"Long before it's in the papers"

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“Quantum chemistry” a new window into lives of molecules

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Courtesy NIST
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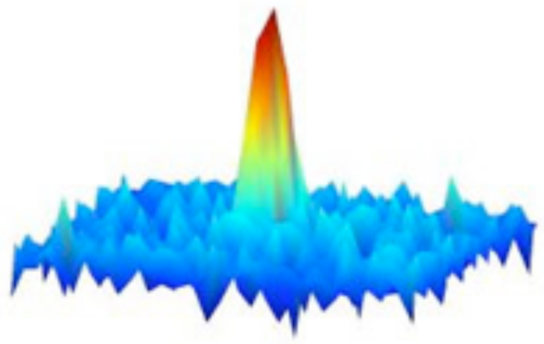
Physicists have detected molecules interacting with each other near the coldest possible temperature, where by the “classical” laws of physics they should be motionless, according to a report.

The chemical reactions are explained by the bizarre rules of quantum mechanics, which govern matter at the sub-microscopic level. These rules allow particles to go into places where they don’t have enough energy to go, by very briefly “borrowing” energy seemingly from nowhere. Quantum mechanics also requires particles to be sometimes considered as waves rather than as solid grains.



A map of the density of a molecular gas in which each molecule is in its lowest possible energy state. The gas has just been released from a trap created by lasers. The molecules are near absolute zero, a temperature at which quantum properties reign. The image -- made by detecting the absorption of laser light by the molecules -- reveals their spatial distribution, with density indicated by peak height and false color. (Credit: D. Wang/JILA).

Physicists don’t know what it is about atoms that makes them manifest themselves in such bizarre ways, but nonetheless, based on many decades of experiments, they do. The more sensible “classical” laws of physics, which reigned in science until the 20th century, apply only to more ordinary-sized objects.

The new findings, described in the Feb. 12 issue of the research journal *Science*, will help scientists understand previously unknown aspects of how molecules interact, a key to advancing biology, creating new materials, producing energy and other research areas, physicists said.

The work has practical applications for chemists in that it shows chemical reaction rates can be controlled using quantum mechanics, added the researchers, from JILA, a joint institute of the U.S. National Institute of Standards and Technology and the University of Colorado at Boulder.

It's "reasonable to expect that when you go to the ultracold regime there would be no chemistry to speak of," because atoms should be motionless, said physicist Deborah Jin, leader of one JILA group involved in the experiments. But "this paper says no, there's a lot of chemistry going on."

The experiments examined molecules near absolute zero, the theoretically lowest possible temperature, in which molecules would have no energy to move. Absolute-zero conditions can't be created in practice, but physicists can get there to within a tiny fraction of a degree. Absolute zero lies at minus 273 degrees Celsius, minus 460 degrees Fahrenheit, or zero on the so-called Kelvin scale.

Scientists have long known how to control molecules' internal states, such as the energies that determine their rotation and vibration. In addition, the field of quantum chemistry has existed for decades to study the effects of the quantum behavior of subatomic particles, components of molecules.

But until now scientists have been unable to observe direct consequences of quantum mechanical motions of whole molecules on the chemical reaction process, according to the scientists. Creating simple molecules and chilling them almost to a standstill makes this possible by presenting a simpler and more placid environment that can reveal subtle, previously unobserved chemical events, according to Jin and colleagues.

By precisely controlling the molecules' internal states while also controlling the molecular motions at the quantum level, scientists also say they can study how the molecules scatter or interact with each other quantum mechanically.

The physicists could observe, they explained, how the quantum effects of the molecule as a whole dictate reactivity. This window into molecular behavior has allowed the observation of long-range interactions in which quantum mechanics determines whether two molecules should come together to react or stay apart. Thus the work expands the standard conception of chemistry, according to the group.

The experiments are done with a gas containing up to a trillion molecules within a space the size of a small die. Each molecule consists of one potassium atom and one rubidium atom. The molecules have a negative electric charge on the potassium side and a positive charge on the rubidium side, so they can be controlled with electric fields.

By measuring how many molecules are lost over time from a gas confined by lasers within a trap, at different temperatures and under various other conditions, the team found evidence of heat-producing chemical reactions in which the molecules must have swapped atoms, broken chemical bonds, and forged new bonds. Theoretical calculations of long-range quantum effects agree with the observations, they noted.

In conventional chemistry at room temperature, molecules can collide and react to form different compounds, releasing heat.

In the ultracold experiments, quantum mechanics reigns and the molecules spread out as ethereal rippling waves instead of acting like solid grains. They don't collide in the conventional sense. Rather, as their wave aspects overlap, the molecules "sense" each other from as much as 100 times farther apart than would be expected normally. At this distance the molecules either scatter from one another or, if conditions are right, swap atoms. Scientists expect to be able to control long-range interactions by creating molecules with specific internal states and “tuning” their reaction energies with electric and magnetic fields.

The JILA team produced a dense molecular gas and found that, although molecules move slowly in the cold, reactions can occur quickly. But they can be suppressed using quantum mechanics. For instance, a cloud of molecules in the lowest-energy electronic, vibrational and rotational states reacts differently if the nuclear “spins” of some molecules are opposite. If the molecules are divided 50/50 into two different nuclear spin states, reactions proceed up to 100 times faster than if all molecules have the same spin. Thus, by preparing all molecules in the same spin state, scientists can deliberately suppress reactions.

The experimental team attributes these results to the fact the molecules are fermions, one of two types of quantum particles found in nature. (Bosons are the second type.) Two identical fermions can’t be in the same place at the same time. This quantum behavior of fermions manifests itself as a suppression of the chemical reaction rate in the ultralow temperature gas. That is, molecules with identical nuclear spins are less likely to approach each other and react than are particles with opposite spins.

“We are observing a new fundamental aspect of chemistry—it gives us a new ‘knob’ to understand and control reactions,” said institute physicist Jun Ye, leader of a second group involved in the research.