

## Physics Nobel spotlights quantum effect

The discovery in 1982 that a cold cloud of electrons in a powerful magnetic field can display unusual behavior came as a great surprise to researchers. At temperatures near absolute zero, the electrons apparently condense to form a quantum fluid made up of ensembles of electrons, each seeming to have a fractional electric charge (SN: 6/25/83, p. 405; 8/25/84, p. 116).

This week, the Royal Swedish Academy of Sciences in Stockholm awarded the 1998 Nobel Prize in Physics to Daniel C. Tsui of Princeton University and Horst L. Störmer, now at Columbia University, for discovering this so-called fractional quantum Hall effect, and to Robert B. Laughlin of Stanford University for explaining the experimental findings.

The Hall quantum fluid is related to the quantum fluids that occur in superconductivity and in liquid-helium superfluidity (SN: 10/19/96, p. 247). "Events in a drop of quantum fluid can afford . . . profound insights into the general inner structure and dynamics of matter," the academy says.

The previously known quantum Hall effect occurs when electrons are trapped at the interface between two semiconductor crystals. That confinement restricts electron motion to two dimensions. A strong magnetic field at right angles to the interface causes electrons to drift sideways compared with the direction of electric current flow. At very low temperatures, gradually increasing the magnetic field causes the electric resistance in the direction of the drifting electrons to increase in steps rather than continuously. Those steps indicate that the resistance is quantized.

In their detailed probes of the quantum Hall effect at very low temperatures, Tsui and Störmer found, to their surprise, additional steps. They therefore named the new phenomenon the fractional

quantum Hall effect.

About a year later, Laughlin proposed that the confined electrons, interacting with the magnetic field, coordinate their movements in specific ways. Such collective behavior can be interpreted as belonging to quasiparticles—entities that behave as if they were particles—each having a precise fraction of the electric charge of an electron.

Recent measurements by other researchers have turned up additional fractionally charged steps. So far, Laughlin's model has explained all the findings.

Last year, two groups working indepen-

dently detected the noise—tiny fluctuations in electric current—produced by quasiparticles making up the fractional quantum fluid. Those experiments showed directly that the current was carried by objects with one-third the charge of an electron.

The physics of systems exhibiting the fractional quantum Hall effect remains an active field both experimentally and theoretically. In one offshoot, researchers are using nuclear magnetic resonance techniques to probe electrons trapped in semiconducting layers. Those studies enable them to determine the spins of electrons. Such data are useful to researchers developing quantum computers (SN: 1/18/97, p. 37). —I. Peterson

## Chemistry computations earn Nobel prize

Computers have revolutionized many scientific disciplines, and the field of chemistry is no exception. In recognition of that fact, the 1998 Nobel Prize in Chemistry was awarded to two scientists for their development of computational methods that describe the properties of molecules. Walter Kohn, a physicist at the University of California, Santa Barbara, and John A. Pople, a chemist at Northwestern University in Evanston, Ill., share the honor.

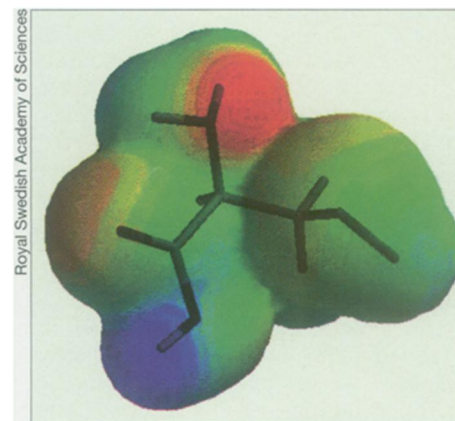
Based on quantum mechanics, the pair's techniques allow chemists to understand the shapes of molecules, how molecules interact, and the results of chemical-identification techniques. Kohn's work and Pople's are "two faces of the [same] coin," says Christopher J. Cramer, a computational chemist at the University of Minnesota in Minneapolis. Both scientists' approaches "have reached very sophisticated levels. This is just the right time for the Nobel prize" for computational chemistry, he says.

In the mid-1960s, Kohn greatly simplified the calculations needed to describe the quantum mechanics of molecules. Previous techniques required scientists to account for the motions of individual electrons, making it nearly impossible to analyze large molecules.

Kohn proved mathematically that it's enough to know the average number of electrons at any one point—the electron density. "His real contribution was in seeing a very different twist to quantum mechanics," says Cramer.

It took about 25 years, however, for scientists to learn how to apply Kohn's method to practical problems. Now known as density-functional theory, it's one of the main theoretical tools of chemists.

Also in the 1960s, Pople developed his novel approach to analyzing the electronic structure of molecules, which he called theoretical model chemistry. He constructed a computational method, applied it to a variety of calculations, and, over time, corrected its weak points.



Colors indicate electron densities around atoms of the amino acid cysteine (stick figure), as calculated by a quantum chemistry computer program.

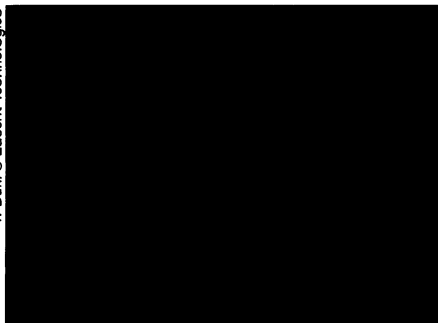
In 1970, Pople packaged the modeling tools he had developed into a computer program called Gaussian, which he distributed free for many years. In 1992, he incorporated Kohn's density-functional theory into the program, allowing chemists easy access to both techniques. Continually updated, today's commercial version, sold by Gaussian Inc. in Pittsburgh, is one of the most popular quantum chemistry programs available.

Pople was "almost always about 5 years ahead of everyone else in seeing what was possible with digital computing," says Cramer. "The vision he had was just spectacular."

Pople's program gave computational tools to chemists who might not have benefited from them otherwise. Gaussian is "so user-friendly," says Cramer, that "lots of experimental chemists—people who are not theorists—are able to apply these theories and interpret them."

Awarding this year's prize to both Kohn and Pople makes sense, says George W. Flynn of Columbia University. "It represents a good example of how, in [the study of] condensed matter, physics and chemistry are tightly coupled." —C. Wu

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In this visualization of the electron state underlying the fractional quantum Hall effect, the height of the blue-green landscape gives the probability of finding a single, representative electron moving in relation to its momentarily pinned companions (green spheres) and to the direction (black arrows) of the magnetic field associated with the electrons.