Electronic Nirvana

In January 1986, Georg Bednorz and Karl Müller found that a novel copper-oxide compound chilled to 30 degrees above absolute zero allowed electricity to flow without resistance. Their discovery, which won a 1987 Nobel Prize, brought an exotic, quantum phenomenon into public consciousness and awakened a dream of technological nirvana—room-temperature superconductivity.

To transmit electrical current without the slightest loss of energy is magic without trickery, perhaps the closest thing to a free lunch Mother Nature offers. A material that is superconducting at room temperature would likely lead to high-speed trains that levitate on superconducting magnets, practical electric cars and superfast networks and computer chips.

Although room-temperature superconductivity remains an elusive quest, the 1986 breakthrough jump-started research around the globe that continues today. Within a few years, scientists found other copper-oxide materials and soon pushed the critical temperature, $T_c$, where resistance drops, well above 100 degrees Kelvin (100 K).

Along with furious laboratory efforts to find ever higher $T_c$ materials, the 1986 breakthrough stirred intensive theoretical work. One leader in the field, David Pines, staff scientist at Los Alamos National Laboratory, says that understanding high-temperature superconductivity is “arguably the major problem in physics today” with thousands of published papers a year contributing to the effort.

“If we can arrive at a complete theoretical explanation of high-temperature superconductivity,” says solid-state physicist Mark Jarrell of the University of Cincinnati, “then we should be able to design and synthesize a room-temperature superconductor, which would have tremendous technological implications.”

Superconductivity is a quantum phenomenon in the solid state, and theoretical formulations to describe it depend on high-performance computing to solve the equations. The solid state, which includes metals, semiconductors and insulators, is a densely packed, regularly spaced lattice of atoms with electrons moving among them. The electrons and electron states that must be accounted for are, like fish in the sea, essentially infinite, and it’s not possible, therefore, even with the most powerful supercomputers, to exactly calculate all the interactions that bear on the electronic properties. The theoretical challenge is to develop computational approaches that can reasonably approximate the complex physics and produce reliable predictions.

Within the past few years, Jarrell has developed an original approach that overcomes a serious limitation of another approach. Using the prototype Terascale Computing System at PSC, he and his colleague, post-doctoral fellow Thomas Maier, carried out computations with a theoretical model, the two-dimensional Hubbard model, that has gained general acceptance as a theoretical framework for high-$T_c$ materials. Structurally, the high-$T_c$ materials are a series of copper-oxide planes, with apparently no interaction between the planes, so they can be modeled as 2-D systems. Jarrell’s computations indicate, nevertheless, that the 2-D Hubbard model is incomplete as a description of high-temperature superconductivity.

**SOMETHING HAPPENING HERE**

BCS theory, which described the electron-pairing phenomenon that underlies low-temperature superconductivity, doesn’t work for high-$T_c$ materials, although some version of electron pairs still appears to be the joy juice of the new superconductivity. In the words of a 60s song, “There’s somethin’ happening here. What it is ain’t exactly clear.”

Fifteen years of prodigious work on high-$T_c$ materials has established that they constitute a new realm of solid-state physics. In virtually every respect, their normal state—behavior above $T_c$—differs markedly from conventional superconductors. The big job of finding a theory that pulls this exotic new solid-state world into a coherent picture has gone in many directions, but the most widely accepted starting place has been the 2-D Hubbard model.

“It’s the simplest possible model you could construct,” says Jarrell. Despite its relative simplicity, the 2-D Hubbard model has shown an ability to accurately calculate many of the strange properties associated with high-$T_c$ superconductors, at least in the normal state. The main problem has come in finding a way to solve the Hubbard model under conditions that replicate the transition to superconductivity.

Solution of the Hubbard model for the infinite number of electrons in a solid-state lattice requires an approximation scheme. An approach called the Dynamical Mean Field has proven useful in many calculations, but is inherently inadequate for the high-$T_c$ transition because it’s “localized.” It accounts for interactions between electrons at one atomic site, while other sites in the lattice are in effect averaged as a mean field. Studies have shown, however, that a fundamental characteristic of high-temperature superconductivity is that the pairing interactions are non-localized—electrons from neighboring atoms, rather than the same atom, interact strongly.
A good deal of activity has gone toward developing non-localized extensions to the DMF approximation. Jarrell has developed a sophisticated approach, the Dynamical Cluster Approximation, that incorporates non-local corrections by mapping the problem onto a cluster of sites, which is itself embedded within the mean field. In 2000, he used the DCA approach to solve the 2-D Hubbard model on a CRAY T3E at Ohio Supercomputer Center. With a four-site cluster, the smallest possible, his results showed properties in good agreement with high-T_c materials, including transition to the superconducting state.

The computational load increases dramatically with larger clusters, and Jarrell was temporarily precluded from looking at the effect of larger cluster sizes. In spring 2001, he and Maier gained access to the prototype Terascale Computing System, facilitating a series of calculations with cluster sizes up to 16. The increase in computational capability introduced a decisive change in the theoretical picture. “As we systematically increased cluster size,” says Jarrell, “superconductivity systematically went away. That tells you something fundamental. We believe that the 2-D Hubbard model is not sufficient by itself. Something new has to be introduced.”

Among several possibilities, Jarrell notes that a fully accurate model of superconductivity may need to add coupling between copper-oxide planes. Another possibility is “chemical disorder,” variation in the number of oxygen atoms from region to region. It’s impossible to predict how much computing it will take to thoroughly explore these questions, says Jarrell, but the full-scale TCS will allow him to get started.

More information: http://www.psc.edu/science/jarrell.html