Computing Limits to Superconductivity

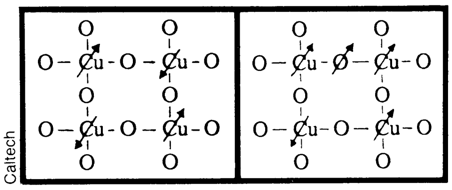
Intuition and guesswork have played a major role in the discovery of new superconducting materials. To reduce the amount of time and effort spent trying out candidates, experimentalists have long sought some theoretical guidance on where to look for materials that lose all resistance to electrical current, especially at temperatures higher than the present record: 125 kelvins, or -234°F. The latest attempt to provide such help combines extensive quantum-mechanical calculations with a rudimentary model of how magnetic interactions may lead to superconductivity. The result is a simple equation that predicts the temperature at which a given copper-based material becomes a superconductor.

"We start with the basics and derive the interactions," says physical chemist William A. Goddard III of the California Institute of Technology in Pasadena. "We solve the equations, plug in numbers and get results in the right ball park. That's really not been done before." Goddard and his colleagues presented their theory this week in Los Angeles at an American Chemical Society meeting.

Copper oxide superconductors have a distinctive layered structure. Each layer consists of a checkerboard of copper atoms separated by oxygen atoms. Each copper atom has a magnetic moment, or spin, that is either up or down. Normally, spins on adjacent copper atoms point in opposite directions to produce an antiferromagnetic state (see diagram, left). The oxygen atoms have no spin.

In a compound such as lanthanum copper oxide, replacing some lanthanum atoms by strontium upsets the charge balance, and forces either a few oxygen or some copper atoms to lose electrons. Goddard's calculations, based on the quantum-mechanical interactions between electrons on neighboring atoms, show for the first time that oxygen rather than copper is the loser. Each oxygen atom, with the loss of a single electron, develops a spin and influences the spins of neighboring copper atoms, making them line up in the same direction (see diagram, right). This creates a local pocket of ferromagnetism within the copper-oxygen sheet.

The small proportion of oxygen atoms missing an electron from their normal state can be thought of as having "holes." Because holes can migrate freely from atom to atom (equivalent to electrons hopping from one oxygen atom to another), the material is an electrical conductor. "What leads to superconductivity, despite the repulsion between conduction electrons, is an effective attractive interaction between those holes as



Caltech

they move around," Goddard says. Simply put, one hole, by creating ferromagnetic pockets as it flits about, blazes a trail that other holes can readily follow.

Goddard's equation for the temperature at which a material becomes a superconductor suggests that the highest temperature attainable with a copper-oxygen system is 225 kelvins, 30 kelvins higher than the temperature of dry ice. According to the equation, that happens in a material in which the magnetic spins are as disordered as possible. The equation also suggests that replacing oxygen with sulfur would lead to even higher transition temperatures, but no one has yet found a copper-sulfur compound with the right layered structure.

"The really important thing in advancing the science is having a theory that provides a greater understanding of the parameters: what would change if you changed the elements," Goddard says. "That would give you a better shot at looking for new systems." He adds, "Our theory makes very specific predictions. This means that if there is something wrong with the theory, experiments will disprove it quickly."

"It's true that some of the beginning assumptions that Goddard makes in his model, which are supported by his calculations, are plausible," says Robert J. Birgeneau of the Massachusetts Institute of Technology. "The fact is, however, that there is as yet no convincing experimental evidence that the beginning assumptions are correct." Birgeneau and his collaborators have independently developed a theory similar to Goddard's.

"Goddard has done some very useful calculations," says physicist Paul M. Grant of the IBM Almaden Research Center in San Jose, Calif. However, Goddard's method for incorporating magnetic interactions leading to superconductivity is only one of several different possibilities proposed by theorists. The issue of how superconductivity arises in copper-based superconductors remains controversial, Grant says.

For example, Richard L. Martin of the Los Alamos (N.M.) National Laboratory and his colleagues also did quantum-mechanical calculations. However, their theory emphasizes the importance of electron movements rather than magnetic, or spin, interactions in superconductivity. Their calculations show that electrons can shuttle back and forth between oxygen and copper atoms in such a way that their motions are coordinated and reinforce each other to produce an electron flow without resistance.

"We have quite a number of experimental results that limit what could be going on," says Victor J. Emery of the Brookhaven National Laboratory in Upton, N.Y. At the same time, neither the theoretical calculations nor the experimental measurements are precise enough to support one theory rather than another.

"People are now trying to do the hard work of figuring out their models in more detail," Emery says. But with so many competing theories, a clear picture of how high-temperature superconductors work still seems far away. "Things are in a state of turmoil at the moment," Emery says.

"This is a phenomenal problem," Birgeneau says. "It involves most of the important unsolved problems in solid-state physics, all realized in one material." — *I. Peterson*

Largest engineering prize

With visions of the prestige bestowed on Nobel laureates, the National Academy of Engineering (NAE) in Washington, D.C., will award $350,000 and a gold medal every two years to an individual or team whose engineering or technology achievements benefit society. NAE President Robert M. White says the prize is the largest financial award offered exclusively for accomplishments in engineering and technology. The recipient of the first Charles Stark Draper Prize, named in honor of the engineer who developed the navigational systems used aboard U.S. spacecraft, will be announced in October 1989 at the academy's 25th-anniversary annual meeting.

A 13-member committee formed to select award recipients includes representatives of leading U.S. academic institutions, research and development companies and the National Science Foundation. Robert C. Seamans Jr. of the Massachusetts Institute of Technology will chair the committee, which will solicit candidate nominations from 31 professional organizations in 24 countries. However, the committee may offer the prize to any living person, and the award carries no stipulations regarding its use.

The Charles Stark Draper Laboratory of Cambridge, Mass., will provide funding for the prize, which White says the NAE hopes will attain the recognition accorded to the Nobel prizes. □