

Gentle warning on fractal fashions

The novel idea that fractal structures can support high-energy lattice vibrations may not be the philosophers' stone that some have suggested.

FRactal structures are understandably one of the captivating fashions of our times. Even without the proselytizing of B.b. Mandelbrot (as in *The Fractal Geometry of Nature* (Freeman, New York; 1983)), the subject would by now have been dragged into prominence by the host of practical applications to which it lends itself. The simplest problems are those of the aggregation of particles onto a growing aggregate, where there is now a host of demonstrations that the density of such a structure is a decreasing function of its size, most graphically described by means of a "dimension" smaller than that of the space in which it grows. But it is plain that biological applications must also abound. For are not large polymer molecules put together by the aggregation of monomers onto a growing backbone candidate fractal structures?

This line of enquiry has already been productive. Some polymer structures do indeed turn out to be fractal structures, while the suspicion has grown up that the properties of some important biological molecules are in many ways a consequence of their supposed inherent fractal character. But fashions that are too pervasive can also be misleading, and require occasional correction. That is the chief interest in an elegant paper by J.A. Krumhansl (*Phys. Rev. Lett* **56**, 2696; 1986) of Cornell University which, in the gentlest manner, warns people against the tendency to look for fractal explanations everywhere.

Krumhansl's topic is also interesting and potentially important. His starting-point is a series of speculations about the interaction in molecules such as those of haemoglobin of the central iron atoms with the surrounding ring of porphyrin rings and the protein structures to which they are in turn attached. Changing the spin states of the central iron atoms requires a substantial amount of energy, greater than that corresponding to the mostly low-energy vibrations of the usual protein chain. So how can a larger amount of energy be exchanged with a protein environment? Fashionably, there seems recently to have been a tendency to invoke fractal phenomena of a new kind, those pertaining to the vibration of fractal structures of various kinds.

The mere idea that it might be possible to calculate the vibration frequencies of a fractal structure is naturally surprising. To be sure, it should in principle be possible

to deal with any specific fractal structure provided there is enough computer power to hand. One common model is that in which the particles in an aggregate are replaced by masses (all of the same size) which are then supposedly connected to their neighbours with springs with identical elastic properties. Since most simulations of fractal structures begin life on an underlying lattice with well-defined properties, solving the vibrational problem is essentially a calculation of the vibrations of a lattice in which there are patches missing. And even though each different arrangement of patches should in principle give rise to a distinctive set of vibration frequencies, the fact that the geometrical properties of aggregates can be described in gross terms (by their fractal geometry) means that it is reasonable to look for general properties of the vibrational spectrum of a fractal lattice.

It is nevertheless remarkable that so much has been accomplished in just over a decade. The frequency spectrum of a reasonably well-behaved solid (with three space dimension) is a function proportional to the square of the frequency. So much has been known since Debye and others took up the question of the specific heat of solids early in this century. At low frequencies, fractal structures have the same kind of vibrational spectrum; longer waves do not recognize that there are patches of the lattice missing.

The surprise (but a little thought will show that it is not really that surprising) is that the vibrational spectrum of a fractal structure includes a large proportion of high-frequency vibrations. Crudely, there must be within a fractal structure patches filled with particles which are nearly isolated from the rest of the structure, and which then perforce vibrate internally at lower frequencies because they are denied the opportunity for taking part in the large-scale long-wavelength vibrations involving the operation of the lattice as a whole.

This conclusion obviously neatly fills the bill required by the haemoglobin problems. If fractal structures not merely admit but require an unexpectedly large proportion of vibrations at high frequency (or, more strictly, short wavelength), there will be opportunities for the exchange of relatively large amounts of energy between, say, haem iron atoms and the surrounding haemoglobin molecule. But there is one snag: the peculiarly

fractal vibrations are also localized (to the patches of the lattice which are themselves almost geometrically isolated), so that the rate of energy exchange will not be great. Is it possible to circumvent that difficulty?

Krumhansl's paper is not so much a protest as a demurring. He does not question the possibility that fractal structures may sustain short wavelength vibrations (which, being cousins of more familiar photons, have inevitably been called fractons), but he does insist that the statement cannot be turned around in such a way that every solid with an anomalous vibration spectrum can be inferred to be a fractal structure of some kind.

The issue is of some importance because of the way in which estimates of the vibrational spectra of real solids (most simply made by measuring the specific heat as a function of temperature) have been used to make structural inferences. This has become especially fashionable in the study of amorphous solids, often said to be fractal over short distances. For starters, Krumhansl offers the example of the monatomic indubitably three-dimensional solid selenium, whose vibrational spectrum is as anomalous as it could be.

Krumhansl's explanation is both simpler and more persuasive. The anomalous vibrational frequency-spectra are often merely consequences of anisotropy of the forces between the atoms in a vibrating structure. Where proteins are concerned, for example, the forces are not central but are directed along the chemical bonds by which atoms are joined. And, in other circumstances, bond-bending forces become dominant.

The effect of Krumhansl's gentle broadside will not be to discourage interest in fractal structures. Quite possibly, the effect may be the reverse of that (no bad thing in itself). But this is an interesting case, which seems to happen more and more often, of how an explanation in search of a phenomenon may lay claim to far more territory than it can handle.

For the time being, and perhaps for a long time to come, progress in the field of fractals hangs crucially on numerical simulation. The results are convincing but not suggestive. They tend to confirm conjectures but not to suggest them. One day, it may all be different. Let us hope so.

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