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It is a quantum fractal algorithmic universe

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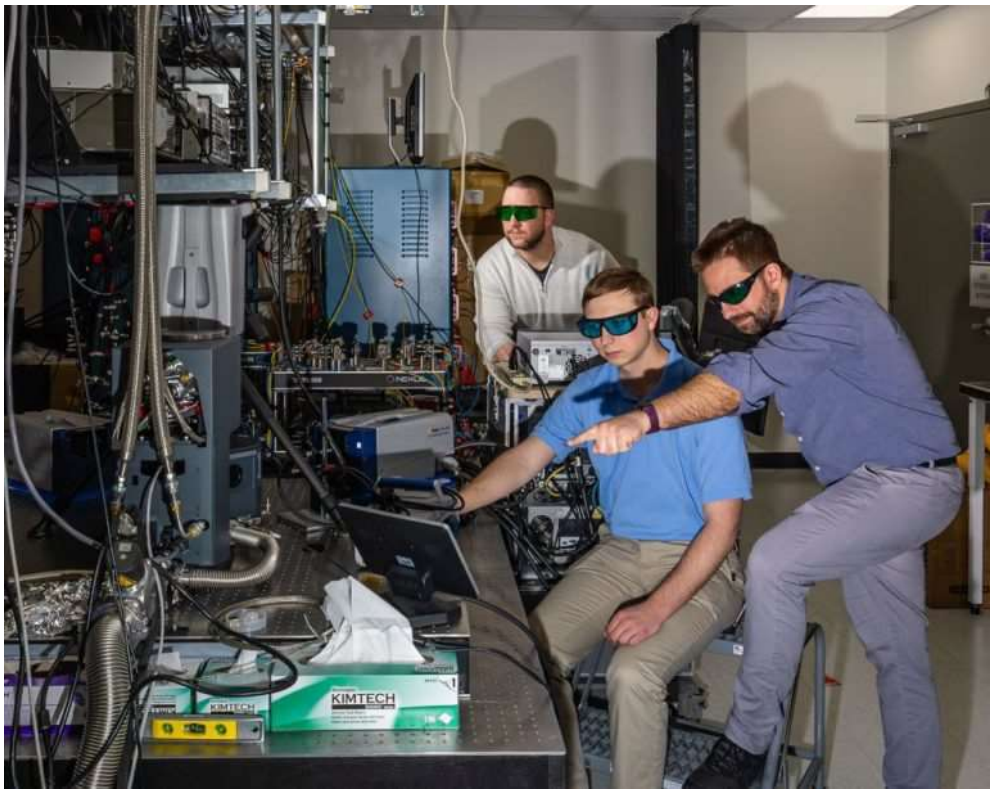
From Massive Structures To Nanometers: ORNL's Scanning Vibrometer Used In Quantum Research

The last time this team used Oak Ridge National Laboratory's 3D scanning vibrometer, it was to measure a gigantic composite panel.

This time, they're measuring the vibration amplitudes of a cryogenic ion trap – around 10 nanometers, peak to peak.



From left, J.D. Rice, Trevor Michelson and Chris Seck look at a monitor in Seck's lab. The three are wearing safety glasses to protect against the laser beams used by the scanning vibrometer, which is helping Seck quantify vibration of an appliance in his lab. Carlos Jones/ORNL, U.S. Dept. of Energy

“This is the first real test of the absolute limits of the machine,” said researcher Blake Van Hoy of the Isotope Science and Engineering Directorate’s Enrichment Science and Engineering Division, or ESED.

Van Hoy is the resident expert on the 3D scanning vibrometer. After he wrote a plant capital equipment proposal pitching it as a long-term infrastructure investment, the lab in 2021 purchased the specialized equipment, which uses visible or infrared lasers from three heads to build a geometric matrix, scattering light and assessing vibration to produce high-fidelity measurements of just about any object – enormous to tiny, any shape.
Its primary use at ORNL so far has been to help ESED with research and development. The composite panel, for example, was measured along with other types of panels to see which was best at reducing vibration energy.

But Van Hoy has advocated for more widespread use of the scanning vibrometer, which belongs to the lab, not specifically to ESED.

That’s why he was excited to hear from Chris Seck, a research scientist in the Computing and Computational Sciences Directorate’s Quantum Sensing and Computing group.

Seck is leading a project to engineer and develop a cryogenic ion trap apparatus to simulate quantum spin liquids, a key research area in materials science and neutron scattering studies. In the simulator, Seck can manipulate the trapped ion qubits – or quantum bits, the basic unit of information in quantum computing − to behave similarly to quantum materials that would be difficult to study in a lab.

But a common source of error in using cryogenic ion traps is the vibration of the actual apparatus, which factors into how the ions behave.

Seck is using a custom-built vacuum system inside a commercial cryo cooler to cool the apparatus, but he needs to be able to quantify the vibration of the mechanical cooler. When Seck read about the lab’s laser scanning vibrometer, he thought it could be used to quantify the vibrations. Not only would that give him a baseline for his own research, it also could help with engineering of future systems to further reduce vibrations.

“But this is much smaller than what they’re used to measuring,” Seck said.

It’s also different in other ways. For one, the team – which also includes ESED’s Trevor Michelson and J.D. Rice − will shoot at the tiny target area through glass. And while often the three laser heads are pointed at a single target, to provide a 3D model, in this case each head will point to an individual measurement point.

“This is going to be an interesting experiment for us because it’s pushing the absolute limits of everything we could think of to do,” Van Hoy said. “It’s going to be a good learning experience to know what the limits are.”

Many of the exceedingly detailed measurements the system can perform were once attempted with accelerometers, expensive and fragile button-size sensors that were placed in multiple locations to measure vibration frequency and damping.

But in this case, that would never be an option, Michelson said, because the accelerometers would be too big to use in the small space, and their added weight would invalidate the experiment by changing the dynamic behavior of the ion trap and associated vacuum chamber.

If not for the availability of the vibrometer, which recently had been calibrated, Seck would have had to order parts and construct an optical beamline to measure the vibrations, investing both time and money. But Michelson and Rice were easily able to set up the vibrometer system in his Building 5700 lab.

Since Seck’s is a long-term project, Michelson and Rice said the vibrometer can be moved if it’s needed for another project in the meantime; it can be set up again in Seck’s lab in a matter of hours. Seck said he hopes the measurements, besides informing his research, will lead to an article in the *Review of Scientific Instruments*.
And the team said they hope increased work for the vibrometer will lead to a dedicated lab space that specifically can accommodate measuring any size – enormous to tiny.

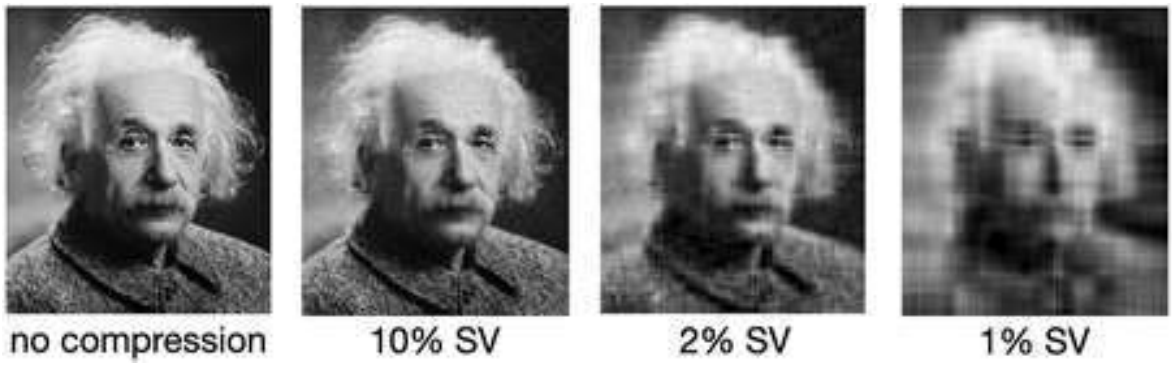
“What’s fascinating to me is the versatility of this equipment,” Rice said. “The first thing we ever did out of the gate with it was a large plate from 12 feet away – but I can take the mechanical pencil and ping it and get a measurement almost to the tip. Literally everything from tiny little components, all the way up to big structures, as long as you can get a good line of sight between the laser and what you need to test, you can get incredibly detailed measurements.

“We’re still barely scratching the surface of its capabilities, and it’s already blowing me away.”

Speeding Up Calculations That Reveal How Electrons Interact in Materials

Materials scientists and engineers would like to know precisely how electrons interact and move in new materials **and how the devices made with them will behave. Will the electrical current flow easily within the material? Is there a temperature at which the material will become superconducting, enabling current to flow without a power source? How long will the** quantum state of an electron spin be preserved **in new electronic and quantum devices?**

A community of materials physicists attempt to address such questions by understanding what takes place inside materials, calculating their behavior down to the level of individual electron interactions and atomic motions.

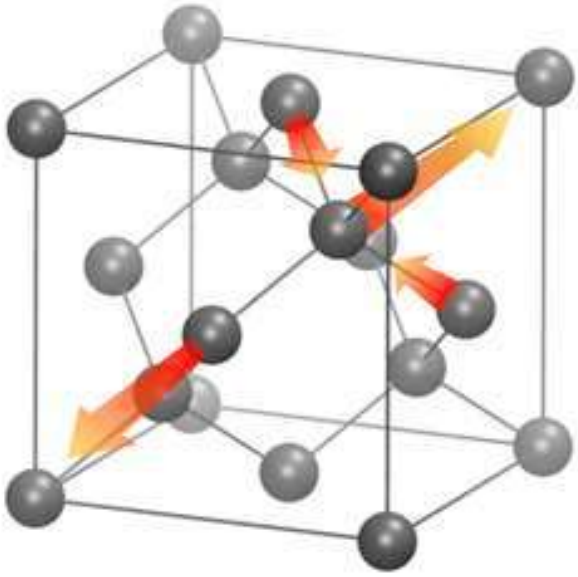


To understand the SVD method the Caltech team used, suppose you wanted to compress an image of Albert Einstein. This well-known photograph could be represented as a matrix. At each x and y coordinate, you could assign a value—that is, a number—that describes the gray scale of that pixel, perhaps 1 for white, 5 for medium gray, and 10 for black. SVD compresses the matrix by then providing singular values that describe both the color value and how important each pixel is with relation to certain features. In this case, perhaps it would give more importance or weight to pixels related to the outline of the face, hair, eyes, nose, and shoulders, for example. When the program keeps only 10 percent of those singular values from the original image, you can still make out that this is the well-known photo of Feynman. Even when only 1 percent of the singular values are kept, there is still a resemblance to the original image. Surprisingly, such a 1 percent level of compression is sufficient to reconstruct electron interactions in materials accurately.

Now a Caltech team has made a key discovery that helps simplify such calculations, speeding them up by a factor of 50 or more while maintaining accuracy. As a result, it is possible to compute electron interactions in more complex materials and devices and develop new calculations that were previously thought impossible.

In a new paper published in the journal *Physical Review X*, Caltech's Yao Luo, a graduate student in applied physics; his advisor Marco Bernardi, professor of applied physics, physics and materials science; and colleagues describe a new data-driven method that has enabled these advances. Their approach simplifies the dense computational matrices used to represent the interactions that take place in a material between electrons and atomic vibrations (or phonons, which can be thought of as individual units of vibrational energy).
Luo and Bernardi say that the new method allows them to use only 1 to 2 percent of the data typically used to solve such problems, greatly accelerating calculations and, in the process, revealing the most important interactions that dictate the properties of materials.

"This was very surprising," says Bernardi. "The electron–phonon interactions computed with the compressed matrices are nearly as accurate as the full calculation. This reduces the computing time and memory usage tremendously, by about two orders of magnitude in most cases. It's also an elegant example of Occam's razor, the idea of favoring simple physical models with minimal numbers of parameters."



The SVD method gives researchers a "physical intuition" about electron interactions in a material, something that has been missing from the first principles calculations in the past. For example, in a calculation involving silicon, it became clear that the dominant singular value was associated with the stretching and squeezing of a particular bond. Image credit: Caltech

Finding a New Middle Ground for the Field

Researchers in this field generally follow one of two approaches to understand materials on this most fundamental level. One approach emphasizes building minimal models, reducing the complexity of the system, so that researchers can tweak a handful of parameters in pen-and-paper calculations to get a qualitative understanding of materials. The other begins with nothing more than the structure of a material and uses so-called “first principles” methods—quantum mechanical calculations requiring large computers—to study materials properties with quantitative accuracy.

This latter set of methods, which Bernardi’s group focuses on, use extremely large matrices featuring billions of entries to compute electron interactions that control a wide range of physical properties. That translates to thousands of hours of computing time for each calculation. The new work suggests a kind of middle ground between the two approaches, Bernardi says. “With our new method you can truncate the size of these matrices, extract the key information, and generate minimal models of the interactions in materials.”

Rooting Out the Most Important Singular Values

His group’s approach is based on applying a method called singular value decomposition (SVD) to the electron–phonon interactions in a material. The SVD technique is widely used in fields like image compression and quantum information science. Here, it allows the authors to separate, or disentangle, the electronic and vibrational components in a matrix of thousands or millions of electron–phonon interactions and to assign each fundamental interaction a number.

These real positive numbers are called singular values and rank the fundamental interactions in order of importance. Then the program can eliminate all but a few percent of the interactions in each matrix, leaving only the leading singular values, a process that makes the determination cheaper by a factor proportional to the amount of compression. So, for example, if the program keeps only 1 percent of the singular values, the calculation becomes faster by a factor of 100. The researchers have found that keeping only a small fraction of singular values, typically 1 to 2 percent, the approximate result retains nearly the same accuracy as the full calculation. (See sidebar below)

“By using SVD, you can cut the number of singular values and capture only the main features of the matrices representing electronic interactions in a given material,” says Luo, lead author on the paper who is in his third year in Bernardi’s group. “This truncates the original matrix, thus speeding up the algorithm, and has the added benefit of revealing which interactions in the material are dominant.”

Bernardi notes that this latter benefit of the SVD method gives the researchers a “physical intuition” about electron interactions in a material, something that has been missing from the first principles calculations in the past. For example, in a calculation involving silicon, it became clear that the dominant singular value was associated with the stretching and squeezing of a particular bond. “It’s something simple, but before doing the calculation, we didn’t know that was the strongest interaction,” explains Bernardi.

In the paper, the researchers show that the compression of matrices related to electron–phonon interactions using the SVD method provides accurate results for various properties of materials researchers might want to calculate, including charge transport, spin relaxation times, and the transition temperature of superconductors.

Bernardi and his team are extending the SVD-based calculations to a wider range of interactions in materials and developing advanced calculations that were previously thought impossible. The team is also working to add the new SVD method into its open source Perturbo code, a software package that helps researchers calculate how electrons interact and move in materials. Bernardi says that this will enable users in the scientific community to predict material properties associated with electron–phonon interactions significantly faster.

Physicists Create A Five-Lane Superhighway For Electrons

MIT physicists and colleagues have created a five-lane superhighway for electrons that could allow ultra-efficient electronics and more.

Caption: Artist's rendition of a newly discovered superhighway for electrons that can occur in rhombohedral graphene. "We found a goldmine, and every scoop is revealing something new," says MIT Assistant Professor Long Ju. Image credit: Sampson Wilcox/Research Laboratory of Electronics

The work, reported in the Science issue, is one of several important discoveries by the same team over the past year involving a material that is a unique form of graphene.
"This discovery has direct implications for low-power electronic devices because no energy is lost during the propagation of electrons, which is not the case in regular

materials where the electrons are scattered," says Long Ju, an assistant professor in the Department of Physics and corresponding author of the *Science* paper.
The phenomenon is akin to cars traveling down an open turnpike instead of those moving through neighbourhoods. The neighbourhood cars can be stopped or slowed by other drivers making abrupt stops or U-turns that disrupt an otherwise smooth commute.

A new material

The material behind this work, known as rhombohedral penta-layer graphene, was discovered two years ago by physicists led by Ju. "We found a goldmine, and every scoop is revealing something new," says Ju, who is also affiliated with MIT's Materials Research Laboratory.

In a *Nature Nanotechnology* paper last October, Ju and colleagues reported the discovery of three important properties arising from rhombohedral graphene. For example, they showed that it could be topological, or allow the unimpeded movement of electrons around the edge of the material but not through the middle. That resulted in a superhighway, but required the application of a large magnetic field some tens of thousands times stronger than the Earth's magnetic field.
In the current work, the team reports creating the superhighway without any magnetic field.

Tonghang Han, an MIT graduate student in physics, is a co-first author of the paper. "We are not the first to discover this general phenomenon, but we did so in a very different system. And compared to previous systems, ours is simpler and also supports more electron channels." Explains Ju, "other materials can only support one lane of traffic on the edge of the material. We suddenly bumped it up to five."

Additional co-first authors of the paper who contributed equally to the work are Zhengguang Lu and Yuxuan Yao. Lu is a postdoc in the Materials Research Laboratory. Yao conducted the work as a visiting undergraduate student from Tsinghua University. Other authors are MIT professor of physics Liang Fu; Jixiang Yang and Junseok Seo, both MIT graduate students in physics; Chiho Yoon and Fan Zhang of the University of Texas at Dallas; and Kenji Watanabe and Takashi Taniguchi of the National Institute for Materials Science in Japan.

How it works

Graphite, the primary component of pencil lead, is composed of many layers of graphene, a single layer of carbon atoms arranged in hexagons resembling a honeycomb structure. Rhombohedral graphene is composed of five layers of graphene stacked in a specific overlapping order.

Ju and colleagues isolated rhombohedral graphene thanks to a novel microscope Ju built at MIT in 2021 that can quickly and relatively inexpensively determine a variety of important characteristics of a material at the nanoscale. Pentalayer rhombohedral stacked graphene is only a few billionths of a meter thick.

In the current work, the team tinkered with the original system, adding a layer of tungsten disulfide (WS_2). "The interaction between the WS_2 and the pentalayer rhombohedral graphene resulted in this five-lane superhighway that operates at zero magnetic field," says Ju.

Comparison to superconductivity

The phenomenon that the Ju group discovered in rhombohedral graphene that allows electrons to travel with no resistance at zero magnetic field is known as the quantum anomalous Hall effect. Most people are more familiar with superconductivity, a completely different phenomenon that does the same thing but happens in very different materials.

Ju notes that although superconductors were discovered in the 1910s, it took some 100 years of research to coax the system to work at the higher temperatures necessary for applications. "And the world record is still well below room temperature," he notes.

Similarly, the rhombohedral graphene superhighway currently operates at about 2 kelvins, or -456 degrees Fahrenheit. "It will take a lot of effort to elevate the temperature, but as physicists, our job is to provide the insight; a different way for realizing this [phenomenon]," Ju says.

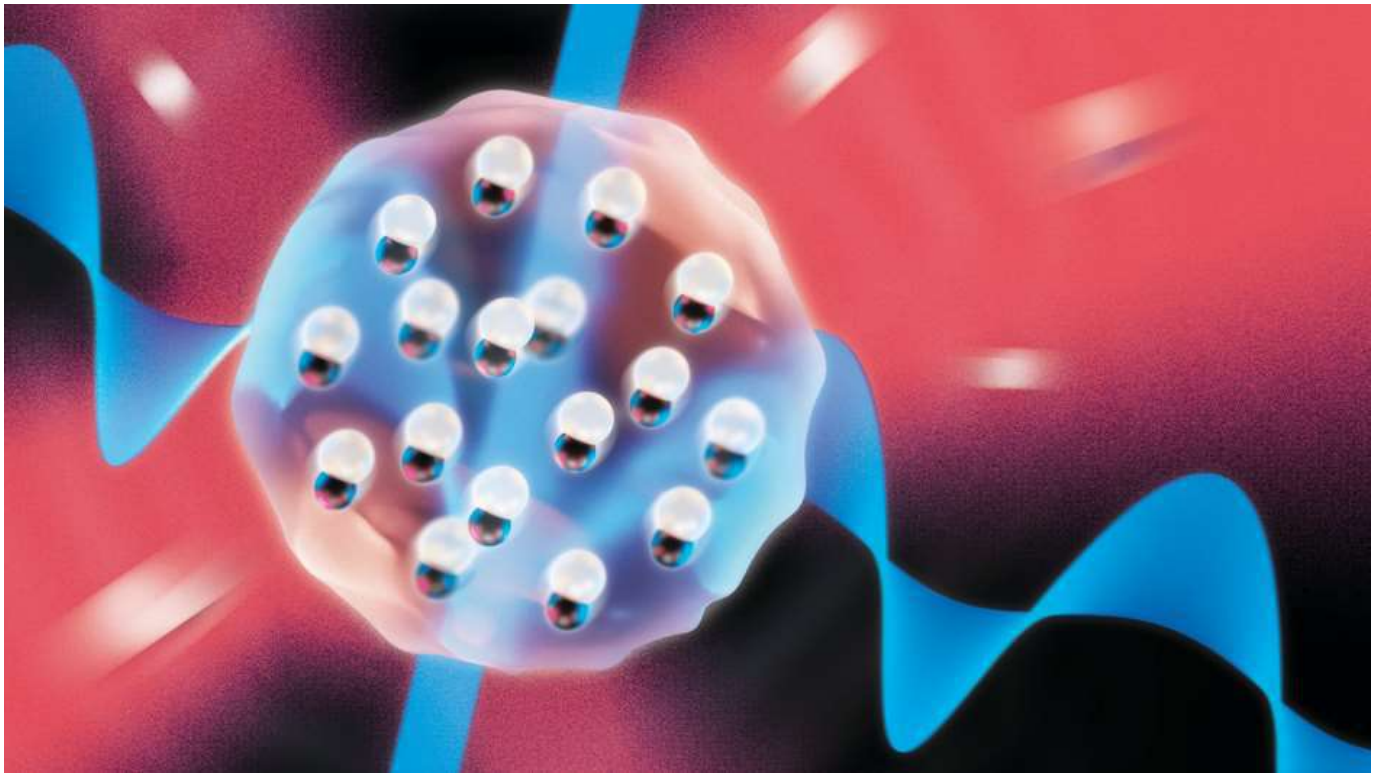
Very exciting

The discoveries involving rhombohedral graphene came as a result of painstaking research that wasn't guaranteed to work. "We tried many recipes over many months," says Han, "so it was very exciting when we cooled the system to a very low temperature and [a five-lane superhighway operating at zero magnetic field] just popped out."

Says Ju, "it's very exciting to be the first to discover a phenomenon in a new system, especially in a material that we uncovered."

The Coldest Lab in New York Has a New Quantum Offering

A hot new BEC in town has nothing to do with bacon, egg, and cheese. You won't find it at your local bodega, but in the coldest place in New York: the lab of Columbia physicist Sebastian Will**, whose experimental group specializes in pushing atoms and molecules to temperatures just fractions of a degree above absolute zero.**



With the help of microwaves, Columbia physicists have created a Bose-Einstein Condensate, a unique state of matter, from sodium-cesium molecules. Image Credit: The Will Lab/Myles Marshall

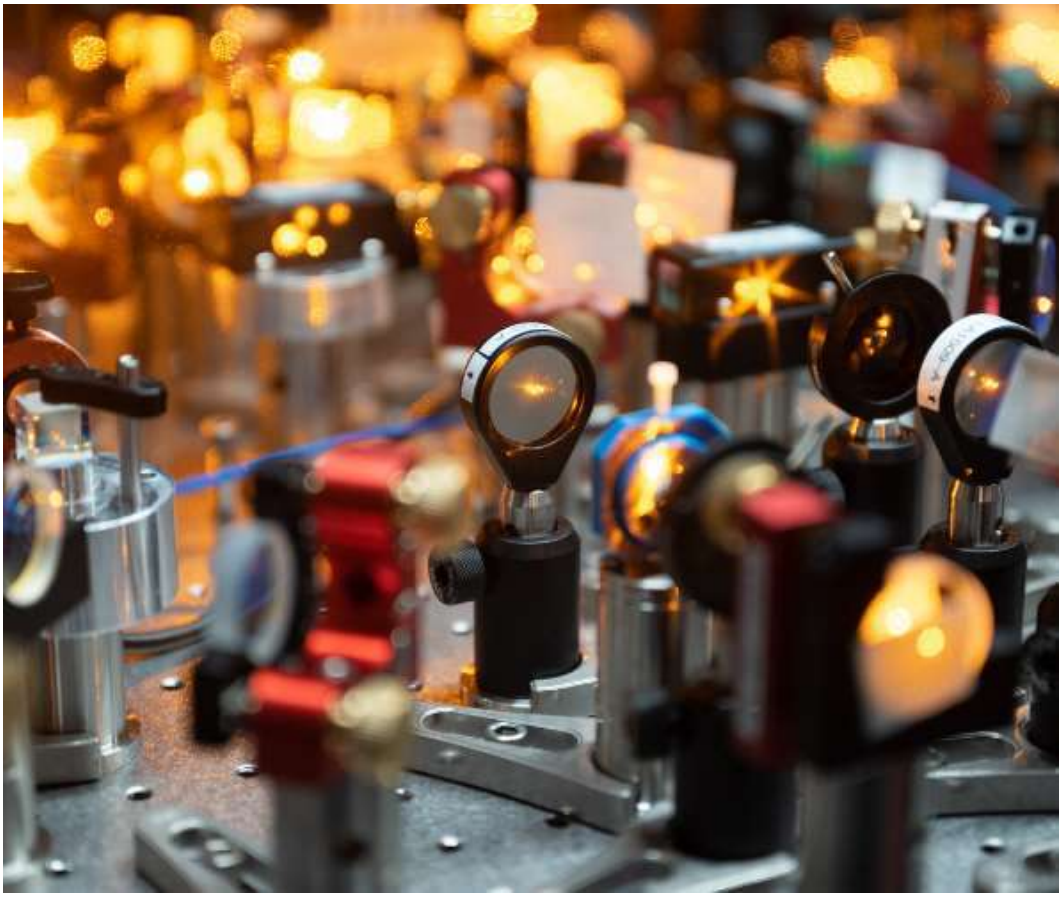
Writing in *Nature*, the Will lab, supported by theoretical collaborator Tijs Karman at Radboud University in the Netherlands, has successfully created a unique quantum state of matter called a Bose-Einstein Condensate (BEC) out of molecules.

Their BEC, cooled to just five nanoKelvin, or about -459.66 °F, and stable for a strikingly long two seconds, is made from sodium-cesium molecules. Like water molecules, these molecules are polar, meaning they carry both a positive and a negative charge. The imbalanced distribution of electric charge facilitates the long-range interactions that make for the most interesting physics, noted Will.

Research the Will lab is excited to pursue with their molecular BECs includes exploring a number of different quantum phenomena, including new types of superfluidity, a state of matter that flows without experiencing any friction. They also hope to turn their BECs into simulators that can recreate the enigmatic quantum properties of more complex materials, like solid crystals.

“Molecular Bose-Einstein condensates open up whole new areas of research, from understanding truly fundamental physics to advancing powerful quantum simulations,” he said. “This is an exciting achievement, but it’s really just the beginning.”

It’s a dream come true for the Will lab and one that’s been decades in the making for the larger ultracold research community.



The Will lab uses a series of lasers and optical elements as part of their cooling experiments.

Ultracold Molecules, a Century in the Making

The science of BECs goes back a century to physicists Satyendra Nath Bose and Albert Einstein. In a series of papers published in 1924 and 1925, they predicted that a group of particles cooled to a near standstill would coalesce into a single, larger superentity with shared properties and behaviors dictated by the laws of quantum mechanics. If BECs

could be created, they would offer researchers an enticing platform to explore quantum mechanics at a more tractable scale than individual atoms or molecules.

It took about 70 years from those first theoretical predictions, but the first atomic BECs were created in 1995. The achievement was recognized with the Nobel Prize in Physics in 2001, just around the time Will was getting his start in physics at the University of Mainz in Germany. Labs now routinely make atomic BECs from several different types of atoms. These BECs have expanded our understanding of concepts such as the wave nature of matter and superfluids and led to the development of technologies such as quantum gas microscopes and quantum simulators, to name a few.
But atoms are, in the grand scheme of things, relatively simple. They are round objects and usually do not feature interactions that may arise from polarity. Since the first atomic BECs were realized, scientists have wanted to create more complicated versions made from molecules. But even simple diatomic molecules made of two atoms of different elements bonded together had proved tricky to cool below the temperature needed to form a proper BEC.

The first breakthrough came in 2008 when Deborah Jin and Jun Ye, physicists at JILA in Boulder, Colorado, cooled a gas of potassium-rubidium molecules down to about 350 nanoKelvin. Such ultracold molecules have proved useful to perform quantum simulations and to study molecular collisions and quantum chemistry in recent years, but to cross the BEC threshold, even lower temperatures were needed.

In 2023, the Will lab created the first ultracold gas of their molecule of choice, sodium-cesium, using a combination of laser cooling and magnetic manipulations, similar to Jin and Ye's approach. To go colder, they brought in microwaves.

To Go Colder, Add Microwaves

Microwaves are a form of electromagnetic radiation with a long history at Columbia. In the 1930s, physicist Isidor Isaac Rabi, who would go on to receive the Nobel Prize in Physics, did pioneering work on microwaves that led to the development of airborne radar systems. "Rabi was one of the first to control the quantum states of molecules and was a pioneer of microwave research," said Will. "Our work follows in that 90-year-long tradition."

While you may be familiar with the role of microwaves in heating up your food, it turns out they can also facilitate cooling. Individual molecules have a tendency to bump into each other and will, as a result, form bigger complexes that disappear from the samples. Microwaves can create small shields around each molecule that prevent them from colliding, an idea proposed by Karman, their collaborator in the Netherlands. With the molecules shielded against lossy collisions, only the hottest ones can be preferentially removed from the sample—the same physics principle that cools your cup of coffee

when you blow along the top of it, explained author Niccolò Bigagli. Those molecules that remain will be cooler, and the overall temperature of the sample will drop.

The team came close to creating molecular BEC last fall in work published in *Nature Physics* that introduced the microwave shielding method. But another experimental twist was necessary. When they added a second microwave field, cooling became even more efficient, and sodium-cesium finally crossed the BEC threshold—a goal the Will lab had harbored since it opened at Columbia in 2018.
"This was fantastic closure for me," said Bigagli, who graduated with his PhD in physics this spring and was a founding lab member. "We went from not having a lab set up yet to these fantastic results."

In addition to reducing collisions, the second microwave field can also manipulate the molecules' orientation. That in turn is a means to control how they interact, which the lab is currently exploring. "By controlling these dipolar interactions, we hope to create new quantum states and phases of matter," said co-author and Columbia postdoc Ian Stevenson.

A New World for Quantum Physics Opens Up

Ye, a pioneer of ultracold science based in Boulder, considers the results a beautiful piece of science. "The work will have important impacts on a number of scientific fields, including the study of quantum chemistry and exploration of strongly correlated quantum materials," he commented. "Will's experiment features precise control of molecular interactions to steer the system toward a desired outcome—a marvelous achievement in quantum control technology."

The Columbia team, meanwhile, is excited to have a theoretical description of interactions between molecules that have been validated experimentally. "We really have a good idea of the interactions in this system, which is also critical for the next steps, like exploring dipolar many-body physics," said Karman. "We've come up with schemes to control interactions, tested these in theory, and implemented them in the experiment. It's been really an amazing experience to see these ideas for microwave 'shielding' being realized in the lab."

There are dozens of theoretical predictions that can now be tested experimentally with the molecular BECs, which co-first author and PhD student Siwei Zhang noted, are quite stable. Most ultracold experiments take place within a second—some as short as a few milliseconds—but the lab's molecular BECs last upwards of two seconds. "That will really let us investigate open questions in quantum physics," he said.

One idea is to create artificial crystals with the BECs trapped in an optical lattice made from lasers. This would enable powerful quantum simulations that mimic the interactions in natural crystals, noted Will, which is a focus area of condensed matter physics. Quantum simulators are routinely made with atoms, but atoms have short-range interactions—they practically have to be on top of one another—which limits how well they can model more complicated materials. “The molecular BEC will introduce more flavor,” said Will.

That includes dimensionality, said co-first author and PhD student Weijun Yuan. “We would like to use the BECs in a 2D system. When you go from three dimensions to two, you can always expect new physics to emerge,” he said. 2D materials are a major area of research at Columbia; having a model system made of molecular BECs could help Will and his condensed matter colleagues explore quantum phenomena including superconductivity, superfluidity, and more.

“It seems like a whole new world of possibilities is opening up,” said Will.

Cutting-Edge Mathematics Provides New Tool For Particle Collision Puzzle

Sebastian Mizera**, Member in the** School of Natural Sciences**, and his collaborators Claudia Fevola (Université Paris-Saclay, Inria) and Simon Telen (Max Planck Institute for Mathematics in the Sciences), have used computational algebraic geometry to study predictions for particle** physics **experiments, such as those at the Large Hadron Collider (LHC), which first detected the Higgs particle in 2012.**

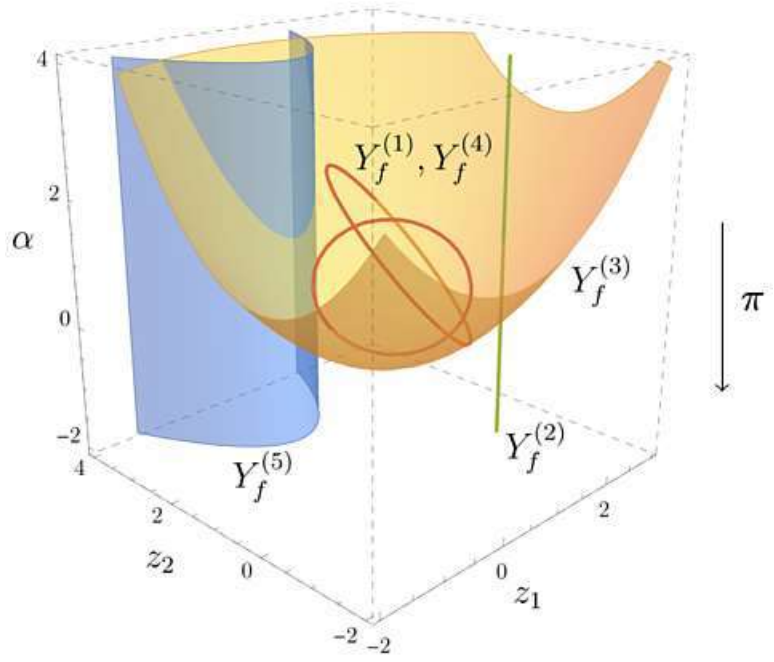
These experiments, combined with new mathematical tools, help solve unanswered questions in physics much faster and have a profound impact on our understanding of nature. The team's results were published in *Physical Review Letters*.

“Our progress was made possible by utilizing recently developed tools in computational algebraic geometry,” said Mizera, who is concluding his five-year term at IAS this summer. “It’s a rare example where using cutting-edge tools from mathematics has a direct impact on practical computations in particle physics.”

When studying particle collisions, physicists seek to describe the probability of particles arriving at certain states: whether they pass through each other, transform, or scatter at different angles, for example. This allows them to identify new particles or classify characteristics of existing ones. In order to do this, they must study particle interactions at the quantum level.

However, in quantum theory, it is impossible to predict the outcomes of particle collision with total certainty. Instead, physicists compute “scattering amplitudes,” which are mathematical expressions that encode the likelihood of different possible outcomes occurring when particles interact or collide. One of the characteristic features that physicists look for in these amplitudes are their “singularities,” which are points or regions where the probability amplitudes become infinite or undefined.

In their paper, Mizera and his colleagues used mathematical tools including topology, geometry, and algebra to better understand a particular kind of singularity, namely Landau singularities. Landau singularities are geometric objects that quantify when virtual particles (those limited by the uncertainty principle) become observable particles. By understanding the implications of Landau singularities, physicists can identify the energy scales and kinematic regimes where new phenomena, such as the production of new particles, may become possible. This plays an important role in interpreting and making predictions for experiments.



A representation of Landau singularities, described by algebraic equations

An algebraic variety called the “principal Landau determinant,” introduced by Mizera and his collaborators in their paper, is likely to be even more helpful in this regard. The principal Landau variant finds singularities even in the presence of massless particles. This is significant: locating singularities in the presence of massless particles is simultaneously the case most important to understanding the physics of the LHC and the most difficult to compute from a mathematical perspective.

This ability was demonstrated in the paper with a number of examples, including calculations needed to understand Higgs boson production in the presence of strong nuclear forces. It is a major step in the ongoing progress by physicists worldwide to increase the high-precision computational capability used to verify predictions of the Standard Model of particle physics at the LHC. Theoretical physicists like Mizera and his collaborators are an essential piece of this particle puzzle.

About the Institute

The Institute for Advanced Study has served as one of the leading independent centers for theoretical research and intellectual inquiry since its establishment in 1930, advancing the frontiers of knowledge across the sciences and humanities. From founding IAS Faculty Albert Einstein, Erwin Panofsky, and John von Neumann to influential figures Emmy Noether, George Kennan, and J. Robert Oppenheimer to the foremost thinkers of the present, IAS is dedicated to enabling independent inquiry and fundamental discovery.

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Faculty, each of whom are preeminent leaders in their fields. Among present and past Faculty and Members, there have been 35 Nobel Laureates, 44 of the 62 Fields Medalists, and 23 of the 27 Abel Prize Laureates, as well as winners of the Pulitzer Prize in History; the Wolf, Holberg, and Kluge prizes; and many MacArthur and Guggenheim fellows, among other honors.

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