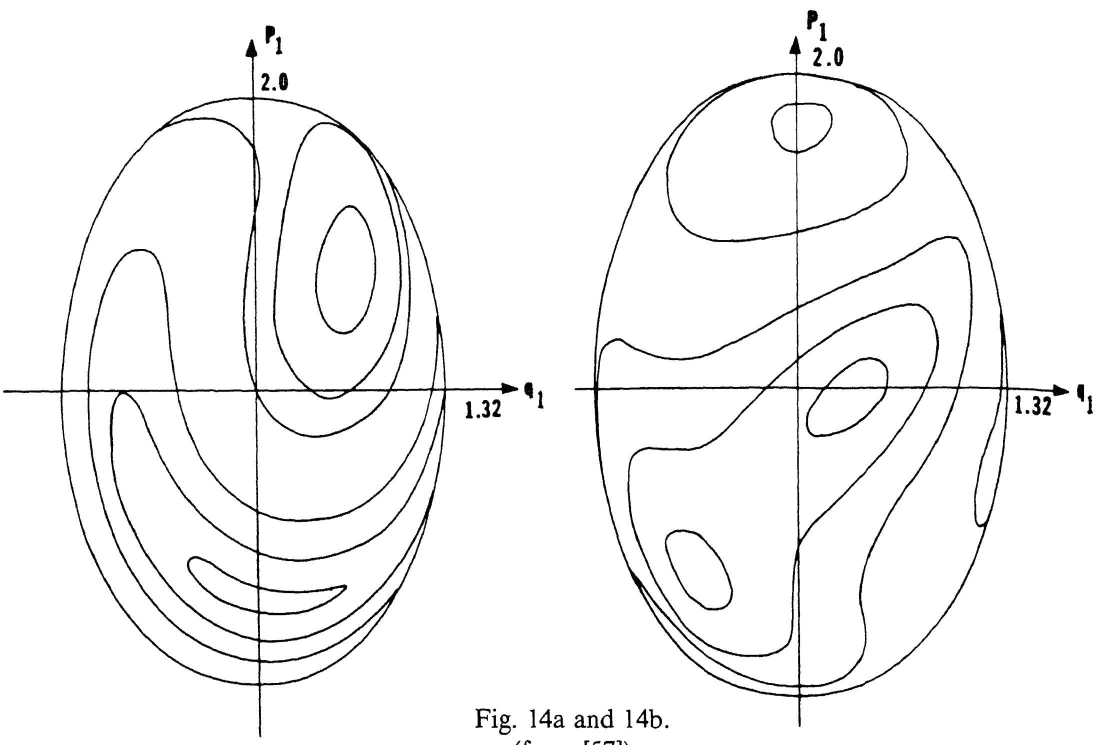


Fig. 14a and 14b.
(from [57])

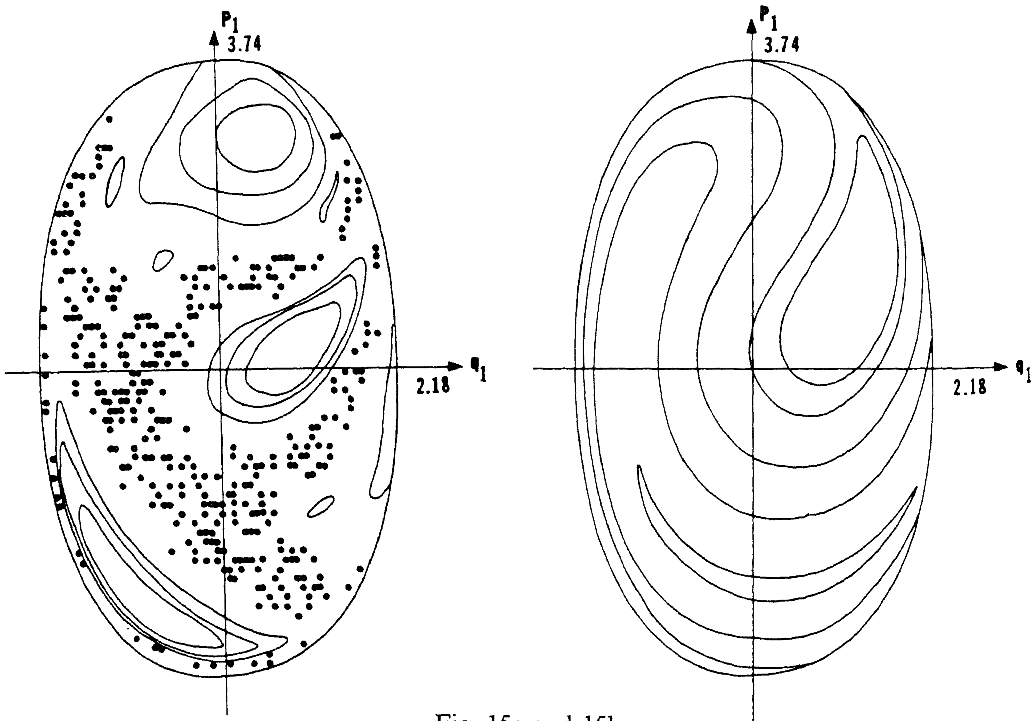


Fig. 15a and 15b.
(from [57])

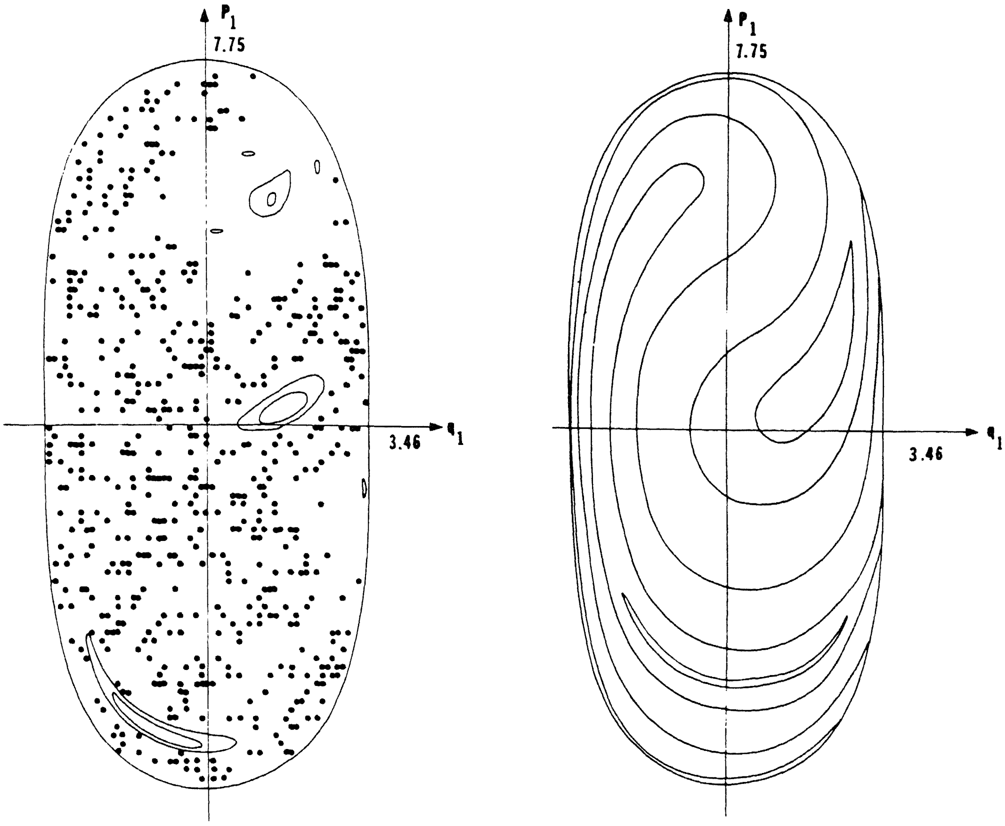


Fig. 16a and 16b.
(from [57])

7. SOME MORE EXAMPLES IN BRIEF

The three examples described above are simply three examples, if rather important ones. There are many more. Eleven stimulating computer experiments are discribed in an uncommonly interesting book by U. Grenander (Mathematical experiments on a computer, Acad. Pr., N.Y., 1982) and both this work and, so far, this article have totally ignored the role of computer experiments and verifications in number theory [20] and algebraic geometry. As an example of the latter, it was a computer which came up with the fact that $27^5+84^5+110^5+133^5=144^5$, thus disproving Euler's assertion (circa 1769) that it is also impossible to find three fourth powers whose sum is a fourth or four fifth powers whose sum is a fifth power.

7.1. The Atkin-Swinnerton Dyer conjectures.

Another example involves the so-called Atkin Swinnerton Dyer conjectures. Associated to an elliptic curve over $\mathbb{Z}$ -whatever that is -, there is its Artin L-function-whatever that is-, which can be developed into a power series in a certain way. The coefficients obtained in this way turned out numerically to satisfy certain congruences of the form

$$a_{np}-\alpha(p)a_n+\beta(p)a_{n//p}\equiv 0 \; mod \; p^{v_p(n)}, \quad n=1,2 \;\cdots$$

Here p is a prime number, $p^{v_p(n)}$ is the largest power of p dividing n and $a_{n//p}=a_{n/p}$ if p

divides n, and $=0$ otherwise. The first numerical work in this direction was done by A.O.L. Atkin; cf. also various papers by P. Swinnerton Dyer and N. Stephens for further high powered numerical algebraic geometry and the conjectures arising from, or supported by, this work. The Atkin Swinnerton Dyer conjectures were first discovered numerically and later indeed proved, cf. e.g., [61] for a proof.

7.2. Julia sets

Consider a complex polynomial $p(z)$. In 1879, Cayley proposed to extend Newton's method for calculating the roots of a polynomial to the complex case. This gives the formula

$$N(z_k) = z_k - p(z_k)/p'(z_k) \tag{7.1}$$

and he posed the problem of determining for each root a of $p(z)$ its set of attraction, $A(a)$, and is boundary $\partial A(a)$. These boundaries are socalled Julia sets and one of their more remarkable properties is, e.g., in the case of the cubic z^3-1, that one has $\partial A(1)=\partial A(-\frac{1}{2}+\frac{1}{2}i\sqrt{3})= \partial A(-\frac{1}{2}-\frac{1}{2}i\sqrt{3})=J$. To see what happens pictorially, PEITGEN c.s. [62] defined level sets of equal attraction as follows: let $0<\epsilon<<1$, $L_0(a)=\{z:|z-a|\leqslant\epsilon\}$, $L_{k+1}(a)=\{z\in L_0(a): N(z)\in L_k(a)\}$, and in their various pictures they coloured $z\in L_k(a)$ black if $\mathrm{Im}(N^k(z))$ is positive and white if $\mathrm{Im}(N^k(z))$ is negative(21). The resulting picture for the polynomial z^2-1 with roots ± 1 is shown in Fig. 17.

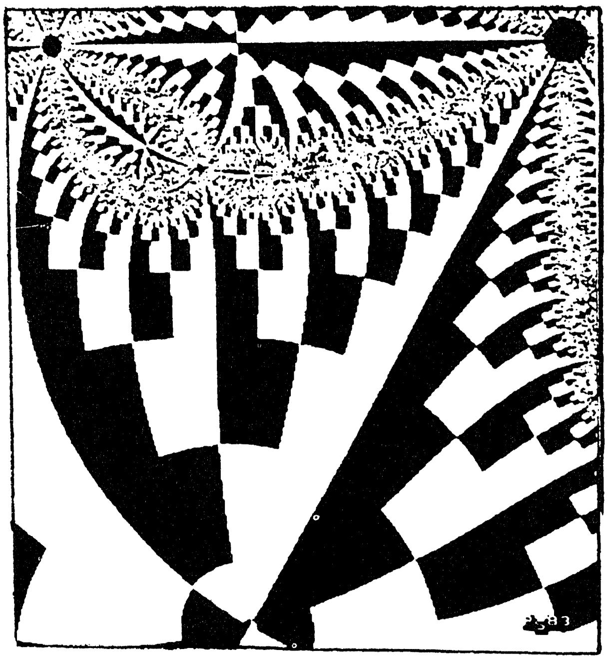


Fig. 17. from [93]

Apparently each point of the Julia set, in this case the imaginary axis, comes, so to speak, with a binary address. Figure 18 shows part of the picture for the third degree polynomial z^3-1. In the upper third of this picture one discerns what looks like a curved version of a neighbourhood of the imaginary axis in Fig. 17. It seems as if the dynamical system for

$z^3 - 1$ in this neighbourhood behaves like the system of a quadratic polynomial, instead of a third degree one. This has since been proved.

7.3. *Formal groups*

A commutative formal group of dimension 1 over a ring R is a formal power series in two variables $F(X,Y)$ which satisfies

$$F(0,Y)=Y,\ \ F(X,0)=X,\ \ F(X,Y)=F(Y,X), \qquad (7.2)$$
$$F(F(X,Y),Z)=F(X,F(Y,Z)).$$

One way to obtain such a thing if R is an integral domain, e.g. $R=\mathbb{Z}=$ the ring of integers, is to take a power series $f(X)$ over the quotient field $Q(R)$ which looks like $f(X)=X+a_2X^2+\cdots$ and to define $F(X,Y)=f^{-1}(f(X)+f(Y))$ where f^{-1} is the inverse function of $f(X)$, i.e., $f^{-1}(f(X))=X$. For suitable $f(X)$, the coefficients of $F(X,Y)$ are then miraculously in $R\subset Q(R)$, and it is a theorem that every one dimensional formal group over an integral domain can be obtained in this way.

There exist universal formal groups from which every such animal can be obtained by assigning particular values to parameters $V_1,V_2\cdots$. These universal examples can be recursively calculated. One such universal formal group is given by

$$\begin{aligned}
F_V(X,Y) = {} & X+Y-V_1(XY^2+X^2Y)+V_1^2(XY^4+X^4Y)\\
& +3V_2^2(X^2Y^3+X^3Y^2)-V_1^3(XY^6+X^6Y)\\
& -6V_1^3(X^2Y^5+X^5Y^2)-13V_1^3(X^3Y^4+X^4Y^3)\\
& -3V_2(XY^8+X^8Y)+(6V_1^4-12V_2)\\
& (X^2Y^7+X^7Y^2)+(27V_1^4-28V_2)(X^3Y^6+X^6Y^3)\\
& +(52V_1^4-42V_2)(X^4Y^5+X^5Y^4)\\
& +(6V_1V_2+V_1^5)(XY^{10}+X^{10}Y)+45V_1V_2(X^2Y^9+X^9Y^2)\\
& +(163V_1V_2-27V_1^5)(X^3Y^8+X^8Y^3)\\
& +(362V_1V_2-27V_1^5)(X^3Y^8+X^8Y^3)\\
& +(362V_1V_2-106V_1^5)(X^4Y^7+X^7Y^4)\\
& +(532V_1V_2-192V_1^5)(X^5Y^6+X^6Y^5)+\cdots\\
& +(-105\,024\,048V_1^3V_2^2+954\,161\,30V_1^7V_2+213\,396\,72V_1^{11})\\
& (X^{10}Y^{13}+X^{13}Y^{10})+\cdots
\end{aligned}$$

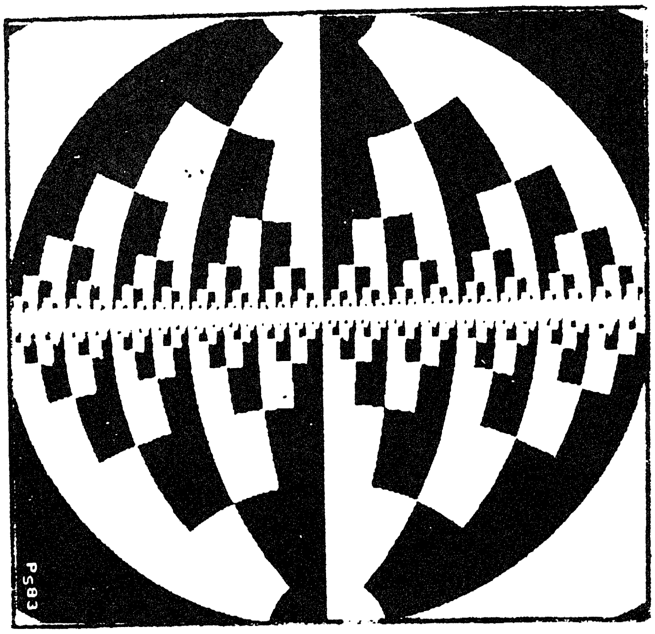


Fig. 18. (from [62])

and I challenge anyone to see the regularity in this [(22)].

This shows that playing experimental mathematics games on a computer is fine but will not lead to stimulating results unless a) one has a good idea of what should be calculated and b) the results are presented in a form suitable for the superior human pattern recognition faculties.[(23)]

In this particular case, the formal group $F_V(X,Y)$ itself is simply totally the wrong thing to look at. The power series $f_V(X)$ such that $F_V(X,Y)=f_V^{-1}(f_V(X)+f_V(Y))$ looks like

$$f_V(X) = X+\frac{V_1}{3}X^3+(\frac{V_1^4}{9}+\frac{V_2}{3})X^9+ \tag{7.3}$$
$$\left(\frac{V_1^{13}}{27}+\frac{V_1V_2^3}{9}+\frac{V_2V_1^9}{9}+\frac{V_3}{3}\right)X^{27}+\ \cdots$$

and here one can see the hidden regularity; especially when one reflects that we are dealing with the prime number $p=3$ and if one substitutes $3=p$, $9=p^2$, $27=p^3$, $4=1+p$, $13=1+p+p^2$. And, as a matter of historical fact, this is (essentially) how the general formula for $f_V(X)$ was discovered. In Nov. 1969 I spent a month calculating $f_V(X)$ up to degree 27, removing by means of suitable isomorphisms all terms that I could get rid off. All this in a vain attempt to find a counterexample to something. Formula (7.3) was what I finally found (apart from two sign mistakes). Nowadays such things should be done by machine. Since then the formula has found quite a few applications in various parts of mathematics [61].

This also brings me to another point I wish to stress. For problems with a geometric content, colored computer graphics are important for experimental mathematics[(23)] and for problems with a more algebraic or analytic flavour it will be symbolic computation, formula manipulation computation, which will perhaps be more important than number crunching[(24)].

7.4. Anti-diffusions

Consider a process with an autocatalytic component, i.e. such that initial disturbances will tend to grow, up to a certain point. One possible model,

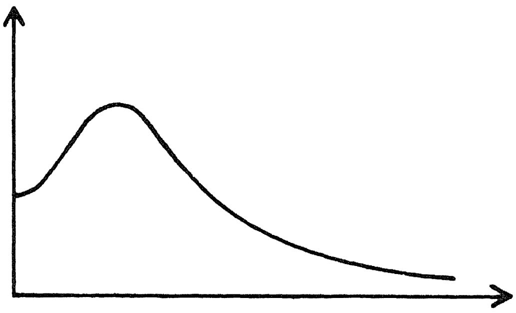


Fig. 19.

at first sight, for such a thing, could be an anti diffusion equation of the form

$$\rho_t = -\frac{\partial^2}{\partial x^2}\phi(\rho) \tag{7.4}$$

where ρ is some sort of density and ϕ is a function of the form shown in Fig. 19. Our hope was that starting from an initially homogeneous ρ and small initial disturbances, or, better, small stochastic disturbances all the time, this would give rise to stable periodic patterns in space(41). Analytically, virtually nothing is known about equations like (7.4), beyond the fact that they are highly unstable. So I suggested to my student to put it on a (small) computer. One of the sequences of pictures he came up with is shown in Fig. 20.

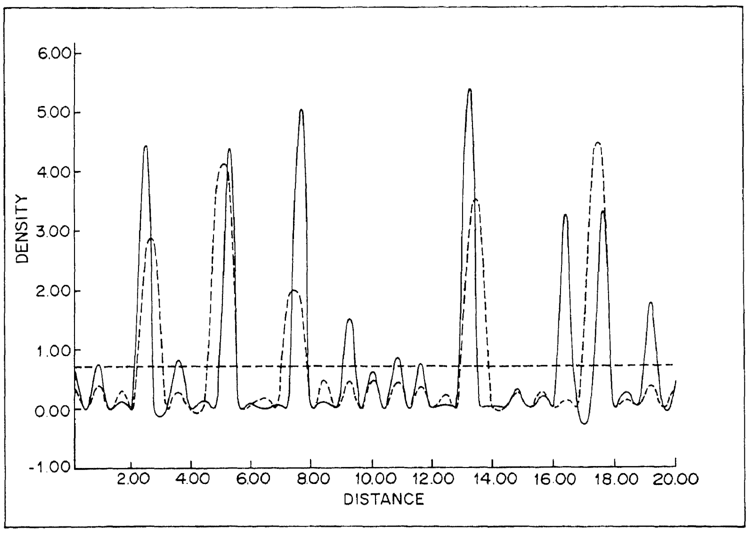


Fig. 20a. from [68]. - horizontal dotted line: starting density; continuous curve: after 1000 periods; dotted curve: after 2000 periods.

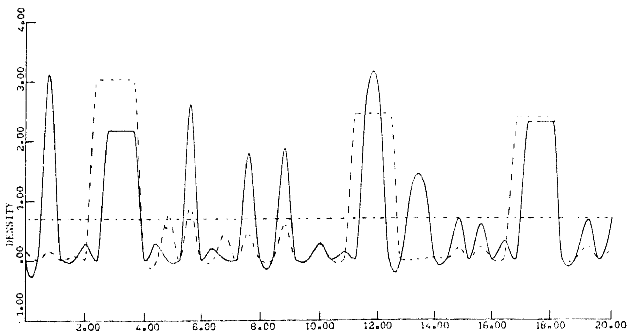


Fig. 20b. As in a) (different parameter value).

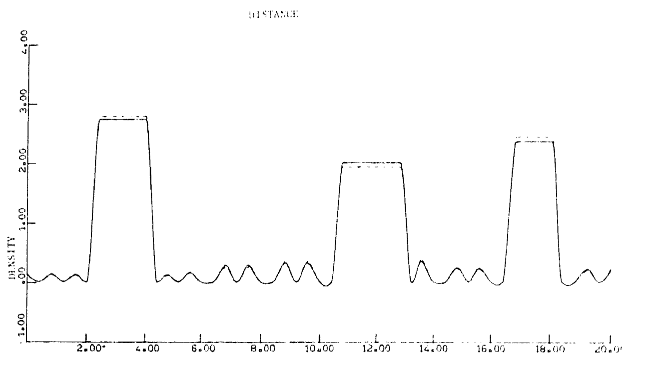


Fig. 20c. continuation of b); continuous curve: after 10000 periods; dotted curve: after 15000 periods.

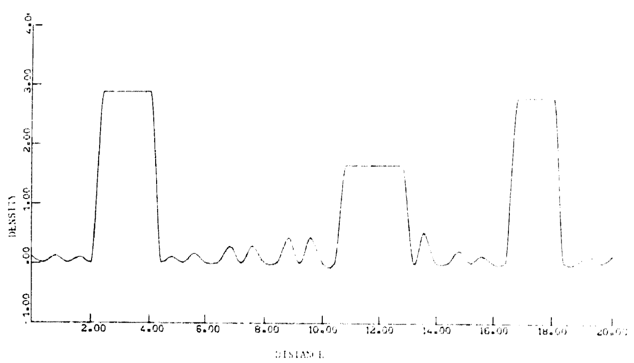


Fig. 20d. continues b) and c): after 25000 periods

Such patterns seem to arise remarkably often in this context and they also persist for long times. They still could be transient phenomena, of course, and indeed there are reasons to believe so (no proof). Even so, they persist for very long times. Similar phenomena occur in [64][25], for example, and they pose the general problem of how to deal mathematically with such "patterns" which are semistable in the sense of persisting for very long times (also in the face of disturbances) but eventually disappear, or which persist only in a looser sense, in that there are always the same number of bumps at roughly the same equal distance, but they keep moving and changing shape slightly and never settle down.

7.5. *Traveling salesman*(26)

The traveling salesman problem is the following. Consider n cities, n large, and the distances between them. Find the shortest circuit which passes through each of them once. This can be viewed as a programming problem with decision variables x_{ij}, $x_{ij}=1$ if the stretch from city i to city j is to be included in the circuit and 0 otherwise, and a large number of restrictions to make the path a so-called Hamiltonian one, i.e., one which passes through each vertex precisely once. The convex hull of all admissible integral vectors constitutes a polytope in $\mathbb{R}^{n^2}$, which has not yet been characterized. Early in the game Dantzig, Fulkerson, and Johnson developed a quite successful algorithm which approached the problem as a (continuous) linear programming problem with $0 \leqslant x_{ij} \leqslant 1$ and with a smaller set of the restrictions than the set defining the original polytope. They started with the trivial restrictions $\Sigma_i x_{ij}=1$, $\Sigma_j x_{ij}=1$ and then if a "subcircuit" came out (e.g. $x_{12}=1=x_{21}$), a new restriction (here $x_{12}+x_{21} \leqslant 1$) was added. This approach got neglected when branch and bound became more successful.

In 1953, Alan Hoffman and Harold Kuhn carried out an experiment.(38) Stand in the middle of the polytope and fire a gun at random in all directions. All shots turned out to pass through a part of the "wall" defined by facets of the trivial type $x_{ij}=0$. These "experiments" contributed to new insight in the structure of the traveling salesman polytope and the best algorithms anno 1983 are based on a combination of the Dantzig c.s. 1954 method (initially) followed by branch and bound methods.

8. A FEW FINAL REMARKS

The three main examples of Sec. 4, 5, and 6 above are but a random selection dictated by personal taste. There are, of course, many more. Indeed, it seems clear by now that experimental mathematics is developing very fast and that it is already generating conjectures, results, and challenging problems at a higher rate than can be handled by the theoreticians. Here are some more challenges posed by experimental results (besides the ones already mentioned).

There is a wealth of material, bifurcation pictures, and phase diagrams, concerning the so-called Josephson - junction , an equation which probably will play the role of *the* well studied and illustrative example which in the past has been played by the VAN DER POL equation [65-68]. It is perhaps also interesting to remark that the so-called "breather solutions" of the Josephson- junction were first discovered numerically(30).

As a rule, if a Hamiltonian system is not integrable, its behaviour becomes more and more chaotic as energy is increased. No proof is available. Exceptions are, of course, systems which decouple into integrable subsystems as $E \to \infty$. There are, however, also systems which do not have this property and still show a return to more regular behaviour as E increases [69, 70].

There is quite a bit of numerical evidence for various kinds of universal behaviour for iterated maps of more dimensional objects, e.g., subsets of the plane, which awaits theoretical elucidation [50-54].

There are literally masses of experimental results dealing with percolation through porous media and associated phenomena like clogging of throats of pores and "fingering", both computer generated and as a result of real hydrology experiments. Mostly, again, awaiting analysis and concept formation to bring some order and classification. [33]

Stimulated by a hypothesis of CRICK and MITCHISON [71] to the effect that one of the functions of dream sleep might be an "unlearning process", HOPFELD a.o. [72] carried out mathematical and computer modelling on networks of neurons. I quote:

> "Although our model was not motivated by higher nervous function, our system displays behaviours which are strikingly parallel to those needed for the hypothesized role of 'unlearning' in rapid eye movement sleep".

Here again is a conceptual and mathematical challenge[32].

Before finishing, let me stress again that "user-friendly" outputs like colour graphics and movies are likely to be more important in experimental mathematics than rows and rows of numbers[34]. Also, symbolic calculation and formula manipulation is likely to grow in relative importance, again because symbolic formulae are better suited to human pattern recognizing abilities than numbers. Also, we really need the computer assistance at this point, again because we seem to have, in many cases, reached a sort of natural limit of what can be done by hand[25].

Let me also remark on the pleasing fact that all three main examples I discussed above have as much to do with classical pure mathematics as with classical applied mathematics and that, thus, it seems that experimental mathematics is doing much to remove the silly and distressing distinction between the two.

Finally, let me close with expressing the hope that what has been said above will have helped to make it clear that experimental mathematics is a vigorous, fast growing subject, synergetically related to its scientific neighbours. Indeed, I have the feeling that we are at the beginning of what may well turn out to be a heroic period in mathematics comparable in significance and future influence to the 1920s in physics. In any case, I hope to have helped to make it clear that von Neumann appears to have been absolutely right in his predictions of 1946.

NOTES

1) The Littlewood- Richardson rule deals with the question of the multiplicities of the representation $\Lambda^{\gamma}E$ of $GL(E)$, E a vectorspace, in the direct sum decomposition of $\Lambda^{\alpha}E\,\Lambda^{\beta}E$. Here α,β, and γ are partitions.

2) I owe the information about Bockwinkel and Lorentz to Jaap J. Seidel and F. Alberto Grünbaum.

3) Hahn uses this phrase in the context of a critique of the Kantian idea that mathematics, especially geometry, is completely based on intuition a priori. To this end, he discusses the counterintuitive properties of such things as Peano and Sierpinsky curves and noneuclidean geometry. Such logical constructs are, of course, equally intuition- and mind-enriching as computer experiments.

4) Cf. also *Computer graphics comes to statistics* (Gina Kolata), Science 217 (1982), 919-920. By means of three dimensional projections generated by means of computer motion graphics from multi-dimensional data sets, combined with human pattern recognition abilities, it seems to be possible to detect previously unrecognized interesting phenomena. (Discrepancies in this case).

5) Later in this article, discussing renormalization-group ideas and "the new physical principle of scale invariance" the author remarks: "In this example it was a new physical principle that permitted computation capable of solving a previously intractable set of problems. The initial computational test of the principle played a mayor role in establishing its utility." This is an aspect of experimental mathematics that I do not stress in this article, though of course it is similar to experiments - as discussed in 3.10 - to find out whether a given type of model is capable of producing the phenomena it is designed to "explain". However, to the remark of Donald R. Hamann on renormalization ideas I would like to add that, from a lecture of Kenneth G. Wilson in Los Alamos in 1972, I have the impression that, at least in the case he was discussing (the Kondo problem), the desire to find some computational scheme to handle the problem had a lot to do with the genesis of Wilson's renormalization group ideas.

6) The "soliton story" and the "iterated maps and chaos story" which are the subject matter of Sec. 6 and 5 of this article are also briefly mentioned in [14].

7) As I have remarked before [73], unaided intuition or common sense are poor instruments of thought when confronted with cause and effect relations which cannot be linearly ordered, i.e., when there are mutual interactions and/or feedback loops present. From this point of view, mathematics is a highly necessary tool for finite human brains. A God would have no need of it. And within mathematics itself, experimental mathematics is proving to be an equally necessary tool for helping our mathematical intuition. Mathematics also does a tool-for-thinking and pointing-out-flaws-in-common sense-reasoning job in geology, physics, chemistry, etc. Examples are, e.g., the Phillips stabilization paradox of economics [74] (dealing with Goverment spending to stabilize an economy), the fact that monopoly positions can very well be disadvantageous [75], and the Arrow impossibility theorems, see, e.g., [76] and [77], (dealing with the design of democratic voting systems). As Eric T. Bell [78] says: "One service mathematics has rendered the human race: it has put common sense back where it belongs, on the top shelf next to the dusty canister labelled 'discarded nonsense'."

8) The picture has to do with studies by S. White, M. Davis, and C. Frank (Berkeley); other studies were done by S. Djorgovsky (Berkeley), J. Centrella and A. Melott (Lawrence-Livermore Lab.). The so-called inflationary cosmogonical model of A. Gut (M.I.T.) is important here.

9) In a short "News and Views" report on the work of C. M. Bender and D. H. Sharp, John Maddox [79] comments that the chief value of their method will be to sharpen physical intuition, and that much the same may be true of a new numerical technique of M. Creutz [80] for calculating partition functions in statistical physics.

   In both cases, especially in my view the first, things work so well that one feels to have received a first hint of the presence of some unsuspected physical or mathematical principle.

10) There appear to be even more bonuses coming out of the F.E.M. approach to quantum field theory, (Bender, Milton, and Sharp, to be published), dealing with finding a gauge invariant F.E.M. model and what happens as a certain dimensionless lattice spacing parameter goes to zero.

11) Further developments from the hard hexagon model involve directed lattice animals, polymers, directed percolation theory, etc. Numerical calculations here continue to play a dominant role in finding, formulating, and testing conjectures, as a good look at the following papers will show: D. Dhar, *Phys. Rev. Lett.* 49 (1982), 959-962; V. Hakim, and J. P. Nadal, *J. Phys. A* 16 (1983), L213-L218; J. P. Nadal, B. Derrida, and J. Vannimenus, *J. de Physique* 43 (1982), 1561, B. Dhar, M. K. Phani, and M. Barma,

J. Phys. A 15 (1982), L279-L284; N. Breuer, and H.K. Janssen, *Z. Phys. B* 48, 347-350; F. Family, *J. Phys. A* 15 (1982), L583-L592; J. E. Green, and M. A. Moore, *J. Phys. A* 15 (1982), L597-L599; A. R. Day, and T. C. Lubensky, *J. Phys. A* 15 (1982), L285-L290; J. L. Cardy, *J. Phys. A* 15 (1982), L593-L595; S. Redner, and A. Coniglio, *J. Phys. A* 15 (1982), L273-L278.

Also, finding the exact results has involved (as in the hard-hexagon case) considerable computer assistance. The original version of the bijection between directed lattice animals and certain kinds of discrete paths which is at the basis of a combinatorial approach to these exact results involved first numerical comparison of the respective numbers of animals and paths, respectively, and also considerable numerical search in finding the right "size" parameters for these things (the latter search involved analogues with orthogonal polynomials). These matters will be reported on in G. Viennot, Problèmes combinatores posés par la physique statistique, Sém Bourbaki, Febr. 1984, Exposé 626.

12) Instead of, say, triangular lattice gas with nearest neighbor exclusion.

13) The story as outlined below is the sort of thing which rarily, if ever, gets published in the official journals. As outlined here, it owes very much to a cassette tape and copies of the slides of a lecture that Baxter gave at King's college in London in July 1980. I am extremely grateful to Baxter for sending me this material.

14) Rodney J. Baxter received the much coveted Boltzmann medal for his work on exactly solvable lattice statistical mechanics.

15) The 10×10 approximation figures are even more spectacular.

16) It also illustrates another point. Interesting systems, phenomena, of a particular kind, etc. are (likely to be) rare. For instance (completely) integrable Hamiltonian systems are rare (in the class of all Hamiltonian systems). Another role for the computer in experimental mathematics could be in a searching for interesting unusual phenomena of certain specified kinds. Much as in [81] where it is described how, in astronomy, computers can help in finding interesting stars. However, cf. also note 37.

17) Such deterministic chaos; i.e. chaotic behaviour caused by perfectly deterministic maps, may provide another model for modelling certain random phenomena, i.e., models different from stochastic models. One type of noise which frequently appears in (solid state) electronics is the so-called $1/f$- noise [82] and it may be possible that deterministic chaos will be fruitful in its study and analysis [83, 84, 85]. The problem of how to distinguish, observationally, between deterministic chaos noise and stochastic noise is still open. Conceivably this is not possible (recent work by Krishnaprasad and student).

18) There have, of course, been other inputs than the computer experiments briefly indicated in this section. Notably the invention of "Strange attractors" (E. LORENZ 1963 [86], D. RUELLE and F. TAKENS, 1971 [87]). Lorenz's model of a stange attractor is a severely cut-down approximation of atmospheric flow and the fact that there is (probably) a strange attractor there present illustrates some of the notorious difficulties of wheather prediction.

19) More precisely, it shows the intersection of these orbits with the $p_1 - q_1$ plane. The Toda lattice of Figs. 14, 15, and 16 is the one with Hamiltonian $H = \frac{1}{2}(p_1^2 m_1^{-1} + p_2^2 m_2^{-1}) + \exp(-q_2 + q_1) + \exp(q_2) - 3$. The pictures on the left have mass ratio $m_2/m_1 = 0.33$; the ones on the right $m_2/m_1 = 1.0$.

20) The first 300 million or so of the non real zeros of the Riemann zeta function do, indeed, lie exactly where they should ([88]) and the mathematics developed to prove

such a thing certainly would not have developed without the big machines(40). Another instance of this is the matter of the mathematics of fast prime number tests [89]. Also, the high interest in effective upper bounds for the solutions of diophantine equations (Baker- Gelfond theory) is certainly connected with the availability of lots of computing power. All these, however, I consider instances, like the case of semiparametric statistics discussed in the introduction, where the presense of the big machines enlarged the set of problems which we are willing and interested to think about, rather then examples of experimental mathematics.

21) In "reality" H. O. Peitgen c.s. used colors, and the resulting pictures are really quite beautiful. Four of them occur in the 1984 Springer-Verlag mathematics calender. They have also been the material of an art exhibition in the Sparkasse in Bremen [90] in Jan/Febr. 1984.

22) As a matter of fact, the example shown is a p-typical universal formal group, in this case for $p=3$. These are not truly universal, but are universal for a more restricted class. They are, however, much more regular than a truly universal one can be, essentially because there is, so to speak, only one prime number to worry about.

23) ZABUSKY [11] stresses this particularly and has repeatedly insisted on the desirability of using computer graphics and movies in this connection. The studies hinted at in 7.2 above also illustrate this point.

24) There may be considerable number crunching behind a computer generated picture, of course, and often there is.

25) In this case the phenomenon is definitely transient.

26) This example I owe to Jan Karel Lenstra, CWI, Amsterdam.

27) Another example, besides the ones that follow, is [91]. Here there is a criterium for the existence of a closed orbit for systems with strange attractors. This criterium involves estimates which are designed to be verified by computer. Otherwise one would hardly consider them.

28) Cf. [11] for a detailed account of these happenings.

29) One phenomenon to which we hope to apply ideas along these lines is the phenomenon of Liesegang rings in (colloid) chemistry. Another model designed to deal with this phenomenon is described in [92]. The patterns generated by that model are of a similar nature. They also appear to be transient, but with a very long life. Here, also, a mathematical analysis predicting these patterns is almost completely absent.

30) By two physicists: Imry and Schulman. I owe this bit of information to M. Levi of Boston Univ.

31) A totally different topic, also of high interest, both from a theoretical and practical point of view, coming out of the availability of computer power is the matter of (flexible?) computer design to meet the requirements of certain problems, cf. [93, 94].

32) To illustrate a point, let me quote from [95], noting that this is but one example from very many. "We have performed Monte-Carlo simulations on the Kinetics of .... The extent of reaction ... increases with decreasing fraction of divinyl monomer, with increasing solvent concentration and with increasing initiator concentration. These predictions, and the observed trends for the dependence of the overall polymerization rate on the same concentrations, are in qualitative agreement with laboratory experiments."

This type of work is, of course, most important, e.g., in constructing adequate models and in testing tentative principles and formulating theories. But if things stop right here, progress will soon cease. A model which is conceptually murky but works numerically well is of very limited value unless the challenge posed by an unusually well working model is taken up.

33) Another area of vigorous interaction between numerical experiment and theoretical and applied (in the more traditional sense) mathematics is the physics and mathematics of disordered media. The key words here are "fractals", "percolation", "random walks (especially non-intersecting)", and "chaos". A recent workshop on the topic took place at the IMA in Madison, Wisconsin in Feb. 1983. The proceedings will appear in the *Lect. Notes in Math.* series of Springer-Verlag. Inevitably perhaps — everything relates (strongly) to everything else — this topic has quite a bit to do with the topic of Sec. 4, cf. note 11.

34) Here is another example to illustrate the point. I quote from [95]. "High-performance computer graphic techniques have been developed in the last year or two, and are now taking the place of conventional model building . . . . Sophisticated computer graphics were used to survey the likely active conformations of known inhibitors of the converting enzyme. This survey guided the synthesis of putative inhibitors with functional groups in rigid orientations. It resulted finally in the synthesis of a potent bicyclic inhibitor molecule, and a patent was applied for a few weeks ago."

35) One area where symbolic computation is becoming increasingly important is in describing and calculating the symmetries of important physical models such as Gauge theories. Cf. [96, 97].

36) The sources of all reproduced figures in this article are stated in the captions. I am grateful for the permission to reproduce these.

37) All in all, it seems that this happens quite often, i.e., that computer experiments bring something new to ponder. Rather remarkably often, perhaps, indicating that there are very many interesting phenomena still awaiting discovery. Not only in experimental mathematics but in all of mathematics I often have had the feeling "can one be so lucky". There really is very often something fascinating going on. This does not contradict note 16.

38) Cf. the remark by Kuhn (page 118) in the discussion of [98]. There are more interesting challenges in this area, e.g., the "unreasonable effectiveness" of some assignment problem algorithms. Cf. the discussion between Edmonds and Kuhn, loc. cit..

39) This work was with Mary T. Menzel and published in Adv. Math. 9 (1972), 339-407. I owe this information to N. Zabusky.

40) Cf. also [100].

41) These studies relate to pattern-formation and self-organization phenomena [101, 102].

42) Quite apart from physical unreality, the time is rapidly approaching when, as a rule, it will be much less expensive to construct and experiment with a computer model then to do real experiments. Cf. also [103].

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