# Towards explaining superconductivity

The high-$T_c$ superconductors contain planar sheets of copper atoms, structures on which much attention is being lavished — with some success.

ALTHOUGH it is curious that, almost exactly three years after the discovery of the first ceramic material capable of supporting superconductivity above the temperature of liquid nitrogen, there is still nothing that might be called a simple theory of the phenomenon, at least it becomes progressively easier to understand why that should be so. At first, of course, it seemed that the materials found to be superconducting have a common structural element that would quickly lead to an explanation of their properties. The working elements are two-dimensional sheets in which copper ions of ambiguous valency are linked to others through oxygens. What more reasonable than to suppose that the problem is that of accounting for conduction by electrons in these copper sheets, on the assumption that the function of the other components of the copper oxide superconductors is simply to hold the working sheets together, and in the process to modulate their electrical properties?

The guess may be correct, but the inference is not especially helpful. The copper ions in superconducting sheets do not all have complete shells of electrons, and so have magnetic moments instead. Although the sheets of copper atoms in a compound such as $La_2CuO_4$ — from which superconductors may be derived by replacing some La by Sr for example — may be regarded as simple prototypes for the superconducting structures, this compound is itself an insulator which, at low temperature, has the properties of an antiferromagnet — there is long-range magnetic ordering of the magnetic ions, but neighbouring spins tend to point in opposite directions, so that there is no overall magnetic moment.

By now, it seems to be generally accepted that most of the high-temperature superconductors are converted, by relatively small changes of chemical composition, into materials with long-range antiferromagnetic order (but no superconductivity) at low temperature. But the measurable order of the copper ions can be taken as a proxy for the ordering of whatever electrons they may have released into the electron bands of the lattice. So the problem of accounting for the electrical properties of the superconducting copper sheets may be likened to that of accounting for the properties of a two-dimensional lattice in which there are spins at all (or almost all) the lattice points, and in which the interaction between them predisposes towards antiferromagnetism — the energy of two parallel neighbouring spins is greater than that of two anti-parallel spins at the same location.

If the spins were those of classical objects, there would be no difficulty. Antiferromagnetism on a two-dimensional lattice would be no different from, say, the problem of filling a lattice with equal numbers of atoms of two different kinds, which is the two-dimensional equivalent of the order–disorder transitions found in, for example beta (GK beta)-brass. But, sadly, electrons being electrons, the problem is not classical but quantal, and the problem is no less difficult than that of enumerating the states of a system of spin-½ quantum spins at the vertices of a two-dimensional lattice. Endless assaults on the problem of ferromagnetism have shown how difficult this task can be.

The essence of the difficulty is that, while it may be possible to guess (and even prove) that the ground state of the whole system (and thus that occupied at sufficiently low temperature) may be a ferromagnet or antiferromagnet according to the direction of the coupling feedback, even the low-temperature thermodynamic properties of the system depend on the numbers of states of not much higher energy accessible to the system. The obvious candidates are states in which patches of order are separated by domain boundaries, but enumerating them is not child's play.

Yet some progress seems to have been made. Thus Hong-Qiang Ding and Miloje S. Makivić, from California Institute of Technology, now describe an exceedingly powerful Monte Carlo calculation of an antiferromagnetic lattice designed to allow for the simulation of $La_2CuO_4$ (*Phys. Rev. Lett.* **64**, 1,449; 1990). In this context, a Monte Carlo simulation entails starting with an arbitrary arrangement of spins on the lattice, and then changing them in pairs according to rules that allow all spin states to be reached without violating the overall constraints. The authors rightly boast of their access to Caltech's parallel computer system, but they have also devised a new and efficient algorithm for tracing out the evolution of their system. As is the custom in this part of the trade, they have worked with square patches of two-dimensional lattice with as many as 128 lattice spacings to each side.

The outcome is a relationship between correlation length — the distance over which order, on the average, persists — and temperature; briefly, the logarithm of the correlation length is inversely proportional to the temperature. That, apparently, contradicts other models of the ordering process. In lanthanum copper oxide, the correlation length agrees well with that measured by neutron diffraction below 500 K (where there is a phase transition), provided the interaction energy is chosen appropriately. For what it is worth, that energy is not very different from estimates derived from Raman-scattering experiments, which provide a direct measurement of the energy of interaction by the change of frequency of the scattered light.

All that is encouraging enough, but not every calculation in the field is like that. The same issue of the same journal (**64**, 1445; 1990) describes a different approach to the same problem by H. J. Schulz of the Université Paris-Sud. The starting-point is again an arrangement much like that of lanthanum copper oxide, but the objective is to understand what happens as electrons are added to or subtracted from the system by the substitution of lanthanum atoms by others. The conclusion seems to be that the detailed structure of the magnetic ordering is exquisitely sensitive to the addition or subtraction of electrons from the lattice.

Imbalancing the lattice in one direction or the other will stimulate the formation of domain walls, at decreasing separation from each other as the imbalance grows. Indeed, Schulz suspects that there is no composition except that corresponding to stoichiometrically pure lanthanum copper oxide over which a single antiferromagnetic domain accounts for the whole of the structure. In this picture, the emergence of a conducting, let alone a superconducting, state seems obscure, to say the least.

There is no inconsistency between these approaches, which are complementary to each other. The more frequently domain walls appear in the structure, the less the long-range order and thus the correlation length. But no doubt it is now only a matter of time — time on Caltech's parallel computer — before there is a sequence of calculations at various degrees of imbalance from the model equivalent of lanthanum copper oxide. It will be interesting to see what emerges, but even success will not necessarily imply that there will be an explanation to put in the textbooks.

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