It's just a phase…

The English physician and scientist William Gilbert first proposed in 1600 that the needle of a compass points northwards because of forces issuing from the Earth. Our planet, Gilbert presciently suggested in his masterwork, *De Magnete*, is itself an enormous magnet, and he supported his argument with experiments using an Earth-like sphere of lodestone called a 'terrella'. As he demonstrated, a compass held on the magnetized sphere's surface acted much as one on the Earth.

In *De Magnete*, Gilbert also presented other bold hypotheses, asserting, for example, that quartz and other hard crystals are, despite all appearances, made of ordinary water. Their starkly different properties, he suggested, reflect internal changes in which "the humour or juices [in the water] were shut up in definite cavities" by various geophysical processes. This particular idea seems silly to us now, yet we also know that Gilbert's essential insight was correct; the manifold transformations of physical matter between liquid, solid and gas, between different crystalline phases or many other more exotic phases, often reflect not changes in the constituent particles, but in their collective organization.

Indeed, we know immeasurably more today than Gilbert could have imagined about such phase transitions, and they occupy a special place in science because of their crucial relevance in condensed-matter physics, as well as in astrophysics, cosmology, geophysics, molecular biology and even the study of traffic flows. Even so, 400 years after Gilbert, we may still have a lot to learn.

There is much theoretical literature on phase transitions, largely devoted to their proper taxonomy and to methods for calculating their precise properties. In a system of interacting particles, according to the developed view, it is a singularity in some thermodynamic quantity that signals the existence of a phase transition. For example, a piece of iron is heated and its magnetic susceptibility diverges when the temperature approaches 770 K. The nature of this particular transformation — a continuous phase transition — is known in exquisite detail through the beautiful theory of critical phenomena. Among its more remarkable implications is that of universality — the insensitivity of physics in the critical regime to many of the details of the microscopic interactions, which implies not only that widely different systems reveal strikingly similar behaviour, but that even crude models can produce extraordinarily accurate predictions.

These results issue in part from the application of powerful renormalization group methods, which have been developed with spectacular success and show every sign of being extended to systems away from equilibrium — to phase transitions induced by noise, for example. Still, all this understanding rests on the framework of statistical mechanics, and its essential reliance on a perspective based on probabilities. What about the precise dynamics? It's natural to wonder if, in a system of interacting particles following purely classical dynamics, for example, a phase transition might also reflect some abrupt qualitative transformation in the nature of the particle trajectories.

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This idea undoubtedly has a long history, and before Boltzmann's introduction of statistical hypotheses, would probably have been the default conceptual perspective of most theorists. But its detailed exploration, surprisingly, has only advanced in the past decade, stimulated by the suggestion that topology may play a crucial role. Take a system with a hamiltonian of the standard form $H = \frac{1}{2}\Sigma p_i^2 + V(q_1,\ldots,q_N)$, with V being the N-particle potential energy. Around 1997 Marco Pettini and colleagues first suggested that phase transitions for such a system might be linked to abrupt topological changes in the system configuration space, specifically in the sets M_v defined to contain all points in the configuration space for which V is less than some value v. Suggestively, early numerical simulations of models exhibiting phase transitions showed cusp-like or discontinuous changes in several topological measures of these dynamically important sets.

Based on these initial results, some physicists speculated that it might be possible to give a general and complete explanation of phase transitions in terms of topological changes in dynamics. This was a little premature. But, as Michael Kastner argues in a forthcoming review, recent studies, while showing that this conjecture doesn't hold, also support the value of the general idea (*Rev. Mod. Phys.* in the press; arXiv:cond-mat/0703401v1, 2007). It now seems that topology does give strong signals of phase transitions, but that features vary from one problem to another in a more delicate way. In systems with a finite number of particles, indeed, any topological change in the sets M_v does seem to be linked to an associated phase transition, reflected in a singularity in the system's (microcanonical) entropy. In any infinite system, however, topological changes in the M_v are necessary but not sufficient for a phase transition, at least in the context of short-range particle interactions of the type usually considered in statistical physics.

A fascinating aspect of this work is its reliance on mathematics suited to the description of topology, particularly so-called Morse theory. Morse theory traces topological changes in manifolds by considering functions defined on them; in this case, changes in the configuration space with the function V defined on it. The theory has a disarming simplicity in that topological changes can be followed in terms of critical points of this function — akin to nodes, saddle points and so on — which serves to render questions of topology into more tractable and familiar analytical terms. A quantity known as the Euler characteristic, for example, because it is known to be a topological invariant, can be monitored in numerical simulations as a key flag signalling abrupt topological changes.

I suppose this way of thinking might be criticized with the old naive argument that "we already have a theory for that". But it explores the nature of phase transformations from a complementary point of view, and for that reason may ultimately pay handsome intellectual dividends. We still cannot say with precision what are the necessary conditions for a system to exhibit a phase transition, and that doesn't seem like too much to ask. One day soon we may be able to answer.

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