Physicists quench their thirst for modeling superfluids

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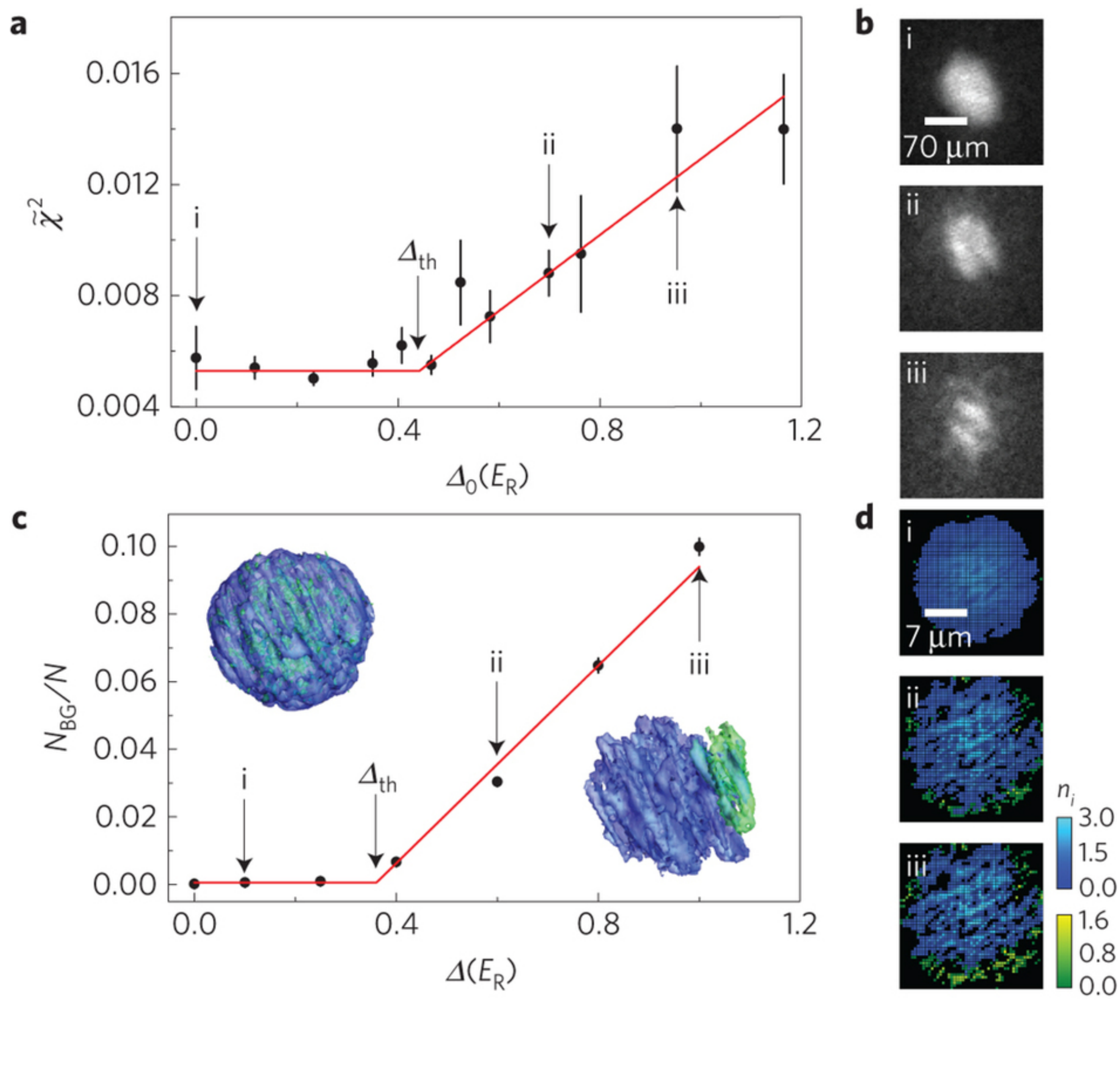

The blue and green images (bottom) are simulation results on Titan. The colors identify separate superfluid puddles coexisting in a trap. The horizontal axis measures the strength of disorder within the trap. The top and bottom figure show different measurements characterizing the state of the system. At a disorder strength of .4, the system fragments from having a single superfluid puddle to multiple. The image series (above right) show experimental measurements while the colored images (below right) show the corresponding simulations on Titan. Credit: C. Meldgin, U. Ray, P. Russ, D. Chen, D. Ceperley, B. DeMarco. "Probing the Bose-Glass—Superfluid Transition Using Quantum Quenches of Disorder." *Nature Physics* (2016). DOI: 10.1038/nphys3695

Simply put, physicists study energy, matter, and how the two interact. Through the years researchers have cataloged countless phenomena relating to these complex interactions.

As science has advanced, researchers have come upon the next frontier of physics research—understanding materials at the most fundamental level and how changes in temperature or pressure can elicit unique, valuable properties in certain materials.

However, studying material properties and interactions under extreme temperature and pressure conditions poses challenges for researchers, as even world-class experimental facilities are unable to recreate sufficiently extreme conditions.

In an effort to improve insight into a broad range of materials exhibiting unique properties, a multi-institution team led by University of Illinois at Urbana-Champaign (UIUC) professor David Ceperley is using high-performance computing resources at the US Department of Energy's (DOE's) Oak Ridge National Laboratory (ORNL) to compare and corroborate experimental findings pertaining to a variety of such materials.

"Our research is fundamental science, helping us understand the origins of planets, among other things," Ceperley said. "This research also has a societal impact on designing new batteries, solar cells, and alloys. There are thousands of applications for this work." In addition, delving more deeply into this state of matter will help researchers better understand how new computer architectures, such as quantum annealing machines, can function.

To simulate these complex atomic interactions, Ceperley's team carries out quantum Monte Carlo simulations using the Cray XK7 Titan supercomputer at the Oak Ridge Leadership Computing Facility (OLCF), a DOE Office of Science User Facility located at ORNL.

Superfluid simulations

When studying materials, researchers often take great interest in phase transitions—the points at which substances change between solid, liquid, gas, or (very rarely) plasma. In addition, certain molecules or their isotopes can enter unique phases when put under certain temperature or pressure states.

Measuring the amount of particle disorder in the atomic structure gives researchers insight into a wide range of materials' properties. Understanding what happens when a material melts, evaporates, or crystalizes is essential when creating certain metal alloys, performing chemical and other industrial processes, or discovering special properties of a material.

For instance, it is well-known that under specific conditions, certain molecules or their isotopes can change from the fluid phase to a superfluid one. As these molecules approach absolute zero—that is, the lowest temperature possible, or -459.67° F—they are able to flow without friction and have zero viscosity. This gives superfluids unique, almost gaslike properties, such as the ability to climb up the walls of a container holding them.

But how can certain molecules exhibit such odd properties? Think of this phenomenon in terms of light. When a person looks out and sees white light, he or she is actually seeing a conglomeration of many different photons at various wavelengths—and, therefore, various colors—converge. When someone looks at a laser, however, he or she typically sees only one color. Photons in a laser almost all have the same wavelength and energy. That uniformity allows humans to perceive laser light as one solid color.

At extremely cold temperatures, particles in a superfluid assume a similarly organized state in which all of the atoms behave like photons in a laser. When the temperature rises, particles become more excited and less organized.

When a superfluid reaches a certain temperature—and, in turn, a certain state of disorder—it enters something called the Bose-glass phase. Rather than exhibiting the constant form of superfluids, molecules in a Bose-glass state have concentrated regions of disordered particles dispersed among the highly ordered regions.

The transition from superfluid to Bose glass happens very quickly, meaning researchers must use computation to corroborate experimental findings.

In order to measure and describe particle positions during the transition between the superfluid and Bose-glass states, the Ceperley team studied the disordered Bose-Hubbard model. For the team's experimental setup, members used the isotope rubidium-87 to test the model. Much of the experimental work was done by former UIUC PhD student Carrie Malden and UIUC professor Brian DeMarco. The bulk of the computations were done by former UIUC PhD student Ushnish Ray.

The team did not want to just simulate the behavior of molecules in a static state, though. They wanted to see if they could manipulate the particles' behavior, and, thereby, a molecule's properties, by changing the system's temperature.

Slaking particle behavior

To study rubidium-87's properties as it transitions from a superfluid to a Bose-glass state, the team wanted to simulate quenching these quantum systems.

The researchers started the experiment with 27,000 rubidium-87 atoms in an ultracold, superfluid state. They then slowly raised the temperature of the system and observed the point at which excited particles' motions started the transition to the Bose-glass phase. Once the system entered that phase, researchers quenched the system by sharply dropping the temperature back near absolute zero.

Using Titan the team can calculate the Bose-glass portion of a system as a function of the degree of its disorder. This approach allows researchers to use computation to emulate the quenching process in real experiments. The group employs a method called quantum Monte Carlo (QMC) to underpin its simulations. Previously when researchers wanted to simulate significant numbers of particles in a quantum state—a "many-body" problem—they would use density functional theory (DFT).

DFT simulations rely on mathematical functions to calculate the properties of the system. While still very useful for gaining some insights, this approach makes certain assumptions that could have impacted the hyperrealistic conditions Ceperley's team hoped to simulate.

QMC simulations, on the other hand, use statistical data and random numbers to plot electrons and give researchers a more realistic view of the particles' positions in an atomic system.

"Think of robotic cars driving down the interstate," Ceperley said. "The car representing DFT drives down the road but doesn't consider where other cars may be driving. QMC is calculating the positions of all the other cars. If the road is crowded, you would clearly choose QMC to get where you are going."

Due to their high accuracy, QMC simulations need to run on the world's fastest computers to achieve results in a timely manner. While the Ceperley team had already scaled its code to perform well on supercomputers, it worked with OLCF staff to improve code performance on Titan's GPU accelerators.

During its simulation of rubidium-87, the team identified superfluid "puddles" that remained as the material transitioned from a superfluid to the Bose-glass state. This finding opens the door for further exploration of materials' individual properties during this complex phase transition and how physicists and materials scientists may understand how disorder, prevalent in nature, affects material properties.

More information: C. Meldgin et al., "Probing the Bose Glass–Superfluid Transition Using Quantum Quenches of Disorder." *Nature Physics* 12, 646–649 (2016), DOI: 10.1038/nphys3695

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