Modelling high-T_c superconductivity?

The ubiquitous Ising lattice has been used to model competitive ordering forces such as may account for some of the properties of the copper-oxide planes in ceramic superconductors.

THE Ising lattice is not so much a model as a notation, it now appears. Originally, in the 1920s, the idea was to make a model of magnetic materials, ferromagnets for example. The procedure was straightforward: represent the structure of the solid by an appropriate geometrical lattice, imagine that there is a magnetic dipole at each of its vertices, define some rule for calculating the total energy of the system from the orientations of the magnetic dipoles at all possible pairs of vertices and then treat the problem as one in statistical mechanics. The hope was that it would be possible to show that such a model would behave as a real ferromagnet does; in other words, that there would be a critical temperature (the Curie temperature) below which magnetic order would be the rule, above which it would not be.

The frustration of this ambition has been amply described. In general, even with simplifying assumptions about the energy of interactions between differently located lattice sites, real three-dimensional problems are not soluble. Even in two dimensions (as with crystalline solids in a plane, Langmuir-Blodgett films perhaps), only drastic simplification will allow analytical solutions of model problems. One powerful simplification is to suppose that only magnetic elements at literally nearest-neighbour vertices contribute to the interaction energy. (On a square lattice, for example, interactions across the diagonal would be counted as zero.) Then, most order-disorder problems on reasonably shaped lattices can be solved exactly.

But do not the simplifying assumptions empty the baby with the bath water, so to speak? A real ferromagnetic material, say a crystal of iron, cannot really be discussed as if it were nothing but a collection of magnetic dipoles sited on the vertices of a geometrical lattice, each of which interacts energetically only with its nearest neighbours in a strictly classical fashion. Indeed, atoms in such a crystal acquire magnetic moments (other than those of their nuclei) by losing electrons to the Fermi sea, which is the means by which the crystals are able to conduct electricity.

The obvious snag is that the ions left behind continue to interact with the electron sea collectively, which means that, at the very least, the problem of ferromagnetism boils down to that of calculating the expectation value of the total electron spin for a system of atoms capable of being ionized and which are located on the vertices of a regular lattice. That is a problem in quantum mechanics, which leads to what is called the Hubbard lattice, a system of quantum spins in a regular array. To tell from the literature, people are still enumerating the eigenstates of such a system. It is even less soluble than the Ising lattice.

That does not mean that the Ising lattice has been of no value. On the contrary, it is a literally exact model of order-disorder in, say, α–brass (Zn to Cu in the ratio 3:1). Measurements show that, in the ordered (and hardened) state, extra energy is needed to melt to solid than when the atoms are randomly arranged. The other side of that coin is that it is possible to measure the latent heat of the phase transition for the disordered to the ordered state when a sample in the disordered solid is annealed. That is something tangible, technically a first-order transition.

The more substantial interest of the Ising lattice has been, over the past several decades, heuristic, as the saying goes. Allowing for the simplifications inherent in any attempt at analytical solutions, it nevertheless emerges clearly that three-dimensional systems allow of first-order phase transitions, the simpler two-dimensional systems allow of only second-order transitions (where there is a specific heat anomaly, but no latent heat, at some critical temperature) and that simple one-dimensional systems in which only nearest neighbours interact do not allow order-disorder phase transitions in either sense. (They cannot, for a single break-point in a linear lattice will destroy long-range order.) None of that is surprising, but it is good that it is confirmed.

By now, there seems to be no limit to the uses of this simple model. It is, for example, a natural description of adatoms on a solid surface (but with inconvenient constraints on the numbers of atoms). More generally, the Ising lattice is potentially a way of modelling continuous systems by discontinuous representations of them, although the difficulty of the algebra in more than two dimensions is an obvious drawback. But should not the model come into its own as a means of dealing with the essentially two-dimensional arrays of atoms in the apparently conducting planes of the new high-temperature superconductors?

That, as it happens, is what U. Löw and V. J. Emery from the Brookhaven National Laboratory, K. Fabricus from the University of Wuppertal and S. A. Kivelson from UCLA have now done (*Phys. Rev. Lett.* **72**, 1918–1921; 1994). The planes containing copper and oxygen atoms in these materials are believed to embody the essence of the superconductivity. It is also known that the electronic state of the atoms is not that of electrical neutrality. When electrons are transferred to the electronic conduction band, the atoms left behind are short of electrons and thus behave as electron "holes". Moreover, in the nature of things, these holes are mobile within the copper-oxygen planes.

It may be that what makes high-temperature superconductivity possible is the formation of physical regions within these planes where the density of holes is greater than expected. But how could such a state of affairs come about? To ask that, in a plane in which positive and negative charges are free to move, the positive charges should congregate together, expelling the others, is to require a great deal of the principle that the energy of a static system tends to a minimum. It can only happen if there is some mechanism that yields an energetic benefit when electron holes are close together.

That is the inspiration for a variation on the Ising theme that, in the short run, will probably do more to command the attention of Isingologists than to throw light on the real mechanism in high-temperature superconductors. The novelty of this version of the model is that it takes account of a short-range interaction between the nearest-neighbour vertices that tends to increase the likelihood that neighbouring vertices will be occupied by holes (and *vice versa*) and a long-range interaction between all vertices which is essentially the Coulomb interaction (like charges repel each other and all that).

Solving this model exactly is a lost cause. What Löw and his colleagues have done it to represent the state of each vertex of their square lattice by a three-valued variable which can take the values +1, 0 and -1, representing a hole, the average state of a vertex and the opposite of a hole respectively.

What they are able to show is that the least energetic state of such a system can consist of rectangular patches in which each vertex is occupied by a hole; that may mildly delight the superconductivity community. They also show that in a system such as this, with contradictory long and short-range ordering forces, there may be many ordered phases related to each other by exceedingly complicated phase diagrams if the relative strengths of the interactions are chosen appropriately. It would be rash to think that this will clear up the scandal of why it has taken ten years not to find an explanation for such an important phenomenon, but it is at least a new approach.

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