FRACTALS AND PHASE TRANSITIONS

D. STAUFFER

Institute for Theoretical Physics, Cologne University, d-W-5000 Köln 41, Germany

ABSTRACT- A wire has a mass proportional to its length, the mass of a disk varies proportional to the squared radius, and the mass of an iron sphere is proportional to the third power of the radius. Therefore these objects have a dimension equal to one, two or three. FRACTALS are objects where the mass varies with some other power of the radius, and that power is called the fractal dimension D. We show examples, in particular from the physics of phase transitions, where D is smaller than the normal dimension by β/ν.

1. INTRODUCTION

Fractals today are spread all over the scientific literature and continents, as is quite appropriate for the person of Mandelbrot (from Lithuania, Poland, France, and the USA) who invented the general concept[1]. Fractal elements appeared centuries ago in Italian church paintings and flood dike constructions [2] and are inherent also in clouds and trees. Fractal Mandelbrot sets have been printed on covers of scientific journals without apparent relation to the content. The present review does not deal with fractals as a new and separate topic. Instead it wants to relate them to examples from traditional physics and their teaching.

2.BASIC CONCEPTS

If you look at the world around you, you can normally distinguish easily between man-made and natural objects: buildings, channels, and streets are Dominated by straight lines, whereas trees, rivers, and coast lines are more complicated. Traditional teaching of mathematics and physics deals with straight lines, circles, spheres and other simple objects; so how can we describe the more complicated objects like trees ? The circumference and area of a circle of radius R are $2\pi R$ and πR^2, whereas surface and volume of a sphere are $4\pi R^2$ and $4\pi R^3/3$, respectively. What are surface and volume of a tree with height R ? Clearly that is a more difficult question, and it is not just of academic interest: due to man-made combustion processes, the carbon-dioxide level in the atmosphere has increased significantly over the last century. This increase may, via the *greenhouse effect*, lead to an increase of the average temperature, causing larger deserts and flooding of low-lying areas. Trees counteract the greenhouse effect by consuming carbon dioxide through the surface of their leaves. So the effect of cutting a tree in the Amazon basin on the atmospheric temperature depends on the surface of a tree.

Many objects follow simple power laws, and so we may generalize the above formulas to a proportionality between mass M and radius R:

$$M \propto R^D$$

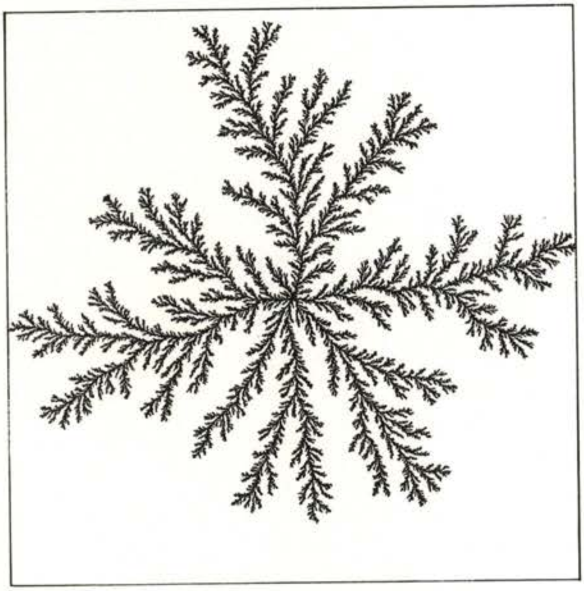
with some empirical exponent D. Thus $D = 2$ and 3 for circle and sphere if we identify the volume with the mass; and $D = 1$ and 2 if instead we identify the surface with the mass. So in these simple artificial examples, D or $D+1$ equals the Euclidean dimension d of the space, depending on whether we look at volume or surface. Such objects are not called fractals. If, however, the exponent above d is different from the Euclidean dimension d or d-1 and thus in general not an integer, then we call these objects fractal with a *fractal dimension D*.

So what about the fractal dimension of plants ? Fig.1 shows diffusion-limited aggregates with 10 and 30 million sites on a plane, and the branches of this figure have a clear similarity with branches of plants. Comparing such aggregates of different mass (the mass is measured by the number of sites) one finds a fractal dimension near 1.7 on a plane, and about 2 on three-dimensional space. The power laws in such computer-generated objects are supposed to be valid only asymptotically, that means for large enough clusters. The author of Fig.1, Peter Ossadnik in Hans Herrmann's group at HLRZ Supercomputer Center Jülich, Germany, competes with Mandelbrot's group for the world record. In natural fractals, as opposed to computer-generated or mathematical objects, the power laws are often valid only in a suitable mass interval: Very young small trees, and extremely high trees, may show deviations.

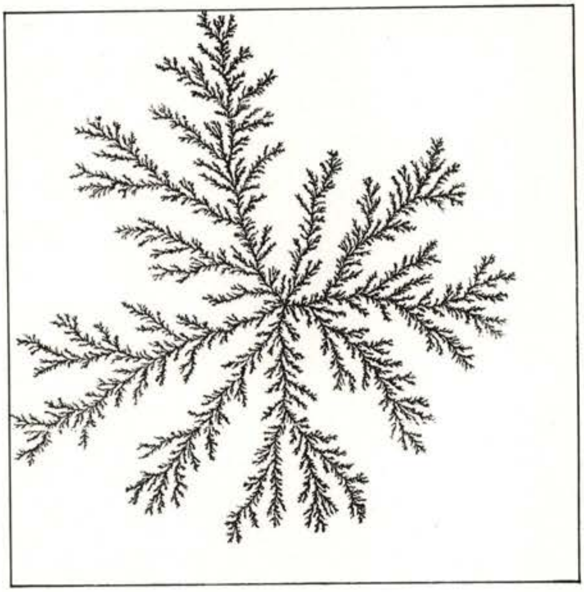
How is Fig.1 generated ? One starts with an occupied site in the center of the plane, and then one adds one particle after the other to the growing cluster in the following way: A new particle is put onto the plane somewhere away from the cluster. Then this new particle diffuses, that means it randomly moves in arbitrary directions like a molecule in the air. Once it hits the cluster it stays at that place forever and becomes part of the cluster. If we simplify the simulation by letting all particles move and sit on a square lattice only, we see the anisotropic lattice structure and get a lower fractal dimension if we simulate multi-million clusters.

Fig.1 also illustrates the concept of *self-similarity*: A big branch looks quite similar to one of its small branches, and this small branch looks similar to a twig emanating from it. Alternatively, whole clusters with different numbers of sites look similar to each other, Fig.1. A mathematical description of "looks similar" is difficult, however, and therefore I recommend to talk about self-similarity only if one knows what it means, e.g for deterministic fractals like the Sierpinski gasket [1].

These diffusion-limited aggregates were invented in 1981 and thus hardly constitute traditional physics subjects. Thus the next two sections instead deal with the phase transition between water and its vapor.



Off-lattice DLA with 30,000,000 particles
Peter Ossadnik, HLRZ, KFA Jülich



Off-lattice DLA with 10,000,000 particles
Peter Ossadnik, HLRZ, KFA Jülich

Fig.1: Diffusion-limited aggregates, by P. Ossadnik, with 10 and 30 million sites ($D = 1.7$).

3. CLOUDS AND PERCOLATION

When water vapor condenses in the atmosphere, it forms small droplets around some solid particles which then grow to micron size. Many of these droplets form a cloud, and if the droplets grow too large they fall down as rain. How do clouds look like ? Clouds move in three dimensions but what we see from them are two-dimensional projections (except if the clouds are very transparent). The interior of these clouds, as projected onto a two-dimensional surface, is usually dense, and thus behaves like a circle: projected area $\propto R^2$ for a cloud of radius R. Thus the area is not fractal. More interesting is the perimeter of the cloud, that means the number of empty sites which touch a cloud site after the projection. [We imagine the coordinates of the clouds to be discretized, where for example each square meter corresponds to one site and is either wet (cloud) or dry (surrounding).] This perimeter for a simple circle would vary as R but for clouds it was found empirically to vary roughly as $R^{1.3}$ or area$^{2/3}$. Fig.2 shows a computer model of the cloud projection[3] which agrees roughly with this fractal dimension.

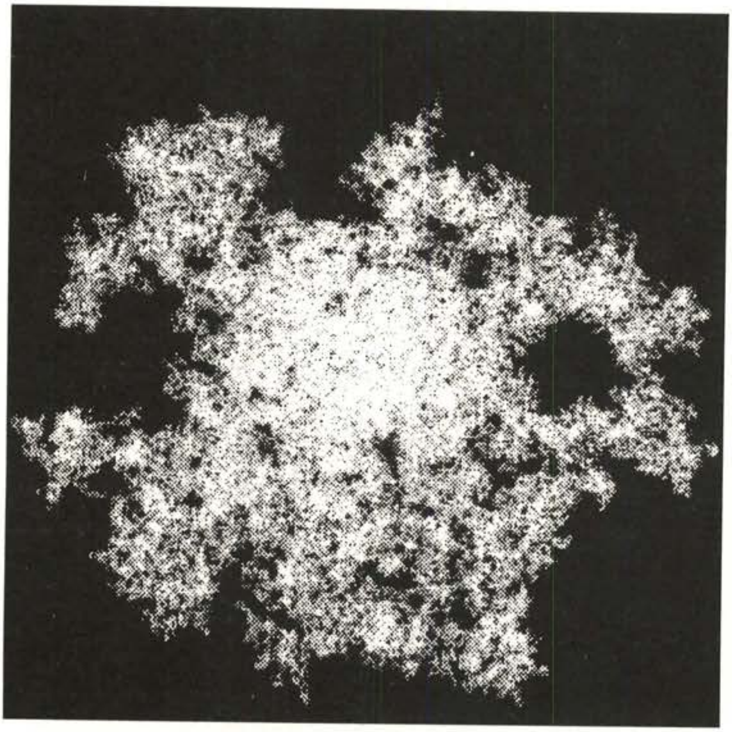


Fig.2: Computer model of three-dimensional cloud projected onto two dimensions (D = 1.3);from ref.3.

A simplified form of this computer model was investigated by two high-school students[4] who had not yet even studied at the university. They looked at percolation[5], a model originally invented by chemistry Nobel laureate Flory to describe the gelation of branched polymers (boiling eggs, milk-to-cheese transition, formation of gelatine pudding). On a simple cubic lattice first occupy the center site. Then add one site after the other by selecting a new neighbor of an already occupied site. Occupy this neighbor with probability p and leave it empty with probability 1-p. After a site is determined as being empty or occupied, it stays in that status during the whole process of building up this cluster. We now observe a transition: For probabilities $p < p_C$ with a threshold p_C near 0.3116 only finite clusters are formed, whereas for $p > p_C$ sometimes this growth process continues up to infinity (i.e. until it touches the borders of the simulated lattice.) Right at $p = p_C$ the clusters are fractal with a fractal dimension D near 2.53. In Ref.4 the authors produced such fractal clusters at $p = p_C$ on an Amiga computer, projected them onto a two-dimensional plane, and found the perimeter of these projections to follow roughly the same power law as a function of radius or area as the clouds and as the more complicated model of ref.3. We see, good physics research can also be done on small computers and without a long university curriculum. Historically, the percolation problem seems to be the first case where phase transitions were coupled to fractal concepts [6].

4.FRACTAL DROPLETS IN ISING MODELS

How can we understand by a simple model the phase transition between a liquid and its vapor ? The Ising model of 1920 allows each site for a large lattice to be either occupied or empty; occupied sites attract each other. Mathematically this model has an interaction energy

$$J = \sum_{i<k} S_i S_k - B \sum_i S_i$$

where the "spin" S_i is +1 for an occupied and -1 for an empty site and where i and k in the double sum correspond to nearest neighbors on the lattice. A simple *cellular automata* simulation for B=0 takes into account the conservation of energy: Starting with a random fraction p of all sites occupied, and the rest empty, we go sequentially through the lattice and flip a spin if and only if it has as many occupied as empty neighbors. Low p correspond to low energies and thus low temperatures, whereas $p \approx 1/2$ corresponds to a high energy at very high temperatures. For p above a critical concentration, 7.55 percent on the square lattice, after many sweeps through the lattice we have as many occupied as empty sites, which corresponds to a supercritical fluid like air at room temperature. For smaller p the majority of sites remains empty, corresponding to the vapor phase below the critical temperature. This model is symmetric with respect to occupied and empty. Thus for p above 92.45 percent, again we will not get a density of 1/2 but a majority of sites occupied, corresponding to the liquid phase at low temperatures, like very cold liquid air. Thus the Ising model, which can also be simulated by other methods, shows one fluid phase above the critical temperature, and two phases (vapor and liquid) below this temperature, just as real fluids so. The Ising behavior very near this critical temperature is known to agree even quantitatively with real fluids.

Fig.3 shows the configuration obtained in a few seconds on a workstation at $p = 0.15$, that means at temperatures somewhat above the critical temperature. (Ref. 2b lists a simple BASIC program; I have used this problem to teach university students even in their first weeks.) Half of the sites are occupied and the other half is empty, but the distribution is not at all random: due to the interaction between neighboring sites the occupied sites tend to cluster together, and to leave large holes. These pictures are very similar to those obtained experimentally for real fluids in recent years[9] and give rise to *critical opalescence*, the strong scattering of light near the fluid critical point.

Fig.3: Ising configuration for part of a 79*79 square lattice after 1000 sweeps through the lattice with the cellular automata algorithm. Only the occupied sites are shown.

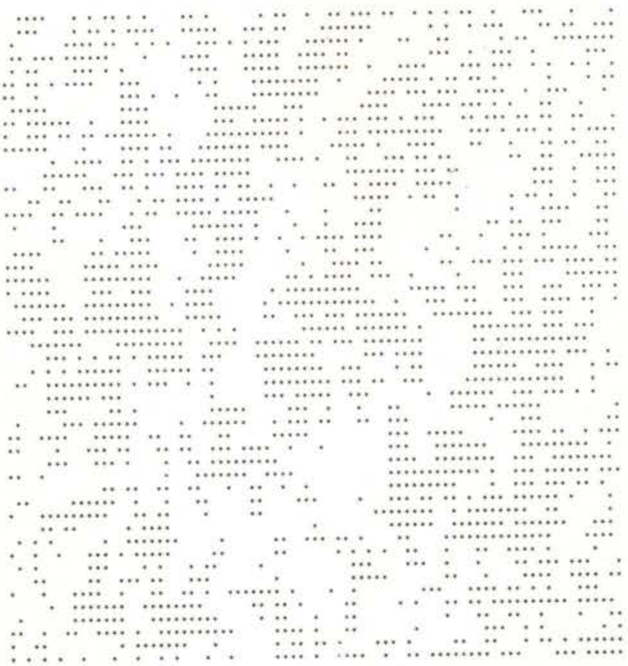


Fig.4: A large droplet from Fig.3 shown isolated after taking into account the helical boundary conditions. The droplet was isolated manually (can you find my error ?); ref.5 gives a computer program.

This critical point is known since more than a century, and van der Waals made the first theory for it in his 1873 thesis. Can we do better today ? Let us transform these impressions into a quantitative droplet picture[5]. A droplet is a group of neighboring occupied sites, as shown in Fig.4.

(Experts require in addition that the sites are connected with a probability 1-exp($-2J/k_BT$).)

In a classical ideal gas we have only single molecules, no larger droplets, and $PV = Nk_BT$ connects pressure, volume, particle number, Boltzmann's constant, and absolute temperature. If we have N_s droplets of s molecules each, due to the clustering shown above, then

$$PV = \sum_s N_s k_B T$$

is a reasonable generalization, neglecting the interactions between different droplets. (Similarly, the total atmospheric pressure is the sum of the partial pressures of nitrogen, oxygen, water vapor, carbon dioxide, etc.) The number of molecules

$$N = \sum_s N_s s$$

is even exact. We know that the density difference N_c-N of a vapor to the critical density N_c (for molecules with unit mass in a unit volume) varies slightly below the critical temperature T_c as $(T_c-T)^{\beta}$. Here $\beta = 1/8$ or 0.32 in two and three dimensions is one of the critical exponents for which Kenneth G. Wilson got the 1982 Physics Nobel prize. Thus

$$\sum_s (N_s(T_c)-N_s(T))s \propto (T_c-T)^{\beta}$$

Another quantity of interest is the spatial extent ξ of the correlations, the correlation length. We expect it to vary as the typical cluster radius R_s, or

$$\xi^2 \propto \sum_s R_s^2 s^2 N_s / \sum_s s^2 N_s$$

The droplet radius then gives a fractal dimension *d* through $R_s^D \propto s$. The correlation length, on the other hand, is known to diverge near the critical point as $(T-T_c)^{-\nu}$. Scaling arguments[5] then give

$$D = d-\beta/\nu$$

for the fractal dimension in *d* dimensions; $D = 15/8$, 2.49, and 3 for $d = 2$ to 4 (in the van der Waals theory, $D = d-1$). The droplet volume varies as R_s^d, and thus the average density within a droplet decays as $s / R_s^d \propto s^{-\beta/D\nu} = s^{-1/\delta}$. (Here the critical exponent δ relates pressure and density on the critical isotherm: $P(T_c) - P_c = (N(T_c)-N_c)^{\delta}$.) due to this decrease of the density with increasing droplet mass the critical droplets are fractal and differ from simple raindrops. [This fractal dimension is valid exactly at the critical point. Below the critical temperature we expect large droplets to be quite spherical, $D = 3$, whereas above the critical temperature they should be similar to the so-called *lattice animals* with $D = 2$ in three dimension.]

Thus we see that the fractal dimension can be expressed as a combination of critical exponents which were of interest to physicists since decades. And more qualitatively, the well-known critical opalescence is the scattering of light on fractal droplets. direct experimental determinations[9] of the droplet radius as a function of the number s of molecules in the droplet have, to my knowledge, not yet been made. Computer simulations[7] in the Ising model, on the other hand, have confirmed within about one percent the predicted values for *D*, nearly two decades after which the first speculations were published. Unfortunately, such accuracy is not yet good enough to distinguish between the fractal dimension of the Ising model and that of percolation, nor has the claim $D=2$ above T_c been confirmed reliably by simulations.

But computers get faster and better every year, equilibrium is reached faster by flipping whole droplets together instead of only single spins[10], and I think that with hundreds of processors, coupled together already today in large parallel computers[8], such accuracy may be possible now. Let us see if the experimental physicists beat the computational physicists in the determination of fractal dimensions at the critical point of fluids. This Ising model is a nice example where old problems are getting solved better and better even today, through new ideas, faster computers, and international cooperation.

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